

# Construction and counting of the number of operators included in a normalized vibrational Hamiltonian with $n$ degrees of freedom with a $p : q$ resonance

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## Abstract

This paper is the second one of two papers aimed at constructing hamiltonian systems of  $n$  degrees of freedom. In molecular spectroscopy, the construction of vibrational Hamiltonians for highly excited molecular systems through algebraic formalism implies to introduce "by hand" the operators reflecting the exchanges of quanta of energy between the different oscillators. It is thus tedious to predict, for any given order of the development of the Hamiltonian, the total number of operators which should appear in the Hamiltonian ([1], [2], [3]). In this second paper, we propose a method of construction of a normalized vibrational Hamiltonian of a highly excited molecular system with  $n$  degrees of freedom in the case of a  $p : q$  resonance. We present also the counting of all the independent operators and the counting of all the parameters included in the Hamiltonian (Counting theorems 1 to 8). The method introduces, on a systematic way, all the operators, in particular the coupling operators, that can be built from the polynomials formed by products of powers of the generators of a Lie algebra: the algebra of the invariant polynomials built in classical mechanics from the kernel  $\text{Ker } ad_{\mathcal{H}_0}$  of the adjoint operator  $ad_{\mathcal{H}_0}$  (see [6] or [4], [5]). Application to the non-linear triatomic molecule ClOH is then given, taking into account the Fermi resonance between the O-Cl stretching oscillators and the bending motion. The study of this molecular system in highly excited vibrational states (until almost the dissociation limit) has been realized in [2], with a fit of 725 levels of energy. On the 86 coefficients (among which 31 coupling coefficients) that we count, and completely compatible with [2], the smallest rms value leads to keep only 28 non-zero coefficients. In the appendix, we explain the vocabulary and the strategy employed in order to demonstrate the theorems of coupling operators included in the Hamiltonian.

*Keywords:* Molecular structure ; Vibrational Hamiltonian ; Lie Algebra ; Polynomial Invariants ; Resonance  $p : q$ .

## 1. Introduction

This second article is the continuation of a first one [6] where we applied an algebraic approach to study highly excited molecular systems with no resonance between two of the oscillators representing the molecular system.

After some basic reminders about the normalization

([7], [8], [9]), we built a vibrational Hamiltonian written as a Dunham expansion on the basis of the generators of the invariant polynomial algebra and we have counted all the operators included in the Hamiltonian developed until the order  $N$  (Eq. (13) of [6]). An application to the non-linear triatomic molecule of ClOH has been performed as the highly excited vibrational states of this molecule have been widely studied ([10], [11], [12]). Thus the Hamiltonian (Table 2 of [6]) allows to reproduce the vibrational

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structure of 314 energy levels (until 70 % of the dissociation energy) with a set of 34 coefficients which is in good agreement with [2]. In order to describe the vibrational structure of more excited levels, it is necessary to take into account a 2 : 1 resonance between the stretching oscillator associated with the O-Cl bond and the bending oscillator associated to the angular deformation between bonds O-Cl and O-H. The coupling operators are then implemented by hand on a more or less arbitrary manner and it is a laborious task to predict in advance the total number of operators appearing in the Hamiltonian.

In the present paper, after some definitions and reminders about the standard normalization of the harmonic oscillator of quadratic part  $\mathcal{H}_0$  (section 2), we present a building method of the normalized vibrational Hamiltonian for a molecular system having two degrees of freedom fulfilling a  $p : q$  resonance condition ( $p$  and  $q$  are positive integers with a gcd equal to 1). We derive also the enumeration of all the independent operators and the number of involved coefficients. Then we extend the method to systems having  $n$  degrees of freedom (section 3). The method introduces on a systematic way all the operators, in particular the coupling operators, which can be obtained from polynomial formed by products of powers of the generators of the invariant polynomial algebra. Then we establish the theorems counting the coupling operators involved in the Hamiltonian (sections 3.4 and 3.5). Demonstration of these theorems imply to implement a specific vocabulary which is given in Appendix. We end our paper with the counting of all the operators and parameters involved in the normalized Hamiltonian describing the vibrational structure of ClOH molecule until 98 % of the dissociation limit (section 4).

## 2. Normalization

### 2.1. Lowest order Hamiltonian: $\mathcal{H}_0$

Suppose  $\mathcal{H}(q_1, \dots, q_n, p_1, \dots, p_n)$  the classical vibrational Hamiltonian of an Hamiltonian system with  $n$  degrees of

freedom, the quadratic part of which is an anisotropic harmonic oscillator  $\mathcal{H}_0 = \sum_{k=1}^n \frac{\omega_k(q_k^2 + p_k^2)}{2}$ , where the  $n$  quantities  $\omega_k$  are characteristic pulsations of the oscillators (with  $1 \leq i, j \leq n$ ,  $\omega_i \neq \omega_j$ ) and  $q_k, p_k$  are the canonical dimensionless variables generalized coordinates and conjugate momenta defined on the phase space  $\Gamma$ .

### 2.2. Definition of the $p : q$ resonance

The hamiltonian  $\mathcal{H}_0$  shows a unique  $p : q$  resonance if two pulsations (refer here-after as  $\omega_1$  and  $\omega_2$ ) are connected through a relation of the form:

$$\frac{\omega_2}{\omega_1} = \frac{p}{q}, \quad (1)$$

$p$  and  $q$  are two positive integers with  $\text{gcd}(p, q) = 1$  and  $p \geq q$  [4], the  $n - 2$  others pulsations  $\omega_k$  satisfying to the condition of non resonance (Equation (3) of [6]).

### 2.3. Equations of motion

We introduce the complex variables  $z_k$  and  $z_k^*$  defined in function of the canonical variables  $q_k$  and  $p_k$  ( $1 \leq k \leq n$ ) as:  $z_k = \frac{1}{\sqrt{2}}(q_k + ip_k)$  and  $z_k^* = \frac{1}{\sqrt{2}}(q_k - ip_k)$ . The lowest order Hamiltonian can be now rewritten  $\mathcal{H}_0 = -i(\omega_1 z_1 z_1^* + \frac{p}{q} \omega_1 z_2 z_2^* + \sum_{k=3}^n \omega_k z_k z_k^*)$ . With these new variables  $z_k$ , the equations of motion reads:

$$\frac{dz_1}{dt} = -i\omega_1 z_1, \quad \frac{dz_2}{dt} = -i\frac{p}{q}\omega_1 z_2, \quad \frac{dz_k}{dt} = -i\omega_k z_k \quad (3 \leq k \leq n). \quad (2)$$

### 2.4. Hamiltonian flow

From an initial condition  $z_0 = (z_{1,0}, \dots, z_{n,0})$ , formally the solution of the equations of motion is written as  $z(t) = \phi_t^{\mathcal{H}_0}(z_0)$ .  $\phi_t^{\mathcal{H}_0} : \Gamma \rightarrow \Gamma$  is the Hamiltonian flow generated by  $\mathcal{H}_0$  ([13, 14, 15])

$$\text{We have: } z(t) = \phi_t^{\mathcal{H}_0}(z_0) \implies \begin{pmatrix} z_1(t) \\ \vdots \\ z_n(t) \end{pmatrix} = \begin{pmatrix} e^{-i\omega_1 t} & 0 & \dots & 0 \\ 0 & e^{-i\frac{p}{q}\omega_1 t} & \dots & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & e^{-i\omega_n t} \end{pmatrix} \begin{pmatrix} z_{1,0} \\ \vdots \\ z_{n,0} \end{pmatrix}. \quad (3)$$

Solutions  $z(t)$  are the trajectories of the Hamiltonian flow or the orbits of the harmonic oscillator with a  $p : q$  resonance.

### 2.5. Hilbert basis

The condition of resonance (1) implies that the kernel  $\text{Ker } ad_{\mathcal{H}_0}$  of the adjoint operator  $ad_{\mathcal{H}_0}$ , (defined by equations (4) and (5) of [6]), is generated by the  $n + 2$  monomials ([4]) ( $n \geq 2$  integer) :

$$\sigma_{-1} = z_1^{*p} z_2^q, \sigma_0 = z_1^p z_2^{*q}, \sigma_1 = z_1 z_1^*, \dots, \sigma_n = z_n z_n^*. \quad (4)$$

The kernel has the structure of a Lie algebra, called algebra of the invariant polynomials. The generators  $\sigma_k$  ( $-1 \leq k \leq n$ ) form a basis of  $\text{Ker } ad_{\mathcal{H}_0}$  called Hilbert basis ([16, 17, 18]). As in the non resonant case, the generators of the Hilbert basis are invariant under the flow of the harmonic oscillator  $\phi_t^{\mathcal{H}_0}$ , which is a symplectic symmetry for the generators [6]. While for the case  $n = 2$ , [15] used  $J = p\sigma_1 + q\sigma_2$ ,  $\Pi_1 = p\sigma_1 - q\sigma_2$ ,  $\Pi_2 = \sqrt{2^{p+q} p^q q^p} \text{Re}(z_1^{*p} z_2^q)$  and  $\Pi_3 = \sqrt{2^{p+q} p^q q^p} \text{Im}(z_1^{*p} z_2^q)$ , we prefer to conserve equations (4) which are more easy to use in order to build a normalized quantum Hamiltonian as we will see in section 3.

### 2.6. Poisson brackets of the generators

The Poisson brackets of the generators are equal to zero except:  $\{\sigma_{-1}, \sigma_1\} = ip\sigma_{-1}$ ,  $\{\sigma_{-1}, \sigma_2\} = -iq\sigma_{-1}$ ,  $\{\sigma_0, \sigma_1\} = -ip\sigma_0$ ,  $\{\sigma_0, \sigma_2\} = iq\sigma_0$  and  $\{\sigma_{-1}, \sigma_0\} = i\sigma_1^{p-1}\sigma_2^{q-1}(p^2\sigma_2 - q^2\sigma_1)$ .

### 2.7. Reduced phase space

The generators of the invariant polynomials algebra,  $\sigma_{-1}$ ,  $\sigma_0$ ,  $\sigma_1$  and  $\sigma_2$  ( $\sigma_1 \geq 0$ ,  $\sigma_2 \geq 0$ ), are not independent. They satisfy the relation:

$$\left(\frac{\sigma_0 + \sigma_{-1}}{2}\right)^2 + \left(\frac{\sigma_0 - \sigma_{-1}}{2i}\right)^2 = \sigma_1^p \sigma_2^q. \quad (5)$$

In the phase space  $\Gamma = \mathbb{R}^{2n}$ , the iso- $\mathcal{K}$ -energy surfaces are hyper-surfaces of  $\mathbb{R}^{2n-1}$ .

For a given value  $h_0$  of  $\mathcal{H}'_0 = -\frac{\mathcal{H}_0}{i}$  (obviously  $h_0 > 0$ ), in the case of a  $p : q$  resonance, (5) becomes:

$$\sigma_0'^2 + \sigma_{-1}'^2 = \sigma_1^p \left( \frac{h_0}{\omega_2} - \frac{q}{p} \sigma_1 - \sum_{k=3}^n \left( \frac{\omega_k}{\omega_2} \right) \sigma_k \right)^q, \quad (6)$$

with  $\sigma_0' = \frac{\sigma_0 + \sigma_{-1}}{2}$  and  $\sigma_{-1}' = \frac{\sigma_0 - \sigma_{-1}}{2i}$  and the condition  $h_0 \geq \omega_2 \frac{q}{p} \sigma_2 + \sum_{k=3}^n \omega_k \sigma_k$ . In the phase space, Eq. (6) defines the reduced phase space [15], on which the dynamics of the motion is reduced to a space of dimension  $n$ .

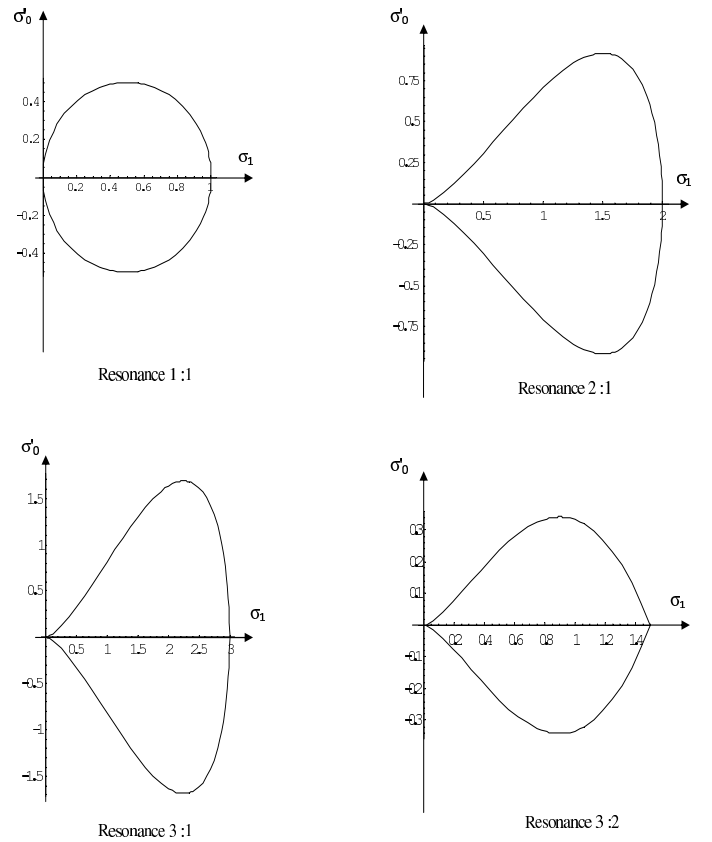


Figure 1: In the plan  $(\sigma_1, \sigma_0')$  for  $\frac{h_0}{\omega_2} = 1$  S.I.: reduced phase space for different  $p : q$  resonance values.

### 2.8. The normalized Hamiltonian $\mathcal{K}$

We want to define a normalized Hamiltonian  $\mathcal{K}$  verifying  $\{\mathcal{H}_0, \mathcal{K}\} = -ad_{\mathcal{H}_0}(\mathcal{K}) = ad_{\mathcal{K}}(\mathcal{H}_0) = 0$ .  $\mathcal{K}$  can be written on the form ([4]):  $\mathcal{K} = \mathcal{H}_0 + f(\sigma_{-1}, \sigma_0, \sigma_1, \dots, \sigma_n)$ , moreover  $\mathcal{K}$  has to be invariant under time reversal operation (TRO). Generators  $\tau(\sigma_k) = \sigma_k$  for  $1 \leq k \leq n$  are

also invariant under TRO except  $\sigma_{-1}$  and  $\sigma_0$  which verify  $\sigma_{-1} \leftarrow \text{TRO} \rightarrow \sigma_0$ .

