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# Quantum conjugate momentum of angular momentum modulus

J Sau

Institut de Physique Nucléaire (and IN2P3), Université Lyon-I, 43, Bd du 11 Novembre 1918, 69621 Villeurbanne, France

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**Abstract.** The quantum conjugate momentum of the angular momentum modulus is derived together with those of  $J_z$  and  $J_3$ . In fact we arrive at the conjugate momentum of the operator j such that  $J^2 = j(j+1)\hbar^2$ .

## 1. Introduction

From a fundamental point of view, it is important to know the canonical set of variables required for the description of a physical system. Concerning rotation it is well known that two components of the angular momentum cannot belong to the same canonical set, since their commutator is not zero, so the prescribed variables are the angular momentum modulus J (or its square  $J^2$ ) and one of its components, say  $J_z$ . Here J is  $J = \sqrt{J^2}$  where  $J^2 = J_x^2 + J_y^2 + J_z^2$ , i.e. it is the operator with the same eigenvectors as  $J^2$  with each eigenvalue of J being the positive square root of the corresponding eigenvalue of  $J^2$ . Now, the conjugate momenta of J and even of  $J_z$  are not known. Moreover, these momenta can have an interesting physical application to the fundamental description of rotation in a many-body system, in order to give explicitly the dependence of the Hamiltonian on the angular momentum modulus J. The method is formally simple and has been applied by Villars (1965) and Rowe (1967) to the very simple cases of centre of mass motion and rotation in a two-dimensional problem.

Sau (1977) has previously generalised in classical mechanics the well known notions of action angle variables (Born 1927). Let us recall here the principal results. Let  $\mathbf{r}$  be a vector so that  $\mathbf{J} \cdot \mathbf{r} = 0$  and  $\{\mathbf{r}, \mathbf{J} \cdot \mathbf{n}\} = \mathbf{n} \times \mathbf{r}$ , where  $\mathbf{n}$  is a constant vector and  $\{\}$  stands for the classical Poisson bracket (CPB). Then, a correct choice for  $\beta_1$  and  $\alpha$ , the respective conjugate variables of  $J_z$  and J, is:

$$\beta_1 = -\tan^{-1}(J_x J_y^{-1}); \qquad \alpha = \tan^{-1}[z J(y J_x - x J_y)^{-1}]. \tag{1}$$

Indeed we get:

 $\{\beta_1, J_z\} = 1,$   $\{\beta_1, J\} = 0,$   $\{\alpha, J_z\} = 0,$   $\{\alpha, J\} = 1.$ 

So  $\alpha$ ,  $\beta_1$ ,  $J_z$  and J fulfil the necessary relations for a canonical set. If we go to quantum mechanics, we have always  $[\beta_1, J_z] = i\hbar$  but not  $[\alpha, J] = i\hbar$ , where [] is the commutator. We remark that  $[\beta_1, J_z] = i\hbar$  because the CPB algebra  $\{J_x, J_y\} = J_z$  (and cyclic

permutations) has its quantum equivalent  $[J_x, J_y] = i\hbar J_z$  (and cyclic permutations). If we define

$$A_1 = i(yJ_x - xJ_y)/r, \qquad A_2 = izJ/r \qquad A_3 = J$$
 (2)

we have a similar CPB algebra:

 $\{A_1, A_2\} = A_3$  (and cyclic permutations)

but with no quantum equivalent. If we put:

$$V'_{+} = A_1 + iA_2$$
  $V'_{-} = A_1 - iA_2$ 

we get:

$$\{J, V'_{+}\} = -iV'_{+} \qquad \{J, V'_{-}\} = iV'_{-}.$$
(3)

In the quantum mechanical case (§ 2), we shall look for operators V' which are, in a way, eigen-operators of J, i.e. such that:

$$[J, V'] = V'\lambda'(J), \tag{4}$$

a relation similar to (3). But now the eigenvalue  $\lambda'$  may be a function of J. This way is interesting since, if relation (4) holds, then V' is also eigen-operator of  $J^2$ ,  $[J^2, V'] = V'\lambda$ , and it is less difficult to work with  $J^2$ . In fact, curiously, as we shall see in § 3, we shall arrive naturally at the conjugate of operator j such that  $J^2 = j(j+1)\hbar^2$  and not of J itself. In § 4, we shall complete the canonical set and give the conjugate momenta of  $J_z$  and also of  $J_3$ , the projection of J on a direction attached to the many-body system.