### 3. Construction of the normalized Hamiltonian

#### 3.1. Case $n = 2$

##### 3.1.1. Development of the Hamiltonian on the Hilbert basis

We show this case as an example of modeling of the vibrational normalized Hamiltonian describing high excited stretching modes of triatomic ABC or AB<sub>2</sub> molecules. The resonant normalized Hamiltonian  $\mathcal{K}$ , with quadratic term  $\mathcal{H}_0 = -i\frac{\omega_1}{q}(q\sigma_1 + p\sigma_2)$  is only function of  $\sigma_{-1}$ ,  $\sigma_0$ ,  $\sigma_1$  and  $\sigma_2$ :  $\mathcal{K} = \mathcal{H}_0 + f(\sigma_{-1}, \sigma_0, \sigma_1, \sigma_2)$ . We expand the normalized Hamiltonian as a polynomial development of powers of the generators until an order  $N$ . In what follows,  $N \geq p + q + 4$ ,  $q_0, q_1, q_2, q_3, \delta$  and  $\beta$  are integers; values of  $Q_0, Q_1, Q_2$  and  $Q_3$  in the sums have to be precise in order that the development based on the generators of the algebra be effectively a polynomial expansion. >From [6] we already know that  $Q_0 = E(\frac{N}{2})$ . In the expression of  $\mathcal{K}$  here-after, we will need to demonstrate that  $Q_1 = E(\frac{N}{p+q})$ ,

$$Q_2 = E(\frac{\delta-(p+q)}{2}) \text{ and } Q_3 = E(\frac{\beta-(p+q)}{2}):$$

$$\begin{aligned} \mathcal{K} &= \mathcal{H}_0 + \sum_{q_0=2}^{Q_0} (\alpha_{q_0}^1 \sigma_1^{q_0} + \alpha_{q_0}^2 \sigma_2^{q_0}) \\ &+ \sum_{r=2}^{Q_0} \sum_{1 \leq i_1 < i_2 \leq 2} \sum_{r_{i_1} \geq 1, r_{i_2} \geq 1}^{r_{i_1} + r_{i_2} = r} \alpha_{r_{i_1}, r_{i_2}}^{i_1, i_2} \sigma_{i_1}^{r_{i_1}} \sigma_{i_2}^{r_{i_2}} \\ &+ \sum_{q_1=1}^{Q_1} (\alpha_{q_1}^0 \sigma_{-1}^{q_1} + \alpha_{q_1}^{\prime 0} \sigma_0^{q_1}) \\ &+ \sum_{\delta=p+q+2}^N \sum_{q_2=1}^{Q_2} \left( \alpha_{E(\frac{\delta-2q_2}{p+q}), q_2}^{-1, 1} \sigma_{-1}^{E(\frac{\delta-2q_2}{p+q})} \sigma_1^{q_2} \right. \\ &+ \left. \alpha_{E(\frac{\delta-2q_2}{p+q}), q_2}^{0, 1} \sigma_0^{E(\frac{\delta-2q_2}{p+q})} \sigma_1^{q_2} \right) \\ &+ \sum_{\delta=p+q+2}^N \sum_{q_2=1}^{Q_2} \left( \alpha_{E(\frac{\delta-2q_2}{p+q}), q_2}^{-1, 2} \sigma_{-1}^{E(\frac{\delta-2q_2}{p+q})} \sigma_2^{q_2} \right. \\ &+ \left. \alpha_{E(\frac{\delta-2q_2}{p+q}), q_2}^{\prime 0, 2} \sigma_0^{E(\frac{\delta-2q_2}{p+q})} \sigma_2^{q_2} \right) \\ &+ \sum_{\beta=p+q+4}^N \sum_{q_3=2}^{Q_3} \sum_{\gamma=1}^{q_3-1} \left( \alpha_{E(\frac{\beta-2q_3}{p+q}), \gamma, q_3-\gamma}^{-1, 1, 2} \sigma_{-1}^{E(\frac{\beta-2q_3}{p+q})} \sigma_1^\gamma \sigma_2^{q_3-\gamma} \right. \\ &+ \left. \alpha_{E(\frac{\beta-2q_3}{p+q}), \gamma, q_3-\gamma}^{0, 1, 2} \sigma_0^{E(\frac{\beta-2q_3}{p+q})} \sigma_1^\gamma \sigma_2^{q_3-\gamma} \right). \end{aligned} \quad (7)$$

In section 3.1.3, we will prove that the invariance of  $\mathcal{K}$  under TRO implies that all the coefficients of  $\mathcal{K}$  are purely imaginary.

Furthermore, one distinguishes in  $\mathcal{K}$  the monomials built as powers of  $\sigma_{-1}$  or  $\sigma_0$  and we will call them coupling monomials between the two resonant oscillators : they appear in the sums  $S_0 = \sum_{q_1=1}^{Q_1} (\alpha_{q_1}^0 \sigma_{-1}^{q_1} + \alpha_{q_1}^{\prime 0} \sigma_0^{q_1})$ ,

$$\begin{aligned} S_{m, \ell}^{(2)} &= \sum_{\delta=p+q+2}^N \sum_{q_2=1}^{Q_2} \alpha_{E(\frac{\delta-2q_2}{p+q}), q_2}^{m, \ell} \sigma_m^{E(\frac{\delta-2q_2}{p+q})} \sigma_\ell^{q_2} \text{ or } S_m^{(3)} \\ &= \sum_{\beta=p+q+4}^N \sum_{q_3=2}^{Q_3} \sum_{\gamma=1}^{q_3-1} \alpha_{E(\frac{\beta-2q_3}{p+q}), \gamma, q_3-\gamma}^{m, 1, 2} \sigma_m^{E(\frac{\beta-2q_3}{p+q})} \sigma_1^\gamma \sigma_2^{q_3-\gamma}. \end{aligned} \quad (m = -1, 0; \ell = 1, 2)$$

Others monomials are the non resonant monomials.

##### 3.1.2. Invariance of $\mathcal{K}$ under TRO

Hypothesis of the invariance of the Hamiltonian  $\mathcal{K}$  under TRO implies the following identification:

$$\begin{aligned} \alpha_{q_1}^0 &= \alpha_{q_1}^{\prime 0} \\ \alpha_{E(\frac{\delta-2q_2}{p+q}), q_2}^{-1, \ell} &= \alpha_{E(\frac{\delta-2q_2}{p+q}), q_2}^{0, \ell} \quad (\ell = 1, 2) \\ \alpha_{E(\frac{\beta-2q_3}{p+q}), \gamma, q_3-\gamma}^{-1, 1, 2} &= \alpha_{E(\frac{\beta-2q_3}{p+q}), \gamma, q_3-\gamma}^{0, 1, 2}. \end{aligned} \quad (8)$$

Taking into account the relations Eq. (8), one may factorize sets of  $\lambda$ -monomials of same coefficients in Eq. (7). These  $\lambda$ -monomials are all real, in particular the following coupling monomials:  $\left(\sigma_{-1}^{E(\frac{\delta-2q_2}{p+q})} + \sigma_0^{E(\frac{\delta-2q_2}{p+q})}\right)\sigma_\ell^{q_2}$  and  $\left(\sigma_0^{E(\frac{\beta-2q_3}{p+q})} + \sigma_{-1}^{E(\frac{\beta-2q_3}{p+q})}\right)\sigma_1^\gamma\sigma_2^{q_3-\gamma}$ . Moreover the transformation of the  $(q_k, p_k)$  in  $(z_k, z_k^*)$  is symplectic of multiplier  $-i$ , like the Hamiltonian  $\mathcal{K}$ . One thus deduce that all the coefficients in Eq. (7) are purely imaginary.

### 3.1.3. Independence of the coefficients

>From the Jacobi identity  $(-1 \leq j \leq 2)$ :  $\{\mathcal{K}, \{\sigma_j, \mathcal{H}_0\}\} + \{\mathcal{H}_0, \{\mathcal{K}, \sigma_j\}\} + \{\sigma_j, \{\mathcal{H}_0, \mathcal{K}\}\} = 0$  and calculating all the Poisson brackets  $\{\mathcal{K}, \sigma_j\}$ , knowing that  $(\mathcal{K}, \sigma_j) \in \text{Ker } \text{ad}_{\mathcal{H}_0}$ , one deduces that none relation exists between the coefficients of the development of Eq. (7): the different  $\lambda$ -monomials are independent between them.

### 3.1.4. Range of variation of the $Q_i$

We will now precise the range of variation of the integers appearing in (7).

- For  $Q_1$ : the monomials  $\sigma_{-1}^{q_1}$  and  $\sigma_0^{q_1}$  are of degree  $d' = (p+q)q_1$ .  $q_1$  takes all integer values from 1 to the maximal value  $Q_1$  satisfying  $(N \geq p+q)$ :  $Q_1 = E(\frac{N}{p+q})$ . If  $N < p+q$ , all the coefficients  $\alpha_{q_1}^0$  are equal to zero.
- For  $Q_2$ : the 2-monomials  $\sigma_{-1}^{p_2}\sigma_1^{q_2}$ ,  $\sigma_0^{p_2}\sigma_1^{q_2}$ ,  $\sigma_{-1}^{p_2}\sigma_2^{q_2}$  and  $\sigma_0^{p_2}\sigma_2^{q_2}$  ( $p_2$  positive integer) are of degree  $(p+q)p_2 + 2q_2$ . In an expansion of  $\mathcal{K}$  to a given order  $\delta$ , the following condition should be verified for the degree of the different 2-monomials:

$$(p+q)p_2 + 2q_2 = \delta. \quad (9)$$

As the products of the powers of these 2-monomials should always appear in  $\mathcal{K}$ , it implies  $p_2 \geq 1$  and  $q_2 \geq 1$ , i.e.  $\delta \geq p+q+2$ . The integer  $q_2$  may vary from 1 to a maximal value  $Q_2$ , obtained for the smallest value of  $p_2$  ( $p_2 = 1$ ). From (9), one deduces

$$\text{that } Q_2 = E\left(\frac{\delta-(p+q)}{2}\right).$$

We determine now the range of variation of the integer  $p_2$ . Conditions (9) and  $p_2$  integer imply that, for a fixed value of  $\delta$ , with  $1 \leq q_2 \leq Q_2$ ,  $p_2$  varies between the integer values of  $E(\frac{\delta-2Q_2}{p+q})$  and  $E(\frac{\delta-2}{p+q})$ . In particular, for  $\delta = p+q+2$  or  $p+q+3$ :  $Q_2 = 1$  and  $p_2 = 1$ ; however for  $\delta = p+q+3$ , the condition (9) is not satisfied. This will not be detrimental to the counting of the coefficients in the sums  $S_{m,\ell}^{(2)}$  but will introduce redundancies among the 2-monomials (See paragraph 3.3) which will then be eliminated (See appendix). Thereafter, we denote  $p_2 = E(\frac{\delta-2q_2}{p+q})$ . Finally  $\delta$  varies from  $p+q+2$  to  $N$  ( $N \geq p+q+2$ ). If  $\delta < p+q+2$ , all the coefficients in the sums involving 2-monomials are equal to zero.

- For  $Q_3$ : the 3-monomials  $\sigma_{-1}^{p_3}\sigma_1^\gamma\sigma_2^{r_3}$  and  $\sigma_0^{p_3}\sigma_1^\gamma\sigma_2^{r_3}$  ( $p_3, \gamma$  and  $r_3$  are positive integers) are of degree  $(p+q)p_3 + 2\gamma + 2r_3$ . As for the 2-monomials, one requires that the following condition is respected:

$$(p+q)p_3 + 2\gamma + 2r_3 = \beta. \quad (10)$$

As the products of powers of the 3-monomials have to be include in  $\mathcal{K}$ :  $p_3 \geq 1, \gamma \geq 1$  and  $r_3 \geq 1$ , thus  $\beta \geq p+q+4$ . We denote  $q_3 = \gamma + r_3$ . For a fixed value of  $q_3$ ,  $\gamma$  takes all the values from 1 to  $q_3 - 1$ . Furthermore we impose no constraint to the integer  $q_3$  which takes all values from 2 ( $r_3 = \gamma = 1$ ) to a maximal value  $Q_3$ , obtained for  $p_3 = 1$ . With (10), we find that  $Q_3 = E(\frac{\beta-(p+q)}{2})$ .

We determine now the range of variation of the integer  $p_3$ . For a fixed value of  $\beta$ , conditions (10) and  $p_3$  integer imply that, for  $2 \leq q_3 \leq Q_3$ ,  $p_3$  varies between the integer values of  $E(\frac{\beta-2Q_3}{p+q})$  and  $E(\frac{\beta-4}{p+q})$ . In particular, for  $\beta = p+q+4$  or  $\beta = p+q+5$ :  $Q_3 = 2$  and  $p_3 = 1$ . For  $\beta = p+q+5$ , condition (10) is not fulfilled, thus the counting of the coefficients in the sums  $S_m^{(3)}$  will show redundancies among the 3-monomials (See section 3.3) that will have to

be removed (See appendix). Thereafter, we denote  $p_3 = E(\frac{\beta-2q_3}{p+q})$ . All the coefficients in the sums involving 3-monomials are *a priori* non equal to zero except if  $p + q + 4 \leq \beta \leq N$ .

### 3.1.5. Counting

For a given value of  $N$ ,  $2E(\frac{N}{p+q})$  monomials appear in the sum  $S_0$ . For given values of  $N$  and  $\delta$ , a sum  $S_{m,\ell}^{(2)}$  contains  $Q_2$  2-monomials. Thus one deduces that it contains  $\Lambda_1 = \sum_{\delta=p+q+2}^N E(\frac{\delta-(p+q)}{2})$  2-monomials. Denoting  $N = p+q+2+K$  with  $K$  integer and  $\delta = p+q+2+k$  with  $k$  an integer such that  $k = 0, \dots, K$ :  $\Lambda_1 = \sum_{k=0}^K E(1+\frac{k}{2})$ . The sum contains  $K+1$  monomials but the calculation of  $\Lambda_1$  depends on the parity of  $K$ :

- if  $K = 2\tilde{p}$  ( $\tilde{p}$  integer) is even, thus for  $k = 0, \dots, K$ , each integer in the sum appears two times: 1 associated to  $E(1), E(3/2), \dots$ , except the last term giving  $E(\tilde{p}+1) = \tilde{p}+1$  which appears only one time, thus we get:

$$\Lambda_1 = \frac{1}{4}[N - (p+q)]^2. \quad (11)$$

- if  $K = 2\tilde{p}+1$  ( $\tilde{p}$  integer) is odd, thus for  $k = 0, \dots, K$ , each integer in the sum appears two times: 1 associated to  $E(1), E(3/2), \dots, \tilde{p}+1$  for  $E(\tilde{p}+1)$  and  $E(\tilde{p}+3/2)$ . After calculations, one obtains:

$$\Lambda_1 = \frac{1}{4}[N - (p+q) - 1][N - (p+q) + 1]. \quad (12)$$

For fixed values of  $N$  and  $\beta$ , a sum  $S_m^{(3)}$  contains  $\sum_{q_3=2}^{Q_3} (q_3 - 1) = \frac{Q_3(Q_3-1)}{2}$ . This sum has

$$\Lambda_2 = \sum_{\beta=p+q+4}^N \frac{\binom{E(\frac{\beta-(p+q)}{2})}{2} \binom{E(\frac{\beta-(p+q)}{2})-1}{2}}{2} \text{ 3-monomials.}$$

We denote now  $N = p+q+4+K$  with  $K$  integer and  $\beta = p+q+4+k$  with  $k$  integer such that  $k = 0, \dots, K$ ,

$$\Lambda_2 = \sum_{k=0}^K \frac{\binom{E(2+\frac{k}{2})}{2} \binom{E(2+\frac{k}{2})-1}{2}}{2}. \text{ Also we denote } \tilde{S}_1 = \sum_{k=0}^K E^2(2+\frac{k}{2}) \text{ and } \tilde{S}_2 = \sum_{k=0}^K E(2+\frac{k}{2}). \text{ The calculation of these two sums depends on the parity of } K:$$

- if  $K = 2\tilde{p}$  ( $\tilde{p}$  integer) is even, then for  $k = 0, \dots, K$ , the following integers appear two times in the sum  $\tilde{S}_1$ : 4 associated to  $E^2(2), E^2(5/2), 9$  for  $E^2(3), E^2(7/2), \dots$ ; only the last term giving  $E^2(\tilde{p}+2) = (\tilde{p}+2)^2$  appears once. With the same process applied for  $\tilde{S}_2$ , one finally obtains:  $\tilde{S}_1 = \frac{(\tilde{p}+1)(2\tilde{p}^2+4\tilde{p}+3)}{3}$  and  $\tilde{S}_2 = (\tilde{p}+1)(\tilde{p}+2) + \tilde{p}$ .

Thus one deduces that:

$$\Lambda_2 = \frac{1}{24}[N - (p+q) - 2][N - (p+q) - 1][N - (p+q)]. \quad (13)$$

- if  $K = 2\tilde{p}+1$  ( $\tilde{p}$  integer) is odd, for  $k = 0, \dots, K$ , the following integers appear two times in the sum  $\tilde{S}_1$ : 4 associated to  $E^2(2), E^2(5/2), 9$  for  $E^2(3), E^2(7/2), \dots, (\tilde{p}+2)^2$  for  $E^2(\tilde{p}+2)$  and  $E^2(\tilde{p}+5/2)$ . Performing all the calculations, it reads:

$$\tilde{S}_1 = \frac{(\tilde{p}+2)(\tilde{p}+3)(2\tilde{p}+5)}{3} - 2 \text{ and } \tilde{S}_2 = (\tilde{p}+2)(\tilde{p}+3) - 2.$$

Finally, the result is given by:

$$\Lambda_2 = \frac{1}{24}[N - (p+q) - 3][N - (p+q) - 1][N - (p+q) + 1]. \quad (14)$$

The number of others monomials involved in the Hamiltonian  $\mathcal{K}$  is given by  $\Lambda = \sum_{k=1}^2 C_2^k C_{Q_0}^k = \frac{Q_0(Q_0+3)}{2}$  (Eq. (13) of [6] for  $n = 2$ ).

## 3.2. Dissatisfaction of the counting

Eq. (11) to (14) take into account the redundancy of some 2-monomials or 3-monomials in the expression of (7). For instance, for a 1 : 1 resonance, developing  $\mathcal{K}$  until  $N = 7$  ( $K = 3$ ), Eq. (12) predicts six 2-monomials in a sum  $S_{m,\ell}^{(2)}$  instead of three in reality.

## 3.3. Multiplicity of some $\lambda$ -monomials

### 3.3.1. Pointing the problem

In the formula (7), we associate the couple of integers  $C = (p_2, q_2)$  (2-couple) or  $(p_3, q_3, \gamma)$  (3-couple) to a 2-monomial or a 3-monomial. In fact, in the next section, we will count the  $\lambda$ -monomials in the sums  $S_{m,\ell}^{(2)}$  and  $S_m^{(3)}$  ( $m = -1, 0; \ell = 1, 2$ ) step by step from  $\delta = p+q+2$  or  $\beta = p+q+4$  until the desired value of  $N$  ( $N \geq p+q+2$ ) by

eliminating the 2-monomials and 3-monomials which are redundant. Firstly, we will define the necessary definitions and tools in the sections 3.3.2 until 3.3.4.

### 3.3.2. Definitions

- We call main interval, any set of values taken by the integer  $N$ , order of development of  $\mathcal{K}$ , between two integers  $N_1$  and  $N_2$  ( $N_2 > N_1$ ):  $N \in [N_1, N_2]$ . The smallest possible value of  $N$  in the relation (7) is  $N = p + q + 2$  for the 2-monomials and  $p + q + 4$  for the 3-monomials.
- For fixed  $\delta$  (respectively  $\beta$ ), we call secondary interval  $IS$ , the set of all the values taken by the integer  $q_2$  (respectively  $q_3$ ) between the integers 1 (respectively 2) and  $Q_2 = E(\frac{\delta-(p+q)}{2})$  (respectively  $Q_3 = E(\frac{\beta-(p+q)}{2})$ ). We denote  $IS_\delta = [1, Q_2]_\delta$  or  $IS_\beta = [2, Q_3]_\beta$  or even more simply  $IS$ .
- For fixed  $\delta$  or  $\beta$ , we will say that a couple of integers  $C$  is present if it appears in the secondary interval  $IS$ . In the opposite case, it will be declared absent.
- A couple of integers  $C$  is said present on a main interval  $[N_1, N_2]$  if it appears at least one time on one of the secondary intervals  $N_2 - N_1 + 1$ , each of these secondary intervals being constituted from one of the  $N_2 - N_1 + 1$  values of  $\delta$  or  $\beta$  composing the main interval. If  $C$  does not appear on all the secondary intervals, it will be said as absent on the main interval  $[N_1, N_2]$ .
- We define the multiplicity  $\mu$  of a couple  $C$  as being the number of times this couple appears in an given interval (main or secondary).
- The cumulative multiplicity (also denoted by  $\mu$ ) of a couple  $C$  on a secondary interval  $IS$  is the number of times this couple appears on the greatest main interval  $[p + q + 2, \delta]$  or  $[p + q + 4, \beta]$  built from this value of  $\delta$  or  $\beta$ .

- The set of couples  $C$  with same value  $p_j = k'$  ( $j = 2, 3$ ) constitutes a class of couples or more simply a class  $C_{k'}$ . The population of a class is the number of couples belonging to this class.
- The set of couples  $C$  with the same cumulative multiplicity on  $IS$  constitutes a class of multiplicity. We denote by  $\tilde{\Lambda}_\mu$  its population.

### 3.3.3. Properties

- By construction, to a given value of  $q_3$  corresponds  $q_3 - 1$  3-couples.
- A 2-couple  $(k', q_2)$  or a 3-couple  $(k', q_3, \gamma)$ , present, appears once and only one on an secondary interval: their multiplicity is thus equal to 1.
- The multiplicity of an absent couple on a main or secondary interval is equal to zero.
- In the case of a resonance  $p : q$ , the cumulative multiplicity of a couple of integers  $C$  may take all integer values from 0 to  $p + q$ . This last value is the maximal cumulative multiplicity of the couple. This result is easily established from Eq. (15). Thus one deduces that the cumulative multiplicity of an absent couple is either zero or maximal. We will call switch-off couple, an absent couple of maximal cumulative multiplicity.

### 3.3.4. Calculation of a cumulative multiplicity

By the same way, we calculate the cumulative multiplicity of a 2-couple  $(k', q_2)$  or a 3-couple  $(k', q_3, \gamma)$ . Also, the couples of integers belonging to a class  $C_{k'}$  ( $k', q_2$ ) or  $(k', q_3, \gamma)$  do not still appear in the counting and are absent (i.e. cumulative multiplicity equal to zero) if  $\delta < k'(p + q) + 2q_j$  ( $j = 2, 3$ ). To the contrary, for  $\delta > (k' + 1)(p + q) + 2q_j - 1$ , they do no more appear: these couples are switch-off; their cumulative multiplicity is maximal. The only main intervals where the couples of integers

are present are of the form:

$$[k'(p+q) + 2q_j, (k'+1)(p+q) + 2q_j - 1]. \quad (15)$$

For a given value of  $N = N_1$  belonging to the interval given by (15), the multiplicity of the present couple  $(k', q_2)$  or  $(k', q_3, \gamma)$  on the main interval  $[k'(p+q) + 2q_j, N_1]$  may be calculated by:

$$\mu = N_1 - N_{app} + 1, \quad (16)$$

with  $N_{app} = k'(p+q) + 2q_j$  the value of  $N$  from which this couple appears on this main interval. Eq. (16) gives also the cumulative multiplicity of the couple present on the secondary interval  $IS_{N_1}$ . Indeed, from the definition, the cumulative multiplicity of the couple  $(k', q_2)$  or  $(k', q_3, \gamma)$  on this secondary interval is its multiplicity on the largest main interval, here  $[p+q+2, N_1]$ . But,  $[p+q+2, N_1] = [p+q+2, N_{app}-1] \cup [N_{app}, N_1]$ , thus from (15), on the main interval  $[p+q+2, N_{app}-1]$ , this couple is absent: its multiplicity is equal to zero. By contrast, it is present on each of the  $N_1 - N_{app} + 1$  secondary intervals associated respectively to the values :  $N_{app}, \dots, N_1$ . Its multiplicity on  $[N_{app}, N_1]$  is equal to  $N_1 - N_{app} + 1$ .

### 3.4. Theorems of the 2-monomials counting

#### 3.4.1. Pointing the problem

The three following theorems about the counting give the number  $\Delta_1$  of independent monomials  $\sigma_m^{E(\frac{\delta-2q_2}{p+q})} \sigma_\ell^{q_2}$  ( $m = -1, 0$  and  $\ell = 1, 2$ ) present in a sum  $S_{m,\ell}^{(2)}$  but also the number  $\tilde{\alpha}_1$  of 2-monomials of degree  $N$ . Without limiting the generality of the problem, we will write  $N = k'(p+q) + 2 + i$  with  $k'$  a positive integer and  $i$  an integer such that  $i \in [0, \dots, p+q-1]$ . *A posteriori* we have to distinguish trois cases in our study according the parity of  $p+q$  and of  $k'$ :  $p+q$  even whatever the parity of  $k'$ ; then for  $p+q$  odd, to study the cases when  $k'$  is even then odd. Demonstration of these theorems is given in Appendix.

**Theorem 1.** *If  $p+q$  is even and  $k'$  an integer  $\geq 1$ :*

$$\Delta_1 = k' \left[ 1 + E\left(\frac{i}{2}\right) + \frac{(k'-1)(p+q)}{4} \right]. \quad (17)$$

**Theorem 2.** *If  $p+q$  odd and  $k'$  an even integer  $\geq 2$ :*

$$\Delta_1 = k' \left[ \frac{(k'-1)(p+q) + 2i + 3}{4} \right]. \quad (18)$$

**Theorem 3.** *If  $p+q$  odd and  $k'$  an odd integer  $\geq 1$ :*

$$\Delta_1 = 1 + E\left(\frac{i}{2}\right) + (k'-1) \left[ \frac{k'(p+q) + 2i + 3}{4} \right]. \quad (19)$$

$N$	$p+q$	$\Delta_1$	$p+q$	$\Delta_1$	$p+q$	$\Delta_1$	$p+q$	$\Delta_1$
4	2	1	3	0	4	0	5	0
5	2	1	3	1	4	0	5	0
6	2	3	3	1	4	1	5	0
7	2	3	3	2	4	1	5	1
8	2	6	3	3	4	2	5	1
9	2	6	3	4	4	2	5	2
10	2	10	3	5	4	4	5	2
11	2	10	3	7	4	4	5	3
12	2	15	3	8	4	6	5	4
13	2	15	3	10	4	6	5	5
14	2	21	3	12	4	9	5	6
15	2	21	3	14	4	9	5	7
16	2	28	3	16	4	12	5	8
17	2	28	3	19	4	12	5	10
18	2	36	3	21	4	16	5	11

Table 1: Counting of the 2-monomials present in a sum  $S_{m,\ell}^{(2)}$  ( $m = -1, 0; \ell = 1, 2$ ) from (7) for  $4 \leq N \leq 18$  and  $2 \leq p+q \leq 5$ .

### 3.5. Theorems of the 3-monomials counting

#### 3.5.1. Pointing the problem

In this section, we give the theorems of the counting of the 3-monomials  $\sigma_m^{E(\frac{\beta-2q_3}{p+q})} \sigma_1^\gamma \sigma_2^{q_3-\gamma}$  ( $m = -1, 0$ ),  $\Delta_2$  in number, appearing in a sum  $S_m^{(3)}$  of (7), but also the number  $\tilde{\alpha}_2$  of 3-monomials of degree  $N$ . Without limiting the generality of the problem, we will write  $N = k'(p+q) + 4 + i$  with  $k'$  a positive integer and  $i$  an integer such that  $i \in [0, \dots, p+q-1]$ . As for the 2-monomials, three cases should be distinguished in our study according to the parity of  $p+q$  and of  $k'$ . In what follows, we denote  $\epsilon = i - 2E(\frac{i}{2})$ :  $\epsilon = 0$  if  $i$  even and  $\epsilon = 1$  if  $i$  odd.