## 2. Eigen-operators of J

We shall follow the same approach as in classical mechanics (Sau 1977). Let  $u_3$  be a vector function of the positions of the particles. We can choose simply the position vector of a given particle, or, more symmetrically, the vector giving a principal direction of the inertial tensor.  $u_3$  is associated with the many-body system. Let  $r_3 = u_3 - [(J \cdot u_3)J/J^2]$ , i.e. classically, the projection of  $u_3$  on the plane orthogonal to J. With this definition  $r_3^+ = r_3$ ,  $J \cdot r_3 = r_3$ , J = 0, but the Cartesian components of  $r_3$  do not intercommute. We have for instance, with  $J_3 = (J \cdot u_3)/u_3$ ,

$$[x_3, y_3] = -i\hbar u_3^2 J_3^2 J_z J^-$$

and formally

$$\boldsymbol{r}_3 \times \boldsymbol{r}_3 = -\mathrm{i}\hbar \frac{u_3^2 J_3^2}{J^4} \boldsymbol{J} = -\mathrm{i}\hbar k \boldsymbol{J}$$

with  $k = u_3^2 J_3^2 / J^4$ . r also fulfils the commutation relation  $[r_3, J.n] = i\hbar(n \times r_3)$ , n being a constant vector. Let us write all the relations we shall need:

$$[\mathbf{r}_{3}, \mathbf{J} \cdot \mathbf{n}] = i\hbar(\mathbf{n} \times \mathbf{r}_{3}) \qquad \mathbf{r}_{3}^{+} = \mathbf{r}_{3} \qquad \mathbf{r}_{3} \cdot \mathbf{J} = \mathbf{J} \cdot \mathbf{r}_{3} = 0$$
  
$$\mathbf{r}_{3} \times \mathbf{r}_{3} = -i\hbar k \mathbf{J} \qquad \text{with } k = u_{3}^{2} J_{3}^{2} / J^{4}. \qquad (5)$$
  
$$\mathbf{r}_{3}^{2} = \mathbf{r}_{3} \cdot \mathbf{r}_{3} = u_{3}^{2} \left(1 - \frac{J_{3}^{2}}{J^{2}}\right).$$

All through this paper we shall deal with operators, so the order of factors is important. But, when we treat expressions of commuting operators, we shall use simple algebraic notation. Now we suppose there exists an operator V' so that  $[J^2, V'] = V'\lambda(J)$ .

As in classical mechanics we try to write V' as a linear combination of operators  $(J_xy_3 - x_3J_y)$  and  $z_3$  (relations (2) and (3)), which are Hermitian. But now the coefficients of the linear combination may depend on J, so we write:

$$V' = (J_x y_3 - x_3 J_y) a_1(J) + z_3 a_2(J).$$

Because of the commutators

$$[J^{2}, z_{3}] = -2i\hbar(J_{x}y_{3} - x_{3}J_{y})$$
  
$$[J^{2}, J_{x}y_{3} - x_{3}J_{y}] = 2i\hbar z_{3}J^{2} + 2\hbar^{2}(J_{x}y_{3} - x_{3}J_{y})$$
  
(6)

we get the eigenvalue problem

$$\begin{pmatrix} 2\hbar^2 & -2i\hbar \\ 2i\hbar J^2 & 0 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \lambda \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$$

with solutions

$$\lambda_{1} = \hbar[\hbar + (\hbar^{2} + 4J^{2})^{1/2}] \qquad a_{1}^{1} = \frac{\hbar + (\hbar^{2} + 4J^{2})^{1/2}}{2J} \qquad a_{2}^{1} = iJ$$
$$\lambda_{2} = \hbar[\hbar - (\hbar^{2} + 4J^{2})^{1/2}] \qquad a_{1}^{2} = \frac{(\hbar^{2} + 4J^{2})^{1/2} - \hbar}{2J} \qquad a_{2}^{2} = -iJ$$