**Theorem 4.** If  $p + q$  even and  $k'$  an integer  $\geq 1$ :

$$\begin{aligned}\Delta_2 &= \frac{[E(\frac{i}{2}) + 1][E(\frac{i}{2}) + 2]}{2} \\ &+ \frac{k'(k' - 1)(p + q)}{48} [(2k' - 1)(p + q) + 6(i + 3 - \epsilon)] \\ &+ \frac{(k' - 1)}{8} [i(i + 6) - 4\epsilon E(\frac{i}{2}) - 7\epsilon + 8].\end{aligned}\quad (20)$$

**Theorem 5.** If  $p + q$  odd and  $k'$  an even integer  $\geq 2$ :

$$\begin{aligned}\Delta_2 &= \frac{[E(\frac{i}{2}) + 1][E(\frac{i}{2}) + 2]}{2} \\ &+ \frac{k'(k' - 1)(p + q)}{48} [(2k' - 1)(p + q) + 3(2i + 5)] \\ &+ \frac{(k' - 1)}{8} [i(i + 6) - 4\epsilon E(\frac{i}{2}) - 7\epsilon + 8] \\ &+ \frac{k'(2\epsilon - 1)}{16} [4E(\frac{i}{2}) + (p + q) + 5 + 2\epsilon].\end{aligned}\quad (21)$$

**Theorem 6.** If  $p + q$  odd and  $k'$  an odd integer  $\geq 1$ :

$$\begin{aligned}\Delta_2 &= \frac{[E(\frac{i}{2}) + 1][E(\frac{i}{2}) + 2]}{2} \\ &+ \frac{k'(k' - 1)(p + q)}{48} [(2k' - 1)(p + q) + 3(2i + 5)] \\ &+ \frac{(k' - 1)}{8} [i(i + 6) - 4\epsilon E(\frac{i}{2}) - 7\epsilon + 8] \\ &+ \frac{(k' - 1)(2\epsilon - 1)}{16} [4E(\frac{i}{2}) - (p + q) + 5 + 2\epsilon].\end{aligned}\quad (22)$$

$N$	$p + q$	$\Delta_2$	$p + q$	$\Delta_2$	$p + q$	$\Delta_2$	$p + q$	$\Delta_2$
6	2	1	3	0	4	0	5	0
7	2	1	3	1	4	0	5	0
8	2	4	3	1	4	1	5	0
9	2	4	3	3	4	1	5	1
10	2	10	3	4	4	3	5	1
11	2	10	3	7	4	3	5	3
12	2	20	3	9	4	7	5	3
13	2	20	3	14	4	7	5	6
14	2	35	3	17	4	13	5	7
15	2	35	3	24	4	13	5	11
16	2	56	3	29	4	22	5	13
17	2	56	3	38	4	22	5	18
18	2	84	3	45	4	34	5	21

Table 2: 3-monomials counting present in a sum  $S_m^{(3)}$  ( $m = -1, 0$ ) of (7) for  $6 \leq N \leq 18$  and  $2 \leq p + q \leq 5$ .

**Theorem 7.** The normalized Hamiltonian  $\mathcal{K}$  given by (7) with a  $p : q$  resonance between its two oscillators, is described by  $N_{coef}$  coefficients,  $N_{op}$  independent monomials among which  $N_c$  are coupling monomials and given by:

$$N_{coef} = \frac{Q_0(Q_0 + 3)}{2} + E(\frac{N}{p + q}) + 2\Delta_1 + \Delta_2, \quad (23)$$

$$N_{op} = \frac{Q_0(Q_0 + 3)}{2} + 2E(\frac{N}{p + q}) + 4\Delta_1 + 2\Delta_2, \quad (24)$$

$$N_c = 2E(\frac{N}{p + q}) + 4\Delta_1 + 2\Delta_2. \quad (25)$$

$\Delta_1$  and  $\Delta_2$  are given by the counting theorems (Theorems 1 to 6).

$p + q$	$N_{coef}$	$N_{op}$	$N_c$
2	55	90	70
3	37	54	34
4	33	46	26
5	27	34	14

Table 3: Counting of the coefficients, monomials and independent coupling monomials in (7) for  $N = 10$  and  $2 \leq p + q \leq 5$ .

### 3.6. The general case

#### 3.6.1. Construction of the normalized Hamiltonian

We consider a Hamiltonian system described by  $n \geq 3$  oscillators among which oscillators "1" and "2" are in  $p : q$  resonance. Hamiltonian  $\mathcal{K}$  is supposed to be invariant under TRO. The quadratic part of  $\mathcal{K}$  is :  $\mathcal{H}_0 = -i \sum_{k=1}^n \omega_k \sigma_k$ . The  $n$  quantities  $\omega_k$  are characteristic pulsations of the oscillators. The Hamiltonian can be expressed as a function of the generators of the Hilbert basis:  $\mathcal{K} = \mathcal{H}_0 + f(\sigma_{-1}, \sigma_0, \sigma_1, \dots, \sigma_n)$ . If we write  $\mathcal{K}$  as a polynomial development of the generators of the Hilbert basis until the order  $N \geq p + q + 4$ , it reads:

$$\begin{aligned}\mathcal{K} &= \mathcal{H}_0 + \sum_{k=1}^n \sum_{q_0=2}^{Q_0} \alpha_{q_0}^k \sigma_k^{q_0} + \\ &\sum_{\ell=2}^n \sum_{r=2}^{Q_0} \sum_{1 \leq i_1 < i_2 < \dots < i_\ell \leq n} \sum_{r_{i_1} \geq 1, \dots, r_{i_\ell} \geq 1}^{r_{i_1} + \dots + r_{i_\ell} = r} \alpha_{r_{i_1}, \dots, r_{i_\ell}}^{i_1, \dots, i_\ell} \sigma_{i_1}^{r_{i_1}} \dots \sigma_{i_\ell}^{r_{i_\ell}}\end{aligned}$$

$$\begin{aligned}
& + \sum_{q_1=1}^{Q_1} \alpha_{q_1}^0 (\sigma_{-1}^{q_1} + \sigma_0^{q_1}) \\
& + \sum_{k=1}^n \sum_{\delta=p+q+2}^N \sum_{q_2=1}^{Q_2} \alpha_{E(\frac{\delta-2q_2}{p+q}), q_2}^{0, k} \left( \sigma_{-1}^{E(\frac{\delta-2q_2}{p+q})} \right. \\
& + \left. \sigma_0^{E(\frac{\delta-2q_2}{p+q})} \right) \sigma_k^{q_2} \\
& + \sum_{i=1}^{n-1} \sum_{j=i+1}^n \sum_{\beta=p+q+4}^N \sum_{q_3=2}^{Q_3} \sum_{\gamma=1}^{q_3-1} \alpha_{E(\frac{\beta-2q_3}{p+q}), \gamma, q_3-\gamma}^{0, i, j} \\
& \left( \sigma_{-1}^{E(\frac{\beta-2q_3}{p+q})} + \sigma_0^{E(\frac{\beta-2q_3}{p+q})} \right) \sigma_i^\gamma \sigma_j^{q_3-\gamma}. \quad (26)
\end{aligned}$$

In Eq.(26), all the coefficients are purely imaginary;  $i_1, \dots, i_\ell$  ( $2 \leq \ell \leq n$ ) are positive integers satisfying the partial order:  $1 \leq i_1 < i_2 < \dots < i_\ell \leq n$ ;  $r_{i_1}, \dots, r_{i_\ell}$  are positive integers satisfying the relation  $r_{i_1} + \dots + r_{i_\ell} = r$ , with  $r$  an integer between 2 and  $Q_0$ ;  $Q_0 = E(\frac{N}{2})$ ,  $Q_1 = E(\frac{N}{p+q})$ ,  $Q_2 = E(\frac{\delta-(p+q)}{2})$  and  $Q_3 = E(\frac{\beta-(p+q)}{2})$ .

$\mathcal{K}$  involves two contributions: a first one corresponding to a Dunham development on the basis of the generators [6] and a second contribution corresponding to a polynomial expansion of the coupling terms.

Furthermore, using the same method as here-before in 3.1.3, one obtains that the different coefficients involved in the normalized Hamiltonian  $\mathcal{K}$  given by Eq. (26) are independent.

**Theorem 8.**  $\mathcal{K}$  is described by  $N_{coef}$  coefficients (among which  $\frac{N_c}{2}$  coupling coefficients),  $N_{op}$  independent monomials whose  $N_c$  are coupling monomials, satisfying the following equations:

$$N_{coef} = \Lambda + E\left(\frac{N}{p+q}\right) + n\Delta_1 + \frac{n(n-1)}{2}\Delta_2, \quad (27)$$

$$N_{op} = \Lambda + 2E\left(\frac{N}{p+q}\right) + 2n\Delta_1 + n(n-1)\Delta_2, \quad (28)$$

$$N_c = 2E\left(\frac{N}{p+q}\right) + 2n\Delta_1 + n(n-1)\Delta_2. \quad (29)$$

$\Delta_1$  and  $\Delta_2$  are given by the counting theorems (Theorems 1 to 6) and  $\Lambda = \sum_{\lambda=1}^{\min(n, Q_0)} C_n^\lambda C_{Q_0}^\lambda$  ([6]).

## 4. Applications

### 4.1. The molecule of ClOH

#### 4.1.1. Conventions of notation

ClOH is a non linear triatomic molecule with 3 vibrational degrees of freedom. ( $n = 3$ ). In the local modes representation, we attach a stretching oscillator to each of the bonds Cl-O (oscillator "1") and O-H (oscillator "3") and a bending oscillator (oscillator "2") to the angle between these bonds.

#### 4.1.2. Quantum vibrational Hamiltonian

The classical relations between dimensionless variables  $\{\underline{z}_j, \underline{z}_k^*\} = -i\delta_{jk}$ , take now the following form:  $\frac{1}{i}[a_j, a_k^+] = -i\delta_{jk}$ , that is  $1 \leq j, k \leq 3$ ,  $[a_j, a_k^+] = \delta_{jk}$ . These operators satisfy the Bose commutation relations and are defined as the Boson creation operator  $a_k^+$  and Boson annihilation operator  $a_j$ .

Generators  $\sigma_k$  and Hamiltonian function  $\mathcal{K}$  are respectively replaced by the number operators  $\hat{N}_k = a_k^+ a_k$ , which physically express the number of quanta of excitation of each oscillator  $k$ , and the Hamiltonian operator  $\hat{K}$ . By convention, for the expression of powers of number operators, we adopt the following form ([19]):

$$\hat{N}_{i_1}^{r_1} \dots \hat{N}_{i_\ell}^{r_\ell} = \underbrace{a_{i_1}^+ a_{i_1} \dots a_{i_1}^+ a_{i_1}}_{r_1 \text{ times}} \dots \underbrace{a_{i_\ell}^+ a_{i_\ell} \dots a_{i_\ell}^+ a_{i_\ell}}_{r_\ell \text{ times}}; \quad (30)$$

but we will write under normal form, as a function of the Bose operators, all the coupling operators:  $\hat{\sigma}_{-1} + \hat{\sigma}_0 = a_1^{+p} a_2^q + a_2^{+q} a_1^p$ ,

$$\begin{aligned}
\hat{\sigma}_{-1}^{q_1} + \hat{\sigma}_0^{q_1} & = \underbrace{a_1^{+p} \dots a_1^{+p}}_{q_1 \text{ times}} \underbrace{a_2^q \dots a_2^q}_{q_1 \text{ times}} \\
& + \underbrace{a_2^{+q} \dots a_2^{+q}}_{q_1 \text{ times}} \underbrace{a_1^p \dots a_1^p}_{q_1 \text{ times}}. \quad (31)
\end{aligned}$$

On a more compact way, Eq. (31) may be rewritten:

$$\hat{\sigma}_{-1}^{q_1} + \hat{\sigma}_0^{q_1} = (a_1^{+p} a_2^q)^{q_1} + (a_2^{+q} a_1^p)^{q_1}. \quad (32)$$

Similarly, the treatment of others coupling operators in  $\hat{K}$  gives:

$$(\hat{\sigma}_{-1}^{p_2} + \hat{\sigma}_0^{p_2})\hat{N}_k^{q_2} = \left( (a_1^{+p} a_2^q)^{p_2} + (a_2^{+q} a_1^p)^{p_2} \right) \underbrace{a_k^+ a_k \dots a_k^+ a_k}_{q_2 \text{ times}}. \quad (33)$$

$$(\hat{\sigma}_{-1}^{p_3} + \hat{\sigma}_0^{p_3})\hat{N}_i^\gamma \hat{N}_j^{q_3-\gamma} = \left( (a_1^{+p} a_2^q)^{p_3} + (a_2^{+q} a_1^p)^{p_3} \right) \underbrace{a_i^+ a_i \dots a_i^+ a_i}_{\gamma \text{ times}} \underbrace{a_j^+ a_j \dots a_j^+ a_j}_{q_3-\gamma \text{ times}}. \quad (34)$$

Hamiltonian  $\hat{K}$  is Hermitian and the  $N_{coef}$  coefficients are real.

#### 4.1.3. Eigen basis of the Hamiltonian $\hat{H}_0$

The eigenstates of  $\hat{H}_0$  are generated from the vacuum state with the relation ( $n_1, n_2, n_3$  are integers):

$$\left| n_1, n_2, n_3 \right\rangle = \frac{1}{\sqrt{n_1! n_2! n_3!}} a_1^{+n_1} a_2^{+n_2} a_3^{+n_3} \left| 0, 0, 0 \right\rangle. \quad (35)$$

>From Theorem 8, the quantum vibrational Hamiltonian, developed until the order  $N = 10$  ( $Q_0 = 5$ ), is described by 115 operators, 60 of which are coupling operators and 85 coefficients; so, we write (with the usual

convention that  $\hbar$  is equal to 1):

$$\begin{aligned} \hat{K} = & \left( \omega_1 \hat{N}_1 + \omega_2 \hat{N}_2 + \omega_3 \hat{N}_3 \right. \\ & + \alpha_2^1 \hat{N}_1^2 + \alpha_3^1 \hat{N}_1^3 + \alpha_4^1 \hat{N}_1^4 + \alpha_5^1 \hat{N}_1^5 \\ & + \alpha_2^2 \hat{N}_2^2 + \alpha_3^2 \hat{N}_2^3 + \alpha_4^2 \hat{N}_2^4 + \alpha_5^2 \hat{N}_2^5 \\ & + \alpha_2^3 \hat{N}_3^2 + \alpha_3^3 \hat{N}_3^3 + \alpha_4^3 \hat{N}_3^4 + \alpha_5^3 \hat{N}_3^5 \\ & + \alpha_{1,1}^{1,2} \hat{N}_1 \hat{N}_2 + \alpha_{1,2}^{1,2} \hat{N}_1 \hat{N}_2^2 + \alpha_{2,1}^{1,2} \hat{N}_1^2 \hat{N}_2 \\ & + \alpha_{1,3}^{1,2} \hat{N}_1 \hat{N}_2^3 + \alpha_{2,2}^{1,2} \hat{N}_1^2 \hat{N}_2^2 + \alpha_{3,1}^{1,2} \hat{N}_1^3 \hat{N}_2 \\ & + \alpha_{1,4}^{1,2} \hat{N}_1 \hat{N}_2^4 + \alpha_{2,3}^{1,2} \hat{N}_1^2 \hat{N}_2^3 + \alpha_{3,2}^{1,2} \hat{N}_1^3 \hat{N}_2^2 + \alpha_{4,1}^{1,2} \hat{N}_1^4 \hat{N}_2 \\ & + \alpha_{1,1}^{1,3} \hat{N}_1 \hat{N}_3 + \alpha_{1,2}^{1,3} \hat{N}_1 \hat{N}_3^2 + \alpha_{2,1}^{1,3} \hat{N}_1^2 \hat{N}_3 \\ & + \alpha_{1,3}^{1,3} \hat{N}_1 \hat{N}_3^3 + \alpha_{2,2}^{1,3} \hat{N}_1^2 \hat{N}_3^2 + \alpha_{3,1}^{1,3} \hat{N}_1^3 \hat{N}_3 \\ & + \alpha_{1,4}^{1,3} \hat{N}_1 \hat{N}_3^4 + \alpha_{2,3}^{1,3} \hat{N}_1^2 \hat{N}_3^3 + \alpha_{3,2}^{1,3} \hat{N}_1^3 \hat{N}_3^2 + \alpha_{4,1}^{1,3} \hat{N}_1^4 \hat{N}_3 \\ & + \alpha_{1,1}^{2,3} \hat{N}_2 \hat{N}_3 + \alpha_{1,2}^{2,3} \hat{N}_2 \hat{N}_3^2 + \alpha_{2,1}^{2,3} \hat{N}_2^2 \hat{N}_3 \\ & + \alpha_{1,3}^{2,3} \hat{N}_2 \hat{N}_3^3 + \alpha_{2,2}^{2,3} \hat{N}_2^2 \hat{N}_3^2 + \alpha_{3,1}^{2,3} \hat{N}_2^3 \hat{N}_3 \\ & + \alpha_{1,4}^{2,3} \hat{N}_2 \hat{N}_3^4 + \alpha_{2,3}^{2,3} \hat{N}_2^2 \hat{N}_3^3 + \alpha_{3,2}^{2,3} \hat{N}_2^3 \hat{N}_3^2 + \alpha_{4,1}^{2,3} \hat{N}_2^4 \hat{N}_3 \\ & + \alpha_{1,1,1}^{1,2,3} \hat{N}_1 \hat{N}_2 \hat{N}_3 \\ & + \alpha_{1,1,2}^{1,2,3} \hat{N}_1 \hat{N}_2 \hat{N}_3^2 + \alpha_{1,2,1}^{1,2,3} \hat{N}_1 \hat{N}_2^2 \hat{N}_3 + \alpha_{2,1,1}^{1,2,3} \hat{N}_1^2 \hat{N}_2 \hat{N}_3 \\ & + \alpha_{1,1,3}^{1,2,3} \hat{N}_1 \hat{N}_2 \hat{N}_3^3 + \alpha_{1,3,1}^{1,2,3} \hat{N}_1 \hat{N}_2^3 \hat{N}_3 + \alpha_{3,1,1}^{1,2,3} \hat{N}_1^3 \hat{N}_2 \hat{N}_3 \\ & + \alpha_{1,2,2}^{1,2,3} \hat{N}_1 \hat{N}_2^2 \hat{N}_3^2 + \alpha_{2,1,2}^{1,2,3} \hat{N}_1^2 \hat{N}_2 \hat{N}_3^2 + \alpha_{2,2,1}^{1,2,3} \hat{N}_1^2 \hat{N}_2^2 \hat{N}_3 \\ & + \alpha_1^0 (a_2^+ a_1^2 + a_1^{+2} a_2) + \alpha_2^0 (a_2^{+2} a_1^4 + a_1^{+4} a_2^2) \\ & + \alpha_3^0 (a_2^{+3} a_1^6 + a_1^{+6} a_2^3) \\ & + \alpha_{1,1}^{0,1} (a_2^+ a_1^2 + a_1^{+2} a_2) \hat{N}_1 + \alpha_{1,2}^{0,1} (a_2^+ a_1^2 + a_1^{+2} a_2) \hat{N}_1^2 \\ & + \alpha_{2,1}^{0,1} (a_2^{+2} a_1^4 + a_1^{+4} a_2^2) \hat{N}_1 + \alpha_{1,3}^{0,1} (a_2^+ a_1^2 + a_1^{+2} a_2) \hat{N}_1^3 \\ & + \alpha_{2,2}^{0,1} (a_2^{+2} a_1^4 + a_1^{+4} a_2^2) \hat{N}_1^2 \\ & + \alpha_{1,1}^{0,2} (a_2^+ a_1^2 + a_1^{+2} a_2) \hat{N}_2 + \alpha_{1,2}^{0,2} (a_2^+ a_1^2 + a_1^{+2} a_2) \hat{N}_2^2 \\ & + \alpha_{2,1}^{0,2} (a_2^{+2} a_1^4 + a_1^{+4} a_2^2) \hat{N}_2 + \alpha_{1,3}^{0,2} (a_2^+ a_1^2 + a_1^{+2} a_2) \hat{N}_2^3 \\ & + \alpha_{2,2}^{0,2} (a_2^{+2} a_1^4 + a_1^{+4} a_2^2) \hat{N}_2^2 \\ & + \alpha_{1,1}^{0,3} (a_2^+ a_1^2 + a_1^{+2} a_2) \hat{N}_3 + \alpha_{1,2}^{0,3} (a_2^+ a_1^2 + a_1^{+2} a_2) \hat{N}_3^2 \end{aligned}$$

$$\begin{aligned}
& + \alpha_{2,1}^{0,3}(a_2^+ a_1^4 + a_1^+ a_2^2) \hat{N}_3 + \alpha_{1,3}^{0,3}(a_2^+ a_1^2 + a_1^+ a_2) \hat{N}_3^3 \\
& + \alpha_{2,2}^{0,3}(a_2^+ a_1^4 + a_1^+ a_2^2) \hat{N}_3^2 \\
& + \alpha_{1,1,1}^{0,1,2}(a_2^+ a_1^2 + a_1^+ a_2) \hat{N}_1 \hat{N}_2 \\
& + \alpha_{1,1,1}^{0,1,3}(a_2^+ a_1^2 + a_1^+ a_2) \hat{N}_1 \hat{N}_3 \\
& + \alpha_{1,1,1}^{0,2,3}(a_2^+ a_1^2 + a_1^+ a_2) \hat{N}_2 \hat{N}_3 \\
& + \alpha_{1,1,2}^{0,1,2}(a_2^+ a_1^2 + a_1^+ a_2) \hat{N}_1 \hat{N}_2^2 \\
& + \alpha_{1,1,2}^{0,1,3}(a_2^+ a_1^2 + a_1^+ a_2) \hat{N}_1 \hat{N}_3^2 \\
& + \alpha_{1,1,2}^{0,2,3}(a_2^+ a_1^2 + a_1^+ a_2) \hat{N}_2 \hat{N}_3^2 \\
& + \alpha_{1,2,1}^{0,1,2}(a_2^+ a_1^2 + a_1^+ a_2) \hat{N}_1^2 \hat{N}_2 \\
& + \alpha_{1,2,1}^{0,1,3}(a_2^+ a_1^2 + a_1^+ a_2) \hat{N}_1^2 \hat{N}_3 \\
& + \alpha_{1,2,1}^{0,2,3}(a_2^+ a_1^2 + a_1^+ a_2) \hat{N}_2^2 \hat{N}_3 \\
& + \alpha_{2,1,1}^{0,1,2}(a_2^+ a_1^4 + a_1^+ a_2^2) \hat{N}_1 \hat{N}_2 \\
& + \alpha_{2,1,1}^{0,1,3}(a_2^+ a_1^4 + a_1^+ a_2^2) \hat{N}_1 \hat{N}_3 \\
& + \alpha_{2,1,1}^{0,2,3}(a_2^+ a_1^4 + a_1^+ a_2^2) \hat{N}_2 \hat{N}_3 \Big). \quad (36)
\end{aligned}$$

#### 4.1.4. Numerical simulations

The vibrational structure of the ClOH molecule has been studied in [2] until almost the dissociation limit. For levels of energy less than 70 % of the dissociation limit, the authors make a Dunham expression based on the number operators (See [6]). But, for highly excited levels, due to the more and more frequent accidentally couplings between levels energetically close, Fermi resonance between oscillators "1" and "2" ( $\frac{\omega_2}{\omega_1} \approx 2$ ) has to be taken into account. Quantum numbers  $n_1$  and  $n_2$  are "no more good quantum numbers", as refers in the literature, and they are replaced by the polyad number  $P = n_1 + 2n_2$  (See for instance [20]). In [2], the authors determine 725 levels of energy, which means to take into account up to 38 quanta of excitation exchanged between oscillator "1" and "2" ( $P \leq 38$ ) and 7 quanta for the oscillator "3", labeling of the states being made with the polyad number  $[P, n_3]$ . Furthermore, these authors add a coupling operator  $\alpha_1^0(a_2^+ a_3 + a_3^+ a_2^3)$  in the Hamiltonian  $\hat{K}$  in order to describe the 3 : 1 resonance between oscillators "2" and "3" ( $\frac{\omega_3}{\omega_2} \approx 3$ ). Our model predicts that the Hamiltonian  $\hat{K}$

$N$	$\Lambda$	coefficients in $\text{cm}^{-1}$
2	3	$\omega_1 = +753.834, \omega_2 = +1\,258.914$ $\omega_3 = +3\,777.067$
4	9	$\alpha_2^1 = -7.123, \alpha_2^2 = +3.204, \alpha_2^3 = -80.277$ $\alpha_{1,1}^{1,2} = -10.637, \alpha_{1,1}^{1,3} = 0, \alpha_{1,1}^{2,3} = -19.985$
6	19	$\alpha_3^1 = +0.0825, \alpha_3^2 = 0, \alpha_3^3 = -0.3619$ $\alpha_{1,2}^{1,2} = -0.2503, \alpha_{1,2}^{1,3} = -0.0532, \alpha_{1,2}^{2,3} = -1.9534$ $\alpha_{2,1}^{1,2} = -0.0802, \alpha_{2,1}^{1,3} = 0, \alpha_{2,1}^{2,3} = 0$ $\alpha_{1,1,1}^{1,2,3} = 0$
8	34	$\alpha_4^1 = -0.00171, \alpha_4^2 = -0.04117, \alpha_4^3 = 0$ $\alpha_{3,1}^{1,2} = 0, \alpha_{3,1}^{1,3} = 0, \alpha_{3,1}^{2,3} = 0$ $\alpha_{2,2}^{1,2} = 0, \alpha_{2,2}^{1,3} = 0, \alpha_{2,2}^{2,3} = -0.15070$ $\alpha_{1,3}^{1,2} = -0.01229, \alpha_{1,3}^{1,3} = 0, \alpha_{1,3}^{2,3} = +0.13189$ $\alpha_{1,1,2}^{1,2,3} = +0.02381, \alpha_{1,2,1}^{1,2,3} = 0, \alpha_{2,1,1}^{1,2,3} = 0$
10	55	$\alpha_5^1 = 0, \alpha_5^2 = +0.00151, \alpha_5^3 = 0$ $\alpha_{4,1}^{1,2} = 0, \alpha_{4,1}^{1,3} = 0, \alpha_{4,1}^{2,3} = 0$ $\alpha_{3,2}^{1,2} = 0, \alpha_{3,2}^{1,3} = 0, \alpha_{3,2}^{2,3} = 0$ $\alpha_{2,3}^{1,2} = 0, \alpha_{2,3}^{1,3} = 0, \alpha_{2,3}^{2,3} = -0.00066$ $\alpha_{1,4}^{1,2} = 0, \alpha_{1,4}^{1,3} = 0, \alpha_{1,4}^{2,3} = 0$

Table 4: List of the Dunham coefficients given by [2]. For a given order  $N$  ( $4 \leq N \leq 10$ ), a line contains the numbers of additional coefficients to the order  $N - 2$ .

has to be described by 86 coefficients (the 85 coefficients of Eq. (36) +  $\alpha_1^0$ ). However the smallest rms value ( $= 5.29 \text{ cm}^{-1}$ ) is obtained for a fit with only 28 coefficients different from zero, some coefficients have been set at zero by a more or less arbitrary way. Results are given in the tables 4 and 5.

## 5. Conclusion and perspectives

We have presented a method of construction of a vibrational normalized Hamiltonian, modeled by a set of  $n$  oscillators until a high order  $N$ . It allows to describe the highly excited vibrational levels in the case of a  $p : q$  resonance. We have also counted all the operators intro-

$N$	$\frac{N_c}{2}$	coefficients in $\text{cm}^{-1}$
3	1	$\alpha_1^0 = 0$
4	1	$(\alpha_1^0 = +0.19520)$
5	4	$\alpha_{1,1}^{0,1} = -0.24939, \alpha_{1,1}^{0,2} = 0, \alpha_{1,1}^{0,3} = -0.76017$
6	5	$\alpha_2^0 = 0$
7	11	$\alpha_{1,2}^{0,1} = +0.00583, \alpha_{1,2}^{0,2} = 0, \alpha_{1,2}^{0,3} = -0.01158$ $\alpha_{1,1,1}^{0,1,2} = +0.04075, \alpha_{1,1,1}^{0,1,3} = 0, \alpha_{1,1,1}^{0,2,3} = 0$
8	14	$\alpha_{2,1}^{0,1} = 0, \alpha_{2,1}^{0,2} = 0, \alpha_{2,1}^{0,3} = 0$
9	24	$\alpha_3^0 = 0, \alpha_{1,3}^{0,1} = 0, \alpha_{1,3}^{0,2} = 0, \alpha_{1,3}^{0,3} = 0$ $\alpha_{1,1,2}^{0,1,2} = 0, \alpha_{1,2,1}^{0,1,2} = 0, \alpha_{1,1,2}^{0,1,3} = 0, \alpha_{1,2,1}^{0,1,3} = 0$ $\alpha_{1,1,2}^{0,2,3} = 0, \alpha_{1,2,1}^{0,2,3} = 0$
10	30	$\alpha_{2,1,1}^{0,1,2} = 0, \alpha_{2,1,1}^{0,1,3} = 0, \alpha_{2,1,1}^{0,2,3} = 0$ $\alpha_{2,2}^{0,1} = 0, \alpha_{2,2}^{0,2} = 0, \alpha_{2,2}^{0,3} = 0$

Table 5: List of the coupling coefficients given by [2]. For a given order  $N$  ( $4 \leq N \leq 10$ ), a line contains the number of additional coefficients to the order  $N - 1$ . The coupling coefficient of the 3 : 1 resonance is in brackets and is not accounting for in the enumeration.

duced in the Hamiltonian, in particular the coupling operators. This building method has been successfully applied to the ClOH molecule taking into account a 2 : 1 resonance. To go further, in a strict manner, for molecular systems having at least 3 oscillators, we should add in the Hamiltonian polynomial expansion, 4-monomials based on the generators of the invariant algebra (Eq.(26)) as soon as  $N \geq p + q + 6$ . If the method of construction is easily adaptable, the counting theorems for these monomials remain to be done.