Let us now look for the commutator between one V' and a function of  $J^2$ . Using relation (A.3) of appendix 1, we get

$$[f(J^2), V'] = V'(f(\lambda + J^2) - f(J^2)) \quad \text{or} \quad f(J^2)V' = V'f(\lambda + J^2).$$
(7)

We now suppose that  $f(J^2) = J = \sqrt{J^2}$  and we find

$$[J, V'] = V'((J^2 + \lambda)^{1/2} - J).$$
(8)

If we let  $\hbar \to 0$  in (8), the quantum Poisson bracket  $(1/i\hbar)[$ ] gives the CPB, with the eigenvalues  $[(J^2 + \lambda)^{1/2} - J]/i\hbar$  giving the classical values +i or -i according to  $\lambda = \lambda_2$  or  $\lambda_1$ ,  $V_1$  and  $V_2$  being then the classical  $V_+$  and  $V_-$  (relation (3)).

Another interesting limiting case is when J is sufficiently great so that:

$$(\hbar^2 + 4J^2)^{1/2} \simeq 2J + O(\hbar^2)$$

then

$$\frac{1}{i\hbar}[(J^2+\lambda)^{1/2}-J]\simeq\pm i+O(\hbar^2)$$

i.e. the classical values, the error being of order  $\hbar^2$ . So we can expect that the classical decomposition of the Hamiltonian would give general features valid for sufficiently great angular momentum. This decomposition will be made in a separate paper.

# 3. The conjugate momentum of j

Let us now return to relations (6) and let us introduce an operator j so that

$$j = \frac{-\hbar + (\hbar^2 + 4J^2)^{1/2}}{2\hbar}$$
(9)

then

$$J^2 = j(j+1)\hbar^2$$

and  $\lambda_1$  and  $\lambda_2$  are rational functions of j so that

$$(\hbar^2 + 4J^2)^{1/2} = (2j+1)\hbar$$
  $\lambda_1 = 2(j+1)\hbar^2$   $\lambda_2 = -2j\hbar^2$ .

We now look for the commutators  $[j, V'_1]$  and  $[j, V'_2]$ . To do this we have to calculate  $[(\hbar^2 + 4J^2)^{1/2}, V']$ . We make use of relations (7) with  $F(J^2) = (\hbar^2 + 4J^2)^{1/2}$ . This function has interesting properties: indeed we get

$$F(J^2+\lambda_1)=F(J^2)+2\hbar.$$

Then

$$[j, V_1'] = V_1'. (10a)$$

A little trouble arises for  $V'_2$  since we have

$$F(J^{2} + \lambda_{2}) = \{ [(\hbar^{2} + 4J^{2})^{1/2} - 2\hbar]^{2} \}^{1/2}.$$

However, we do not always have  $F(J^2 + \lambda_2) = F(J^2) - 2\hbar$ ; the relation is false for J = 0 for instance. So we write

$$F(J^{2} + \lambda_{2}) = F(J^{2}) - 2\hbar + [F(J^{2} + \lambda_{2}) - F(J^{2}) + 2\hbar]$$

replacing  $(\hbar^2 + 4J^2)^{1/2}$  by  $(2j+1)\hbar$ , we get:

$$[j, V_2'] = -V_2'(1-A) \tag{10b}$$

with  $A = \frac{1}{2} \{ [(2j-1)^2]^{1/2} - (2j-1) \}$ . So, applied to an eigenket of *j*, *A* is zero for all values of *j* except for j = 0 where A = 1.  $V'_1$  and  $V'_2$  are then step operators for *j*, built with the physical observables of the system.

Let us rewrite  $V'_1$  and  $V'_2$  using j:

$$V'_{1} = J_{x}y_{3} - x_{3}J_{y} + i\hbar z_{3}j$$

$$V'_{2} = J_{x}y_{3} - x_{3}J_{y} - i\hbar z_{3}(j+1).$$
(11)

We have omitted the factor  $\hbar[(j+1)/j]^{1/2}$  behind  $V'_1$  and  $\hbar[j/(j+1)]^{1/2}$  behind  $V'_2$  since this does not change the commutation relations (10).