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## 7. Appendix

### 7.1. 2-monomials counting

In this section, we present the demonstration of the three counting theorems of the 2-monomials. We denote the order  $N$  of the development of (26) under the form  $N = k'(p+q) + 2 + i$  with  $k'$  and  $i \in [0, \dots, p+q-1]$  two positive integers. Thus we are working on the secondary interval  $IS = [1, Q_2]_{N=k'(p+q)+2+i}$  with  $Q_2 = E(\frac{(k'-1)(p+q)+2+i}{2})$ .

#### 7.1.1. The different classes of couples

On  $IS$ , the different values taken by  $q_2$  belong to different classes of couples:  $C_1, \dots, C_{k'-1}$  and  $C_{k'}$ . We begin by searching the couples belonging to the class  $C_{k'}$  as well as the population  $\tilde{\Lambda}''$  of this class. The couples  $(k', q_2)$  of this class are:  $(k', 1), (k', 2), \dots, (k', \tilde{q}_2)$  with  $\tilde{q}_2$  the highest possible value of  $q_2$  such that  $p_2 = E(\frac{k'(p+q)+2+i-2\tilde{q}_2}{p+q}) = k'$ , that is  $\tilde{q}_2 = 1 + E(\frac{i}{2})$ . the multiplicities of these  $1 + E(\frac{i}{2})$  couples are easily calculated with the Eq. (15) and (16). The cumulative multiplicities of the couples  $(k', 1), (k', 2), \dots, (k', \tilde{q}_2)$  on  $IS$  are respectively equal to  $\mu = i + 1, i - 1, \dots, i + 3 - 2q_2, \dots, 1 + \epsilon$  with  $\epsilon = i - 2E(\frac{i}{2})$ . It is possible now to evaluate the numbers of couples of this class: the population of  $C_{k'}$  is the sum of all the couples present in this class taking into account the cumulative multiplicity of each of the couples on  $IS$ , which is equivalent to calculate the number of times a couple appears on the main interval  $[p + q + 2, k'(p + q) + 2 + i]$ . We get:

$$\begin{aligned} \tilde{\Lambda}'' &= \sum_{q_2=1}^{\tilde{q}_2} (i + 3 - 2q_2), \\ &= [E(\frac{i}{2}) + 1][i + 1 - E(\frac{i}{2})], \end{aligned} \quad (37)$$

or accordingly to the parity of  $i$ :

$$\tilde{\Lambda}'' = \frac{i^2}{4} + i + 1 \quad (i \text{ even}), \quad (38)$$

$$\tilde{\Lambda}'' = \frac{i^2}{4} + i + \frac{3}{4} \quad (i \text{ odd}). \quad (39)$$

Couples of the others different classes of  $IS$  break down as follows:  $(k' - 1, E(\frac{i}{2}) + 2), (k' - 1, E(\frac{i}{2}) + 3), \dots, (k' -$

$1, E(\frac{p+q+i+2}{2})$ ) for the class  $C_{k'-1}$ ,  $(k' - 2, E(\frac{p+q+i+4}{2}))$ ,  $(k' - 2, E(\frac{p+q+i+6}{2}))$ , ...,  $(k' - 2, E(\frac{2(p+q)+i+2}{2}))$  for the class  $C_{k'-2}$ , ...,  $(2, E(\frac{(k'-3)(p+q)+i+4}{2}))$ ,  $(2, E(\frac{(k'-3)(p+q)+i+6}{2}))$ , ...,  $(2, E(\frac{(k'-2)(p+q)+i+2}{2}))$  for the class  $C_2$  and finally  $(1, E(\frac{(k'-2)(p+q)+i+4}{2}))$ ,  $(1, E(\frac{(k'-2)(p+q)+i+6}{2}))$ , ...,  $(1, Q_2 = E(\frac{(k'-1)(p+q)+i+2}{2}))$  for the class  $C_1$ .

Calculation of the cumulative multiplicity of the 2-couples implies to distinguish three cases:  $p+q$  even (case A),  $p+q$  odd with  $k'$  even (case B) and  $p+q$  odd with  $k'$  odd (case C). Results are given in the tables 6 to 10.

### 7.1.2. Case A

We denote by  $\tilde{\Lambda}'$  the population of the classes  $C_{k'-1}$  to  $C_1$ ; on each of these classes, each cumulative multiplicity ( $\frac{p+q}{2}$  in number)  $p+q-1+\epsilon$ ,  $p+q-3+\epsilon$ , ...,  $1+\epsilon$  appears only one time; we may write:

$$\begin{aligned}\tilde{\Lambda}' &= (k' - 1) \sum_{j=0}^{\frac{p+q-2}{2}} (2j + 1 + \epsilon), \\ &= \frac{(k' - 1)(p + q)}{2} \left[ \frac{p + q}{2} + \epsilon \right].\end{aligned}\quad (40)$$

The population  $\tilde{\Lambda}$  of all the classes  $C_j$  ( $j = 1, \dots, k'$ ) is the sum of (37) and (40). In order to obtain the number of 2-monomials, we have first to determine the number of switch-off couples  $\alpha$  on  $IS$ . To do it, depending of the parity of  $K = (k' - 1)(p + q) + i$ , we have to subtract from  $\Lambda_1$  (given by (11) or (12)) the population  $\tilde{\Lambda}$  of all the couples present on  $IS$ . As the cumulative multiplicity of all the switch-off couples is equal to  $p + q$ ,  $\tilde{\Lambda}$  is divisible by  $p + q$ . More precisely, one calculates  $\Lambda_1$  by replacing in (11) or (12)  $N$  by  $k'(p + q) + 2 + i$ ; one obtains:

$$\Lambda_1 = \frac{1}{4}(k' - 1)^2(p + q)^2 + \frac{1}{2}(k' - 1)(p + q)(i + 2) + R, \quad (41)$$

with

$$R = \frac{i^2}{4} + i + 1 \quad (K \text{ even}), \quad (42)$$

$$R = \frac{i^2}{4} + i + \frac{3}{4} \quad (K \text{ odd}). \quad (43)$$

For the case A,  $K$  has the same parity as  $i$  thus  $R$  is canceled by  $\tilde{\Lambda}'$  in  $\alpha = \Lambda_1 - \tilde{\Lambda}' - \tilde{\Lambda}''$ . We obtain:

$$\begin{aligned}\alpha &= \frac{1}{4}(k' - 1)(k' - 2)(p + q)^2 \\ &+ \frac{1}{2}(k' - 1)(i + 2 - \epsilon)(p + q).\end{aligned}\quad (44)$$

To eliminate the redundancies in the switch-off couples in  $IS$ , it is enough to divide  $\alpha$  by  $p + q$ . The number of couples, thus the number of 2-monomials  $\Delta_1$  in a sum  $S_{m,\ell}^{(2)}$  ( $m = -1, 0$ ,  $\ell = 1, 2$ ) is obtained by summing  $\frac{\alpha}{p+q}$  and  $\tilde{\alpha}_1$ , the number of couples present without multiplicity on  $IS$  (to do it, one attributes artificially a cumulative multiplicity of 1 to each of the couples of the  $k' - 1$  different classes  $C_{k'-1}$  to  $C_1$ , each cumulative multiplicity appearing exactly 1 time in each class, and to add the  $\tilde{q}_2$  couples the class  $C_{k'}$ ), that is:

$$\tilde{\alpha}_1 = \left(\frac{p+q}{2}\right)(k' - 1) + E\left(\frac{i}{2}\right) + 1.$$

From which we deduce that:  $\Delta_1 = k'[1 + E(\frac{i}{2}) + \frac{(k'-1)(p+q)}{4}]$ .

Theorem 1 is thus proved.

### 7.1.3. Case B

Compared with case A, for a given class of couples, the cumulative multiplicities are either all even or all odd. We have to distinguish the "sub-cases"  $i$  even and  $i$  odd:

- If  $i$  is even, one counts  $\frac{p+q+1}{2}$  odd cumulative multiplicities 1, 3, ...,  $p + q$ , which appear exactly one time on each of the  $\frac{k'-2}{2}$  even classes  $C_{k'-2}$ , ...,  $C_2$  whereas the odd classes  $C_{k'-1}$ , ...,  $C_1$ ,  $\frac{k'}{2}$  in number, contain the  $\frac{p+q-1}{2}$  even cumulative multiplicities : 2 to  $p + q - 1$ . We denote  $\tilde{\Lambda}'_{odd}$  and  $\tilde{\Lambda}'_{even}$  the number of couples of, respectively, odd and even cumulative multiplicity on  $IS$ , except the couples of the class  $C_{k'}$  which population is given by (37). We have:

$$\begin{aligned}\tilde{\Lambda}'_{odd} &= \frac{(k' - 2)}{2} \sum_{j=0}^{\frac{p+q-1}{2}} (2j + 1), \\ &= \frac{(k' - 2)(p + q + 1)^2}{8}.\end{aligned}\quad (45)$$

$$\begin{aligned}\tilde{\Lambda}'_{even} &= \frac{k'}{2} \sum_{j=1}^{\frac{p+q-1}{2}} (2j), \\ &= \frac{k'(p+q-1)(p+q+1)}{8}.\end{aligned}\quad (46)$$

One deduces:

$$\tilde{\Lambda}' = \frac{(k'-1)(p+q)^2}{4} + \frac{(k'-2)(p+q)}{4} - \frac{1}{4}, \quad (47)$$

then the population  $\tilde{\Lambda}$  of all the classes, the population of  $C_{k'}$  being still given by Eq. (38). The determination of switch-off couples is made analogously to the case *A*. For  $i$  and  $k'$  even,  $K = (k'-1)(p+q) + i$  is odd,  $\Lambda_1$  is obtained with (41) and (43), thus it gives:

$$\alpha = \frac{1}{4}(k'-1)(k'-2)(p+q)^2 + \frac{1}{4}[3k' + 2i(k'-1) - 2](p+q), \quad (48)$$

One checks that (48) is divisible by  $p+q$ ,  $R$  being canceled by the contributions (38) and  $-\frac{1}{4}$  of (47). Eq. (48) divided by  $p+q$  and  $\tilde{\alpha}_1 = (\frac{p+q}{2})(k'-1) + E(\frac{i}{2}) + \frac{1}{2}$  gives:  $\Delta_1 = k'[\frac{(k'-1)(p+q)+2i+3}{4}]$ .

- If  $i$  is odd, there is  $\frac{p+q+1}{2}$  odd cumulative multiplicities 1, 3, ...,  $p+q$ , which appear exactly one time on each of the  $\frac{k'}{2}$  odd classes  $C_{k'-1}, \dots, C_1$  whereas the  $\frac{(k'-2)}{2}$  even classes  $C_{k'-2}, \dots, C_2$  contain the  $\frac{p+q-1}{2}$  even cumulative multiplicity : 2, ...,  $p+q-1$ . We have now:

$$\begin{aligned}\tilde{\Lambda}'_{odd} &= \frac{k'}{2} \sum_{j=0}^{\frac{p+q-1}{2}} (2j+1), \\ &= \frac{k'(p+q+1)^2}{8}.\end{aligned}\quad (49)$$

$$\begin{aligned}\tilde{\Lambda}'_{even} &= \frac{(k'-2)}{2} \sum_{j=1}^{\frac{p+q-1}{2}} (2j), \\ &= \frac{(k'-2)(p+q-1)(p+q+1)}{8}.\end{aligned}\quad (50)$$

It gives:

$$\tilde{\Lambda}' = \frac{(k'-1)(p+q)^2}{4} + \frac{k'(p+q)}{4} + \frac{1}{4}, \quad (51)$$

$\Lambda_1$  is determined by (41) and (42),  $\tilde{\Lambda}''$  by (39), from which one has  $\alpha = \Lambda_1 - \tilde{\Lambda}' - \tilde{\Lambda}''$ :

$$\alpha = \frac{1}{4}(k'-1)(k'-2)(p+q)^2 + \frac{1}{4}[3k' + 2i(k'-1) - 4](p+q), \quad (52)$$

then the sum of  $\tilde{\alpha}_1 = (\frac{p+q}{2})(k'-1) + E(\frac{i}{2}) + \frac{3}{2}$  and (52) divided by  $p+q$  gives:  $\Delta_1 = k'[\frac{(k'-1)(p+q)+2i+3}{4}]$ .

This proves the theorem 2 .

#### 7.1.4. Case *C*

As for case *B*, the study implies to consider all the "sub-cases"  $i$  even and  $i$  odd:

- If  $i$  is even, there is  $\frac{p+q+1}{2}$  odd cumulative multiplicities 1, 3, ...,  $p+q$ , which appear exactly one time on each of the  $\frac{k'-1}{2}$  odd classes  $C_{k'-2}, \dots, C_1$ , the  $\frac{k'-1}{2}$  even classes  $C_{k'-1}, \dots, C_2$  having the  $\frac{p+q-1}{2}$  even cumulative multiplicities: 2, ...,  $p+q-1$ . It gives:

$$\begin{aligned}\tilde{\Lambda}'_{odd} &= \frac{(k'-1)}{2} \sum_{j=0}^{\frac{p+q-1}{2}} (2j+1), \\ &= \frac{(k'-1)(p+q+1)^2}{8}.\end{aligned}\quad (53)$$

$$\begin{aligned}\tilde{\Lambda}'_{even} &= \frac{(k'-1)}{2} \sum_{j=1}^{\frac{p+q-1}{2}} (2j), \\ &= \frac{(k'-1)(p+q-1)(p+q+1)}{8}.\end{aligned}\quad (54)$$

>From which we deduce:

$$\tilde{\Lambda}' = \frac{(k'-1)(p+q)(p+q+1)}{4}, \quad (55)$$

then the population  $\tilde{\Lambda}$  of all the classes, the population of  $C_{k'}$  is determined by (38). The number of switch-off couples is obtained on a analogous way that cases *A* and *B*.  $K = (k'-1)(p+q) + i$  being even,  $\Lambda_1$  is given by (41) and (42),  $\tilde{\Lambda}''$  is given by (38), then  $\alpha = \Lambda_1 - \tilde{\Lambda}' - \tilde{\Lambda}''$ :

$$\alpha = \frac{1}{4}(k'-1)(p+q)[(k'-2)(p+q) + 2i + 3]. \quad (56)$$

Using Eq. (56) and  $\tilde{\alpha}_1 = (\frac{p+q}{2})(k'-1) + E(\frac{i}{2}) + 1$ , one deduces:  $\Delta_1 = (k'-1)[\frac{k'(p+q)+2i+3}{4}] + E(\frac{i}{2}) + 1$ .

- If  $i$  is odd, there is  $\frac{p+q+1}{2}$  odd multiplicities 1, 3, ...,  $p+q$ , which appear exactly one time on each of the  $\frac{(k'-1)}{2}$  even classes  $C_{k'-1}, \dots, C_2$  while the  $\frac{(k'-1)}{2}$  odd classes  $C_{k'-2}$  to  $C_1$  contain the  $\frac{p+q-1}{2}$  even multiplicities 2 to  $p+q-1$ . Populations  $\tilde{\Lambda}'_{odd}$ ,  $\tilde{\Lambda}'_{even}$  and  $\tilde{\Lambda}' = \tilde{\Lambda}'_{even} + \tilde{\Lambda}'_{odd}$  are still given by Eqs. (53), (54) and (55);  $\tilde{\Lambda}''$  is calculated by Eq. (39) and  $\Lambda_1$  deduced by Eqs. (41) and (43). One obtains once again Eq. (56) for  $\alpha$ . From Eq. (56) and  $\tilde{\alpha}_1 = (\frac{p+q}{2})(k'-1) + E(\frac{i}{2}) + 1$ , one may write:  

$$\Delta_1 = (k'-1) \left[ \frac{k'(p+q)+2i+3}{4} \right] + E(\frac{i}{2}) + 1.$$

Theorem 3 is thus demonstrated.

## 7.2. 3-monomials counting

In this section, we give the demonstration of the three 3-monomials counting theorems. For the following, without limiting the generality of the problem, the order  $N$  of the expansion (26) is denoted  $N = k'(p+q) + 4 + i$  with  $k'$  and  $i \in [0, \dots, p+q-1]$  two strictly positive integers. We work on the secondary interval  $IS = [2, Q_3]_{N=k'(p+q)+4+i}$  with  $Q_3 = E(\frac{(k'-1)(p+q)+4+i}{2})$ .

### 7.2.1. The different classes of couples

Successive values taken by the integer  $q_3$  on  $IS$  compose the classes of the couples :  $C_1, \dots, C_{k'-2}, C_{k'-1}$  and  $C_{k'}$  (classes  $C_{k'-1}$  and  $C_{k'-2}$  exist if, respectively,  $k' \geq 2$  and  $k' \geq 3$ ). We begin by giving explicitly the 3-couples belonging to the class  $C_{k'}$  as well as its population  $\tilde{\Lambda}''$ . The 3-couples  $(k', q_3, \gamma)$  ( $\gamma = 1, \dots, q_3 - 1$ ) of this class are:  $(k', 1, \gamma), (k', 2, \gamma), \dots, (k', \tilde{q}_3, \gamma)$  with  $\tilde{q}_3$  the highest integer value of  $q_3$  allowed such that  $p_3 = E(\frac{k'(p+q)+4+i-2\tilde{q}_3}{p+q}) = k'$ , that is  $\tilde{q}_3 = 2 + E(\frac{i}{2})$ . We determine the multiplicities of these 3-couples with the help of (15) and (16). Thus, the cumulative multiplicities of the couples  $(k', 1, \gamma), (k', 2, \gamma), \dots, (k', \tilde{q}_3, \gamma)$  on  $IS$  are, respectively,  $\mu = i+1, i-1, \dots, i+5-2q_3, \dots, 1+\epsilon$  with  $\epsilon = i - 2E(\frac{i}{2})$ . However, to a given value of  $q_3$ , there is  $q_3 - 1$  3-couples  $(k', q_3, \gamma)$ . The counting of the population of  $C_{k'}$  is equivalent to the counting of all the 2-couples

$(k', q_3)$  which cumulative multiplicities on  $IS$  is the product of one of the  $q_3 - 1$  3-couples  $(k', q_3, \gamma)$  which it relates and of  $q_3 - 1$ . It reads:

$$\begin{aligned} \tilde{\Lambda}'' &= \sum_{q_3=2}^{\tilde{q}_3} (i+5-2q_3)(q_3-1), \\ &= \frac{1}{2}(i+7)[E(\frac{i}{2})+1][E(\frac{i}{2})+4] + 2 - (i+5)[E(\frac{i}{2})+1] \\ &\quad - \frac{1}{3}[E(\frac{i}{2})+2][E(\frac{i}{2})+3][2E(\frac{i}{2})+5], \end{aligned} \quad (57)$$

or also, depending of the parity of  $i$ :

$$\tilde{\Lambda}'' = \frac{i^3}{24} + \frac{3i^2}{8} + \frac{13i}{12} + 1 \quad (i \text{ even}), \quad (58)$$

$$\tilde{\Lambda}'' = \frac{i^3}{24} + \frac{3i^2}{8} + \frac{23i}{24} + \frac{5}{8} \quad (i \text{ odd}). \quad (59)$$

The 3-couples of the others different classes of  $IS$  divide as follows:  $(k'-1, E(\frac{i}{2})+3, \gamma), (k'-1, E(\frac{i}{2})+4, \gamma), \dots, (k'-1, E(\frac{p+q+i+4}{2}), \gamma)$  for the class  $C_{k'-1}$ ,  $(k'-2, E(\frac{p+q+i+6}{2}), \gamma), (k'-2, E(\frac{p+q+i+8}{2}), \gamma), \dots, (k'-2, E(\frac{2(p+q)+i+4}{2}), \gamma)$  for the class  $C_{k'-2}$ , ...,  $(2, E(\frac{(k'-3)(p+q)+i+6}{2}), \gamma), (2, E(\frac{(k'-3)(p+q)+i+8}{2}), \gamma), \dots, (2, E(\frac{(k'-2)(p+q)+i+4}{2}), \gamma)$  for the class  $C_2$  and finally  $(1, E(\frac{(k'-2)(p+q)+i+6}{2}), \gamma), (1, E(\frac{(k'-2)(p+q)+i+8}{2}), \gamma), \dots, (1, Q_3 = E(\frac{(k'-1)(p+q)+i+4}{2}), \gamma)$  for the class  $C_1$ . As for the 2-monomials, the calculation of a cumulative multiplicity implies to distinguish the three cases:  $p+q$  even (case A),  $p+q$  odd with  $k'$  even (case B) and  $p+q$  odd with  $k'$  odd (case C). Results are given in the tables 11 to 15.

### 7.2.2. Case A

We denote by  $\tilde{\Lambda}'$  the population of the classes  $C_{k'-1}$  to  $C_1$ ; the counting of  $\tilde{\Lambda}'$  is more tedious than for the 2-monomials, because, for one given class of couples, there is  $q_3 - 1$  3-couples of same multiplicity on  $IS$  and this value varies from a class of couples to another. The method used here, consists in counting successively the populations of the  $\frac{p+q}{2}$  classes of multiplicity  $\tilde{\Lambda}_{p+q-1+\epsilon}, \tilde{\Lambda}_{p+q-3+\epsilon}, \dots, \tilde{\Lambda}_{1+\epsilon}$ . For instance, there is  $E(\frac{i}{2}) + 1 + \frac{j(p+q)}{2}$  3-couples ( $1 \leq j \leq k' - 1$ ) of cumulative multiplicity  $\mu = 1 + \epsilon$  in



each of the classes  $C_j$ . Thus one has:

$$\begin{aligned}\tilde{\Lambda}_{1+\epsilon} &= (1+\epsilon) \sum_{j=1}^{k'-1} [E(\frac{i}{2}) + 1 + \frac{j(p+q)}{2}], \\ &= (1+\epsilon)(k'-1)[E(\frac{i}{2}) + 1 + \frac{k'(p+q)}{4}].\end{aligned}\quad (60)$$

Doing similarly for the others populations:

$$\begin{aligned}\tilde{\Lambda}_{3+\epsilon} &= (3+\epsilon) \sum_{j=1}^{k'-1} [E(\frac{i}{2}) + \frac{j(p+q)}{2}], \\ &= (3+\epsilon)(k'-1)[E(\frac{i}{2}) + \frac{k'(p+q)}{4}],\end{aligned}\quad (61)$$

⋮

$$\begin{aligned}\tilde{\Lambda}_{p+q-1+\epsilon} &= (p+q-1+\epsilon) \sum_{j=0}^{k'-2} [E(\frac{i}{2}) + 2 + \frac{j(p+q)}{2}], \\ &= (p+q-1+\epsilon)(k'-1)[E(\frac{i}{2}) + 2 \\ &\quad + \frac{(k'-2)(p+q)}{4}].\end{aligned}\quad (62)$$

Population  $\tilde{\Lambda}'$  is the sum of Eqs. (60) to (62):

$$\begin{aligned}\tilde{\Lambda}' &= \sum_{j=0}^{\frac{p+q-2}{2}} (\epsilon + 2j + 1)(k'-1)[E(\frac{i}{2}) \\ &\quad + 1 - j + \frac{k'(p+q)}{4}], \\ &= \frac{(k'-1)(p+q)}{2} [(\epsilon + \frac{p+q}{2})(E(\frac{i}{2}) + \frac{k'(p+q)}{4}) \\ &\quad + \frac{(p+q-2)}{12}(5 - 2\epsilon - 2(p+q)) + \epsilon + 1].\end{aligned}\quad (63)$$

The population  $\tilde{\Lambda} = \tilde{\Lambda}' + \tilde{\Lambda}''$  of all the classes  $C_j$  ( $j = 1, \dots, k'$ ) is the sum of Eqs. (57) and (63). To count the number of 3-monomials in a sum  $S_m^{(3)}$ , one has at first to determine the number of switch-off couples  $\alpha$  on  $IS$ , the method remaining the same as for the 2-monomials. It gives:  $\alpha = \Lambda_2 - \tilde{\Lambda}$ , where depending on the parity of  $K = (k'-1)(p+q) + i$ ,  $\Lambda_2$  is given by Eq. (13) or (14). In Eqs. (13) or (14) we replace  $N$  by  $k'(p+q) + 4 + i$ , and one obtains the following equations:

$$\begin{aligned}\Lambda_2 &= \frac{1}{24}(k'-1)^3(p+q)^3 + \frac{1}{8}(k'-1)^2(p+q)^2(i+3) \\ &\quad + \frac{1}{24}(k'-1)(p+q)(3i(i+6) + 26 - 3\epsilon) \\ &\quad + R,\end{aligned}\quad (64)$$

$$R = \frac{i^3}{24} + \frac{3i^2}{8} + \frac{13i}{12} + 1 \quad (K \text{ even}),\quad (65)$$

$$R = \frac{i^3}{24} + \frac{3i^2}{8} + \frac{23i}{24} + \frac{5}{8} \quad (K \text{ odd}).\quad (66)$$

For the case  $A$ ,  $K$  and  $i$  have the same parity, thus  $R$  is canceled by  $\tilde{\Lambda}''$ . All calculations made, it results:

$$\begin{aligned}\alpha &= \frac{1}{24}(k'-1)(p+q) \left( \frac{1}{2}(p+q)^2[2(k'-1)^2 - 3k'] \right. \\ &\quad + (p+q)[3(k'-1)(i+3) - 3\epsilon k' + 2(p+q-2) \\ &\quad - 6E(\frac{i}{2})] + 2(3+i)^2 + (4+i)(2+i) \\ &\quad \left. - 12\epsilon E(\frac{i}{2}) - (p+q-2)(5-\epsilon) - 12(\epsilon+1) \right).\end{aligned}\quad (67)$$

The number of 3-monomials  $\Delta_2$  in a sum  $S_m^{(3)}$ , is obtained by summing  $\frac{\alpha}{p+q}$  and  $\tilde{\alpha}_2$ , the number of couples present without multiplicity on  $IS$  take into account the 3-couples of the classes  $C_j$  ( $1 \leq j \leq k'-1$ ) and of the class  $C_{k'}$ :

$$\begin{aligned}\tilde{\alpha}_2 &= \sum_{j=0}^{\frac{p+q-2}{2}} [E(\frac{i}{2}) + 1 + \frac{k'(p+q)}{4} - j] + \sum_{q_3=2}^{\tilde{q}_3} (q_3 - 1), \\ &= \frac{[E(\frac{i}{2}) + 1][E(\frac{i}{2}) + 2]}{2} + \frac{(k'-1)(p+q)}{2} [E(\frac{i}{2}) \\ &\quad + \frac{3}{2} + \frac{(k'-1)(p+q)}{4}]\end{aligned}$$

One deduces  $\Delta_2 = \frac{\alpha}{p+q} + \tilde{\alpha}_2$  given by Eq. (20); this proves theorem 4.

### 7.2.3. Case B

Compared with case  $A$ , as for the 2-monomials, one has to consider the "sub-cases"  $i$  even and  $i$  odd. Once again, the method consists to begin with the populations of the different classes of multiplicity, to determine  $\tilde{\Lambda}'_{even}$  and  $\tilde{\Lambda}'_{odd}$ , the populations of even and odd cumulative multiplicities on  $IS$ , except the class  $C_{k'}$  which population is known and given by Eq. (57).