In the following we shall need the commutators  $[f(j), V'_1]$ ,  $[f(j), V'_2]$ ,  $[j, z_3]$  where f(j) is a function of j. The first two are easily found using relations (A.3) and (A.4) of the appendix 1, the eigenvalues being now +1 and -(1-A). Thus, we obtain:

$$[f(j), V'_1] = V'_1(f(j+1) - f(j))$$

whence

$$f(j)V'_{1} = V'_{1}f(j+1) \qquad V'^{+}_{1}f(j-1) = f(j)V'^{+}_{1}$$

$$[f(j), V'_{2}] = V'_{2}(f(j-1+A) - f(j)) \qquad (12)$$

whence

$$f(j)V'_2 = V'_2 f(j-1+A).$$

We shall make use of these relations every time we need to pass a function of j from one side of a V' to the other side.

For the third commutator we note that:

$$z_3 = -i(V'_1 - V'_2)(2j+1)^{-1}\hbar^{-1}$$

then

$$[j, z_3] = -i[V'_1 + V'_2(1 - A)](2j + 1)^{-1}\hbar^{-1}.$$
(13)

If we call  $\alpha$  the conjugate momentum of j so that  $[\alpha, j] = i$ , the relations (10) show that  $V'_1$  can be written in the more general form  $V'_1 = e^{i\alpha}g_1(j)$ , where  $g_1(j)$  is a function of j but also, eventually, of the other operators of the canonical set, since they commute with  $\alpha$  and j. We now try to obtain operators  $j_+ = e^{i\alpha}$  and  $(j_+)^+ = j_- = e^{-i\alpha}$  which satisfy  $[j, j_+] = j_+, [j, j_-] = -j_-$ , but also  $j_-j_+ = 1$ . In view of this we first find the relation between  $V_1^{++}$  and  $V_2'$ :

$$V_1^{\prime +} = J_x y_3 - x_3 J_y - i\hbar j z_3 = J_x y_3 - x_3 J_y - i\hbar z_3 j - i\hbar [j, z_3].$$

Using (13) we have

$$V_1^{\prime +} = V_2^{\prime} \frac{2j - 1 + A}{2j + 1}.$$

We now calculate the norm  $N = V_1'^+ V_1'$ :

$$N = V_1'^+ V_1' = V_2' \frac{2j - 1 + A(j)}{2j + 1} V_1' = V_2' V_1' \frac{2j + 1 + A(j + 1)}{2j + 3}.$$

We remark that we shall have always A(j+1) = 0. The product  $V'_2 V'_1$  gives:

$$V'_{2}V'_{1} = (J_{x}y_{3} - x_{3}J_{y})V'_{1} - i\hbar z_{3}(j+1)V'_{1}$$
  
=  $(J_{x}y_{3} - x_{3}J_{y})V'_{1} - i\hbar z_{3}V'_{1}(j+2)$   
=  $(J_{x}y_{3} - x_{3}J_{y})^{2} + i\hbar [J_{x}y_{3} - x_{3}J_{y}, z_{3}]j - 2i\hbar z_{3}(J_{x}y_{3} - x_{3}J_{y}) + \hbar^{2}z_{3}^{2}j(j+2).$ 

The lengthiest calculation is for  $(J_xy_3 - x_3J_y)^2$  since, as we have seen, even  $x_3$ ,  $y_3$  and  $z_3$  do not intercommute. Using relations (5),  $(J_xy_3 - x_3J_y)^2$  can be brought into the form:

$$(J_{x}y_{3}-x_{3}J_{y})^{2}=r^{2}(J^{2}-J_{z}^{2})-z_{3}^{2}J^{2}+2i\hbar z_{3}(J_{x}y_{3}-x_{3}J_{y})+\hbar^{2}r^{2}+\hbar^{2}kJ^{2}.$$

Also, using relations (5), we have:

$$[z_3, J_x y_3 - x_3 J_y] = i\hbar(x_3^2 + y_3^2 + k J_x^2 + k J_y^2).$$

In order to have a compact expression we define the operator M such that  $M\hbar = J_z$ .

Similarly, we remark that  $J_3$  is the projection of J on the direction  $u_3$  associated with the many-body system. So we define  $K = J_3/\hbar$  and so  $k = u_3^2 \hbar^2 K^2/J^4$ . Adding all the terms, replacing  $J^2$  by  $j(j+1)\hbar^2$ , we find after a little algebra:

$$N = \frac{u_3^2 \hbar^2}{(j+1)^2} [(j+1)^2 - M^2] [(j+1)^2 - K^2] \frac{2j+1}{2j+3}.$$
 (14)

The operators  $u_{3}^{2}$ , *j*, *K*, *M* are all Hermitian and intercommute. So if we define:

$$j_{+} = V_1' N^{-1/2} \tag{15}$$

we have  $j_-j_+ = 1$  and  $[j, j_+] = j_+$ ,  $[j, j_-] = -j_-$ . Thus  $j_+$  can be regarded as  $j_+ = e^{i\alpha}$  with  $[\alpha, j] = i$ . K and M commute with  $j_+$ . In order to have a canonical set, the conjugate momenta of K and M must be chosen so as to commute with  $j_+$  and  $j_+$  and so too must the other variables, usually called 'intrinsic'.

Now  $\alpha$  can be given formally by

$$\tan \alpha = \frac{1}{i}(j_+ - j_-)(j_+ + j_-)^{-1}.$$

Later, without loss of generality, we shall suppose that  $u_3$  is unitary.

#### 4. Complete canonical set for rotational motion

#### 4.1. The conjugate variable of M

Although

$$[\tan^{-1}(y_3/x_3), J_z] = i\hbar$$
 and  $[-\tan^{-1}J_xJ_y^{-1}, J_z] = i\hbar$ 

neither of these two angles can belong to the canonical set since the commutators between the first and J, and between the second and  $\alpha$ , are not zero. In order to find  $\beta$ , the conjugate variable of M (and of  $J_z$ ), we shall follow the same approach as for  $\alpha$ , i.e. we look for operators  $M_+$  and  $M_-$  such that  $(M_+)^+ = M_-, M_+M_- = M_-M_+ = 1$  and  $[M, M_+] = M_+, [M, M_-] = -M_-$ .

The problem is now simpler since we already know  $J_+ = J_x + iJ_y$  and  $J_- = J_x - iJ_y$ which satisfy the previous commutation relations.  $M_+$  and  $M_-$  can be taken as:

$$M_{+} = J_{+} \frac{\left[j(j+1) - M(M+1)\right]^{-1/2}}{\hbar} = (M_{-})^{+}.$$
 (16)

We try to identify  $M_+$  with  $e^{i\beta}$ , and so

$$\beta = \tan^{-1} \left( \frac{1}{i} (M_+ - M_-) (M_+ + M_-)^{-1} \right).$$

It can be verified easily that  $[\beta, M] = i$ . Moreover,  $M_+$  commutes with j and K, and so  $\beta$  does also. In order to be a good candidate for the canonical set,  $\beta$  must satisfy the commutation relation  $[\beta, \alpha] = 0$ , or equivalently  $[M_+, j_+] = 0$ . We remark that the pair of operators M,  $J_+$  is of the type discussed in appendix 1 and so relation (A.4) can be used. Then the commutator  $[M_+, j_+]$  can be brought into the form (using relations (14), (15) for the definition of  $j_+$ ):

$$[M_{+}, j_{+}] = [J_{+}V_{1}'(j - M + 1)^{-1} - V_{1}'J_{+}(j - M)^{-1}]F(j, M, K)$$
(17)

with

$$F(j, M, K) = \frac{j+1}{\hbar^2} \left( \frac{2j+3}{(2j+1)[(j+1)^2 - K^2](j+1+M)(j+2+M)} \right)^{1/2}$$

Relation (A.4) has been used once for the pair j,  $V'_1$  and once for the pair M,  $J_+$  in order to get the products  $J_+V'_1$  and  $V'_1J_+$  on the left.

Now we have:

$$(J_x + iJ_y)(J_xy_3 - x_3J_y) = (y_3 - ix_3)(J^2 - J_z^2 + \hbar J_z) - (J_x - iJ_y)z_3(\hbar - J_z)$$
  
$$(J_xy_3 - x_3J_y)(J_x + iJ_y) = (y_3 - ix_3)(J^2 - J_z^2) + (J_y - iJ_x)z_3J_z$$

hence

$$J_{+}V'_{1} = [\hbar^{2}(y_{3} - ix_{3})(j + M) - \hbar(J_{y} - iJ_{x})z_{3}](j + 1 - M)$$
  
$$V'_{1}J_{+} = [\hbar^{2}(y_{3} - ix_{3})(j + M) - \hbar(J_{y} - iJ_{x})z_{3}](j - M).$$

These two relations used in (17) give at once  $[M_+, j_+] = 0$  and so  $[\beta, \alpha] = 0$ .

#### 4.2. The conjugate momentum of K

We shall proceed for K in the same way as for M. Let  $(u_1, u_2, u_3)$  be the Cartesian coordinate system associated with the many-body system  $(u_1 \times u_2 = u_3 \text{ etc})$ . Let  $J_1, J_2, J_3$  be the components of J along the axes; they satisfy the well known anomalous commutation relations:

$$[J_1, J_2] = -i\hbar J_3$$
 (and cyclic permutations).

We define  $J'_{+} = (J'_{-})^{+} = J_{1} - iJ_{2}$  and we get

$$[J_3, J'_+] = J'_+, \qquad [J_3, J'_-] = -J'_-.$$

Hence the operators

$$K_{+} = (K_{-})^{+} = J'_{+} \frac{\left[j(j+1) - K(K+1)\right]^{-1/2}}{\hbar}$$

are such that

$$[K, K_+] = K_+;$$
  $[K, K_-] = -K_-$  and  $K_+K_- = K_-K_+ = 1.$ 

So  $K_+$  can be regarded as  $K_+ = e^{i\gamma}$  with  $[\gamma, K] = i$ ,  $\gamma$  being the conjugate variable of K. Since  $J_1, J_2, J_3$  commute with  $J_+, J_-, J_z, K_+ = e^{i\gamma}$  commute with  $j, M, \beta$  and we must show that  $\gamma$  commutes also with  $\alpha$ . We shall now calculate the commutator  $[K_+, j_+]$ .

First, however, some preliminary relations must be derived. Let us define, analogously to  $r_3$ , the vectors  $r_1(x_1, y_1, z_1)$  and  $r_2(x_2, y_2, z_2)$ , projections of  $u_1$  and  $u_2$  on the plane orthogonal to J:

$$\boldsymbol{r}_1 = \boldsymbol{u}_1 - \frac{J_1 \boldsymbol{J}}{J^2} \qquad \boldsymbol{r}_2 = \boldsymbol{u}_2 - \frac{J_2 \boldsymbol{J}}{J^2}$$

Hence

$$\mathbf{r}_1 J_1 + \mathbf{r}_2 J_2 + \mathbf{r}_3 J_3 = 0 \tag{18}$$

$$[\mathbf{r}_1, J_1] = 0$$

$$[\mathbf{r}_1, J_2] = -i\hbar\mathbf{r}_3$$

$$(and cyclic permutations).$$

$$[\mathbf{r}_1, J_3] = i\hbar\mathbf{r}_2$$

$$(19)$$

The quantity  $J_x y_3 - x_3 J_y$  which appears in  $V'_1$  can be rewritten in a more useful form (with  $u_3 = u_1 \times u_2$ ):

$$J_x y_3 - x_3 J_y = z_1 J_2 - J_1 z_2.$$
<sup>(20)</sup>

Here also the pair of operators  $K, J'_+$  are of the type discussed in appendix 1 so we can use relation (A.4).

From the above relations we obtain for the commutator  $[K_+, j_+]$ :

$$[K_{+}, j_{+}] = [J'_{+}V'_{1}(j - K + 1)^{-1} - V'_{1}J'_{+}(j - K)^{-1}]F(j, K, M)$$
(21)

i.e. K in relation (21) plays the role of M in relation (17). Now with relations (18) and (19) it follows that

$$(J_1 - iJ_2)(z_1J_2 - J_1z_2) = -(z_2 + iz_1)(J^2 - J_3^2 + \hbar J_3) + (J_2 + iJ_1)z_3(\hbar - J_3)$$
  
$$(z_1J_2 - J_1z_2)(J_1 - iJ_2) = -(z_2 + iz_1)(J^2 - J_3^2) - (J_2 + iJ_1)z_3J_3.$$

Hence

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$$J'_{+}V'_{1} = [-\hbar^{2}(z_{2} + iz_{1})(j + K) + \hbar(J_{2} + iJ_{1})z_{3}](j + 1 - K)$$
  
$$V'_{1}J'_{+} = [-\hbar^{2}(z_{2} + iz_{1})(j + K) + \hbar(J_{2} + iJ_{1})z_{3}](j - K).$$

Using these relations in (21) we see immediately that  $[K_+, j_+] = 0$  and so  $[\gamma, \alpha] = 0$ .

#### 5. Conclusion

The three pairs of operators  $(j, \alpha)$ ,  $(M, \beta)$ ,  $(K, \gamma)$  form the complete canonical set for the description of rotational motion. Obviously, all we have said remains valid when we deal with rotational motion around the centre of mass. If we investigate the properties of a rotationally invariant Hamiltonian, we find that the problem can be reduced since  $\alpha$  is a cyclic variable ([H, J] = 0) and so also is M and its conjugate momentum  $\beta$ : since  $[J_z, H] = [J_+, H] = [J_-, H] = 0$  then [M, H] = 0 and  $[\beta, H] = 0$ . This simply demonstrates the well known rotational degeneracy of H.

Concerning the application to rotational motion, since  $\alpha$  is a complicated object, it follows that the method of Villars (1965) cannot be applied. Then, rather than  $\alpha$ , we shall use  $j_+$ . Let H be a rotationally invariant Hamiltonian. In the above method, H is expanded in powers of j, here we try the equivalent series:

$$H = H_0 + H_1 f_1(j) + H_2 f_2(j) + \dots + H_n f_n(j) + \dots$$
(22)

where the unknown coefficients  $H_n$  depend on the 'intrinsic variables' only, and the  $f_n(j)$  are such that:

$$f_n(j) = \frac{j(j-1)(j-2)\dots(j-n+1)}{n!}.$$
(23)

These functions have the interesting property that

$$f_n(j+1)-f_n(j)=f_{n-1}(j),$$

so (relation (A.4))

$$[f_n(j), j_+] = j_+ f_{n-1}(j),$$

Then if  $H^{(0)}, H^{(1)}, H^{(2)}...$  are defined by:

$$H^{(0)} = H,$$
  $[H^{(0)}, j_+] = j_+ H^{(1)},$   $[H^{(1)}, j_+] = j_+ H^{(2)},$  ...

we get:

$$H^{(p)} = \sum_{n=p}^{\infty} H_n f_{n-p}.$$

In order to obtain the  $H_n$ , the above triangular system must be inverted. Let us put:

$$A_{\nu}(j) = (-1)^{\nu} \frac{j(j+1)\dots(j+\nu-1)}{\nu!}$$
(24)

Then (see relation (A.7))

$$\sum_{p=i}^{n} A_{p-i} f_{n-p} = \delta_{n,i}.$$

Hence:

$$H_{n} = \sum_{p=n}^{\infty} H^{(p)} A_{p-n}.$$
 (25)

These results can be verified in the simple case of the one-body kinetic energy. The commutators  $H^{(i)}$  are calculated in appendix 2: we have (relations (A.5), (A.6))

$$H^{(1)} = \frac{\hbar^2(j+1)}{mr^2}, \qquad H^{(2)} = \frac{\hbar^2}{mr^2}, \qquad H^{(i)} = 0, \qquad i \ge 3.$$

This last relation shows, with (23), that expansion (22) stops at  $H_2f_2$ . Using (24) and (25), we get

$$H_2 = \frac{\hbar^2}{mr^2} \qquad H_1 = \frac{\hbar^2}{mr^2}$$

which is the required result.

In fact in expansion (22), the coefficients  $H_n$  can be obtained without introducing the intrinsic coordinates, remaining expressed in the original particle coordinates. Thus the advantage of working with independent-particle wavefunctions is not lost, although the dependence on the collective angular momentum has been extracted explicitly. We think here especially of the nuclear rotational problem. For example, we can hope to realise variational calculations in order to get the lower state of a given angular momentum (the Yrast line), or to obtain the value of the moment of inertia (see Rowe 1967).

# Appendix 1

Suppose there are two operators  $O_1$  and  $O_2$  such that

$$[O_1, O_2] = O_2 \lambda, \tag{A.1}$$

where  $\lambda$  is a function of  $O_1$ . Let us look for the commutator

$$C_{n} = [O_{1}^{n}, O_{2}]$$
  
=  $O_{1}^{n-1}[O_{1}, O_{2}] + [O_{1}^{n-1}, O_{2}]O_{1}$   
=  $O_{1}^{n-1}O_{2}\lambda + C_{n-1}O_{1} = C_{n-1}(\lambda + O_{1}) + O_{2}O_{1}^{n-1}\lambda.$ 

This recurrence relation gives:

$$C_n = O_2[(O_1 + \lambda)^n - O_1^n].$$
(A.2)

Then if  $f(O_1)$  is a function of  $O_1$  we can write

$$[f(O_1), O_2] = O_2[f(O_1 + \lambda) - f(O_1)]$$
(A.3)

or

or

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$$f(O_1)O_2 = O_2 f(O_1 + \lambda).$$

In the special case where  $\lambda = 1$ ,

$$[f(O_1), O_2] = O_2[f(O_1 + 1) - f(O_1)]$$

$$f(O_1)O_2 = O_2f(O_1 + 1).$$
(A.4)

# Appendix 2. The case of one-body kinetic energy

In this case we take  $u_3 = r$ , since  $J = r \times p$ , then K = 0 and the canonical set reduces to  $(\alpha, J), (\beta, J_z)$ .

The part of  $j_+$  which does not commute with

$$T = \frac{p^2}{2m} = \frac{1}{2m} (p_x^2 + p_y^2 + p_z^2)$$

is

$$g_+ = (J_x y - x J_y + \mathrm{i}\hbar z j)r^{-1}$$

so  $g_+$  is sufficient.

Let us calculate  $T^{(1)}, T^{(2)}, \ldots$  defined by  $[T, g_+] = g_+ T^{(1)}, [T^{(1)}, g_+] = g_+ T^{(2)}, \ldots$ . We have

$$[p^{2}, g_{+}] = -2i\hbar[J_{x}(p_{y}r^{2} - yp \cdot r) - (p_{x}r^{2} - xp \cdot r)J_{y} + i\hbar(p_{z}jr^{2} - zp \cdot rj)]r^{-3}$$

since

$$p_y r^2 - y \mathbf{p} \cdot \mathbf{r} = J_z x - z J_x$$
 (and cyclic permutations)

and

$$J_x(J_z x - zJ_x) - (J_y z - yJ_z)J_y = -zJ^2 + i\hbar(J_x y - xJ_y)$$

we get

$$T^{(1)} = \frac{\hbar^2(j+1)}{mr^2}.$$
 (A.5)

Then

$$[T^{(1)}, g_{+}] = g_{+} \frac{\hbar^{2}}{mr^{2}} = g_{+}T^{(2)}$$
  
[T<sup>(2)</sup>, g\_{+}] = 0. (A.6)

# **Appendix 3**

With:

$$f_{\nu}(j) = \frac{j(j-1)\dots(j-\nu+1)}{\nu!}$$

$$A_{\nu}(j) = (-1)^{\nu} \frac{j(j+1)\dots(j+\nu-1)}{\nu!}$$

$$A_{0}(j) = 1$$

$$f_{0}(j) = 1$$

we get the following expansions (for |x| < 1):

$$(1+x)^{j} = \sum_{\nu=0}^{\infty} f_{\nu}(j)x^{\nu}$$
$$(1+x)^{-j} = \sum_{\nu=0}^{\infty} A_{\nu}(j)x^{\nu}.$$

 $f_{\nu}(j)$  and  $A_{\nu}(j)$  are in fact the generalised binomial coefficients  $\binom{i}{\nu}$  and  $(-1)^{\nu}\binom{i+\nu-1}{\nu}$ . Multiplication of the two previous series gives:

$$1 = \sum_{k=0}^{\infty} x^k \sum_{\nu=0}^{k} A_{\nu} f_{k-\nu}$$

Comparison of the coefficients of  $x^k$  in the two terms leads to:

$$\sum_{\nu=0}^{k} A_{\nu} f_{k-\nu} = \delta_{k,0}.$$

Putting k = n - i,  $\nu = p - i$  we get:

$$\sum_{p=i}^{n} A_{p-i} f_{n-p} = \delta_{n,i}.$$
 (A.7)

# References

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