- If  $i$  is even, there is  $\frac{p+q+1}{2}$  classes of odd multiplicities with populations  $\tilde{\Lambda}_{2j+1}$  ( $0 \leq j \leq \frac{p+q-1}{2}$ ), each of these classes appears 1 time on each of the  $\frac{k'-2}{2}$  even classes of couples  $C_{k'-2}, \dots, C_2$ . On the set of these classes, one counts  $E(\frac{i}{2}) + \frac{k'(p+q)}{4} + 1 - j$  3-couples

of cumulative multiplicity  $\mu = 2j + 1$ . It gives:

$$\begin{aligned}
\tilde{\Lambda}'_{odd} &= \frac{(k' - 2)}{2} \sum_{j=0}^{\frac{p+q-1}{2}} (2j + 1) \left( E\left(\frac{i}{2}\right) \right. \\
&+ \left. \frac{k'(p+q)}{4} + 1 - j \right) \\
&= \frac{(k' - 2)(p+q+1)}{4} \left( E\left(\frac{i}{2}\right) + \frac{k'(p+q)}{4} \right. \\
&+ \left. 1 + \frac{(p+q-1)}{4} [2E\left(\frac{i}{2}\right) + 1 + \frac{k'(p+q)}{2}] \right. \\
&- \left. \frac{1}{6}(p+q)(p+q-1) \right). \quad (68)
\end{aligned}$$

One counts also  $\frac{p+q-1}{2}$  classes of even multiplicity with populations  $\tilde{\Lambda}_{2j}$  ( $1 \leq j \leq \frac{p+q-1}{2}$ ), each of these classes appearing 1 time on each of the  $\frac{k'}{2}$  odd classes of couples  $C_{k'-1}, \dots, C_1$ . Furthermore, to a given cumulative multiplicity  $\mu = 2j$ , correspond  $E\left(\frac{i}{2}\right) + \frac{k'(p+q)}{4} + \frac{3}{2} - j$  3-couples, thus:

$$\begin{aligned}
\tilde{\Lambda}'_{even} &= \frac{k'}{2} \sum_{j=1}^{\frac{p+q-1}{2}} (2j) \left( E\left(\frac{i}{2}\right) + \frac{k'(p+q)}{4} + \frac{3}{2} - j \right) \\
&= \frac{k'(p+q+1)}{4} \left( \frac{(p+q-1)}{4} [2E\left(\frac{i}{2}\right) + 3 \right. \right. \\
&+ \left. \left. \frac{k'(p+q)}{2} \right] - \frac{1}{6}(p+q)(p+q-1) \right). \quad (69)
\end{aligned}$$

One deduces the population of all the classes  $C_j$  ( $j = 1, \dots, k' - 1$ ):

$$\begin{aligned}
\tilde{\Lambda}' &= \frac{(k' - 1)(3k' - 4)(p+q)^3}{48} \\
&+ \frac{(k' - 1)(p+q)^2}{8} [2E\left(\frac{i}{2}\right) + 1] + \frac{k'^2(p+q)^2}{16} \\
&+ \frac{(p+q)}{4} \left[ (k' - 2)E\left(\frac{i}{2}\right) + \frac{13k'}{12} - \frac{7}{3} \right] \\
&- \frac{1}{4}E\left(\frac{i}{2}\right) - \frac{3}{8}. \quad (70)
\end{aligned}$$

For  $i$  and  $k'$  even,  $K = (k' - 1)(p+q) + i$  is odd,  $\Lambda_2$  is obtained by Eqs. (64) and (66), thus it results:

$$\begin{aligned}
\alpha &= \frac{(k' - 1)(k' - 2)(2k' - 3)(p+q)^3}{48} \\
&+ \frac{(k' - 1)(p+q)^2}{8} \left[ (k' - 1)(3+i) - 2E\left(\frac{i}{2}\right) - 1 \right] \\
&- \frac{k'^2(p+q)^2}{16} + \frac{(p+q)}{4} \left( \frac{(k' - 1)}{6} [3i(i+6) + 23] \right. \\
&- \left. (k' - 2)E\left(\frac{i}{2}\right) - \frac{13k'}{12} + \frac{7}{3} \right). \quad (71)
\end{aligned}$$

Eq.(71) is divisible by  $p+q$ , the sum of terms  $-\frac{1}{4}E\left(\frac{i}{2}\right) - \frac{3}{8}$  in Eq. (70) and of  $\tilde{\Lambda}''$  (Eq. (58)) cancels  $R$  (Eq.(66)). Moreover, the number of 3-couples present without multiplicity on  $IS$  is:

$$\begin{aligned}
\tilde{\alpha}_2 &= \frac{[E\left(\frac{i}{2}\right) + 1][E\left(\frac{i}{2}\right) + 2]}{2} \\
&+ \frac{(k' - 2)}{2} \sum_{j=0}^{\frac{p+q-1}{2}} \left[ E\left(\frac{i}{2}\right) + \frac{k'(p+q)}{4} + 1 - j \right] \\
&+ \frac{k'}{2} \sum_{j=1}^{\frac{p+q-1}{2}} \left[ E\left(\frac{i}{2}\right) + \frac{k'(p+q)}{4} + \frac{3}{2} - j \right] \\
&= \frac{[E\left(\frac{i}{2}\right) + 1][E\left(\frac{i}{2}\right) + 2]}{2} \\
&+ \frac{(k' - 1)(p+q)}{2} \left[ \frac{(k' - 1)(p+q)}{4} + E\left(\frac{i}{2}\right) + 1 \right] \\
&- \frac{E\left(\frac{i}{2}\right)}{2} - \frac{5}{8}.
\end{aligned}$$

We obtain:

$$\begin{aligned}
\Delta_2 &= \frac{[E\left(\frac{i}{2}\right) + 1][E\left(\frac{i}{2}\right) + 2]}{2} \\
&+ \frac{k'(k' - 1)(p+q)}{48} [(2k' - 1)(p+q) + 3(2i+5)] \\
&+ \frac{(k' - 1)}{8} [i(i+6) + 8] - \frac{k'}{16} [4E\left(\frac{i}{2}\right) \\
&+ (p+q) + 5]. \quad (72)
\end{aligned}$$

This is Eq.(21) for  $i$  even ( $\epsilon = 0$ ).

- If  $i$  is odd, one counts  $\frac{p+q-1}{2}$  classes of odd multiplicity with populations  $\tilde{\Lambda}_{2j+1}$  ( $0 \leq j \leq \frac{p+q-1}{2}$ ), each of these classes appearing one time on each of the  $\frac{k'}{2}$  odd classes of couples  $C_{k'-1}, \dots, C_1$ . On the set of these classes, one counts  $E\left(\frac{i}{2}\right) + \frac{k'(p+q)}{4} + \frac{3}{2} - j$  3-couples of cumulative multiplicity  $\mu = 2j + 1$ . It reads:

$$\begin{aligned}
\tilde{\Lambda}'_{odd} &= \frac{k'(p+q+1)}{24} \left( 3\epsilon [2E\left(\frac{i}{2}\right) + 3] + \frac{3\epsilon k'(p+q)}{2} \right. \\
&- \left. (p+q-1)(p+q) + \frac{3(p+q-1)}{2} [2E\left(\frac{i}{2}\right) \right. \\
&+ \left. \frac{k'(p+q)}{2} + 3 - \epsilon] \right). \quad (73)
\end{aligned}$$

There is also  $\frac{p+q-1}{2}$  classes of even multiplicity with populations  $\tilde{\Lambda}_{2j}$  ( $0 \leq j \leq \frac{p+q-1}{2}$ ), each of these

classes appearing one time on each of the  $\frac{(k'-2)}{2}$  even classes of couples  $C_{k'-2}, \dots, C_2$ . Furthermore, for a given cumulative multiplicity  $\mu = 2j$ , there is  $E(\frac{i}{2}) + \frac{k'(p+q)}{4} + 2 - j$  3-couples. It gives:

$$\begin{aligned} \tilde{\Lambda}'_{even} = & \frac{(k'-2)(p+q-1)}{4} \left( \frac{(p+q-3)}{4} [2E(\frac{i}{2}) + \right. \\ & \left. \frac{k'(p+q)}{2} + 1 - \epsilon] + (1 + \epsilon)[E(\frac{i}{2}) + 1 \right. \\ & \left. + \frac{k'(p+q)}{4}] - \frac{(p+q-2)(p+q-3)}{6} \right). \end{aligned} \quad (74)$$

One deduces successively the populations  $\tilde{\Lambda}$  of all the classes  $C_j$  ( $j = 1, \dots, k'$ ) by summing Eqs. (59), (73) and (74), then  $\Lambda_2$  with the help of Eqs. (64) and (65),  $\alpha = \Lambda_2 - \tilde{\Lambda}$ . One determines then the number of 3-couples present without multiplicity on  $IS$  by:

$$\begin{aligned} \tilde{\alpha}_2 = & \frac{[E(\frac{i}{2}) + 1][E(\frac{i}{2}) + 2]}{2} \\ & + \frac{(k'-1)(p+q)}{2} \left[ \frac{(k'-1)(p+q)}{4} + E(\frac{i}{2}) + 2 \right] \\ & + \frac{E(\frac{i}{2})}{2} + \frac{7}{8}, \end{aligned} \quad (75)$$

It follows that:

$$\begin{aligned} \Delta_2 = & \frac{[E(\frac{i}{2}) + 1][E(\frac{i}{2}) + 2]}{2} \\ & + \frac{k'(k'-1)(p+q)}{48} [(2k'-1)(p+q) + 3(2i+5)] \\ & + \frac{(k'-1)}{8} [i(i+6) - 4E(\frac{i}{2}) + 1] + \frac{k'}{16} [4E(\frac{i}{2}) \\ & + (p+q) + 7]. \end{aligned} \quad (76)$$

$\Delta_2$  is deduced from (21) for the value  $\epsilon = 1$ . Theorem 5 is demonstrated.

#### 7.2.4. Case C

As for the case B, One has to consider the "sub-cases"  $i$  even and  $i$  odd.

- If  $i$  is even, there is  $\frac{p+q+1}{2}$  classes of odd multiplicity with the populations  $\tilde{\Lambda}_{2j+1}$  ( $0 \leq j \leq \frac{p+q-1}{2}$ ), each of these classes appearing exactly one time on each of the  $\frac{k'-1}{2}$  odd classes of couples  $C_{k'-2}, \dots,$

$C_1$ . Furthermore, for a given cumulative multiplicity  $\mu = 2j + 1$ , there is  $E(\frac{i}{2}) + \frac{(k'+1)(p+q)}{4} + 1 - j$  3-couples. Thus one may write:

$$\begin{aligned} \tilde{\Lambda}'_{odd} = & \frac{(k'-1)(p+q+1)}{4} \left( E(\frac{i}{2}) \right. \\ & + \frac{(k'+1)(p+q)}{4} + 1 + \frac{(p+q-1)}{4} [2E(\frac{i}{2}) \\ & + 1 + \frac{(k'+1)(p+q)}{2}] \\ & \left. - \frac{1}{6}(p+q)(p+q-1) \right). \end{aligned} \quad (77)$$

There is also  $\frac{p+q-1}{2}$  classes of even multiplicity with populations  $\tilde{\Lambda}_{2j}$  ( $1 \leq j \leq \frac{p+q-1}{2}$ ), each of these classes appearing exactly one time on each of the  $\frac{(k'-1)}{2}$  even classes of couples  $C_{k'-1}, \dots, C_2$ . Furthermore, for a given cumulative multiplicity  $\mu = 2j$ , there is  $E(\frac{i}{2}) + \frac{(k'-1)(p+q)}{4} + \frac{3}{2} - j$  3-couples. It reads:

$$\begin{aligned} \tilde{\Lambda}'_{even} = & \frac{(k'-1)(p+q+1)}{4} \left( \frac{(p+q-1)}{4} [2E(\frac{i}{2}) + 3 \right. \\ & + \left. \frac{(k'-1)(p+q)}{2}] \right. \\ & \left. - \frac{1}{6}(p+q)(p+q-1) \right). \end{aligned} \quad (78)$$

One deduces  $\tilde{\Lambda}'$ :

$$\begin{aligned} \tilde{\Lambda}' = & \frac{(k'-1)(3k'-4)(p+q)^3}{48} \\ & + \frac{(k'-1)(p+q)^2}{4} [E(\frac{i}{2}) + 1] + \frac{(k'^2-1)(p+q)^2}{16} \\ & + \frac{(k'-1)(p+q)}{4} [E(\frac{i}{2}) + \frac{19}{12}]. \end{aligned} \quad (79)$$

Determination of the number of switch-off couples is made on the same way as for cases A and B. For  $i$  even and  $k'$  odd,  $K = (k'-1)(p+q) + i$  is even, one obtains  $\Lambda_2$  with (64) and (65), thus:

$$\begin{aligned} \alpha = & \frac{(k'-1)(k'-2)(2k'-3)(p+q)^3}{48} \\ & + \frac{(k'-1)(p+q)^2}{8} [(k'-1)(3+i) - 2E(\frac{i}{2}) - \frac{k'}{2} \\ & - \frac{5}{2}] + \frac{(k'-1)(p+q)}{8} [i(i+6) + \frac{11}{2} \\ & - 2E(\frac{i}{2})]. \end{aligned} \quad (80)$$

(80) is divisible by  $p + q$ ,  $\tilde{\Lambda}''$  (Eq. (58)) canceling  $R$  (Eq.(65)). The number of 3-couples present without multiplicity on  $IS$  is given by Eq.:

$$\begin{aligned}\bar{\alpha}_2 &= \frac{[E(\frac{i}{2}) + 1][E(\frac{i}{2}) + 2]}{2} + \frac{(k' - 1)(p + q)}{2} [E(\frac{i}{2}) \\ &+ \frac{(k' - 1)(p + q)}{4} + \frac{3}{2}].\end{aligned}\quad (81)$$

One deduces:

$$\begin{aligned}\Delta_2 &= \frac{[E(\frac{i}{2}) + 1][E(\frac{i}{2}) + 2]}{2} \\ &+ \frac{k'(k' - 1)(p + q)}{48} [(2k' - 1)(p + q) + 3(2i + 5)] \\ &+ \frac{(k' - 1)}{8} [i(i + 6) + 8] \\ &- \frac{(k' - 1)}{16} [4E(\frac{i}{2}) - (p + q) + 5].\end{aligned}\quad (82)$$

It is Eq. (22) for  $i$  even.

- If  $i$  is odd, one counts  $\frac{p+q+1}{2}$  classes of odd multiplicity with populations  $\tilde{\Lambda}_{2j+1}$  ( $0 \leq j \leq \frac{p+q-1}{2}$ ), each of these classes appearing exactly one time on each of the  $\frac{(k'-1)}{2}$  odd classes of couples  $C_{k'-1}, \dots, C_1$ . Moreover, for a given cumulative multiplicity  $\mu = 2j + 1$ , there is  $E(\frac{i}{2}) + \frac{(k'-1)(p+q)}{4} + \frac{3}{2} - j$  3-couples. One has:

$$\begin{aligned}\tilde{\Lambda}'_{odd} &= \frac{(k' - 1)(p + q + 1)}{24} \left( 3[2\epsilon E(\frac{i}{2}) + 3\epsilon] \right. \\ &+ \frac{3(k' - 1)(p + q)}{2} - (p + q - 1)(p + q) \\ &+ \frac{3\epsilon(p + q - 1)}{2} + \frac{3(p + q - 1)}{2} [2E(\frac{i}{2}) \\ &+ \left. 3 - \epsilon + \frac{(k' - 1)(p + q)}{2} \right)].\end{aligned}\quad (83)$$

There is also  $\frac{p+q-1}{2}$  classes of even multiplicity with populations  $\tilde{\Lambda}_{2j}$  ( $1 \leq j \leq \frac{p+q-1}{2}$ ), each of these classes appearing exactly one time on each of these  $\frac{(k'-1)}{2}$  odd classes of couples  $C_{k'-2}, \dots, C_1$ . Furthermore, for a given cumulative multiplicity  $\mu = 2j$ ,

there is  $E(\frac{i}{2}) + \frac{(k'+1)(p+q)}{4} + 2 - j$  3-couples. It gives:

$$\begin{aligned}\tilde{\Lambda}'_{even} &= \frac{(k' - 1)(p + q - 1)}{4} \left( \frac{(p + q - 3)}{4} [2E(\frac{i}{2}) \right. \\ &+ \frac{(k' + 1)(p + q)}{2} + 1 - \epsilon] + (\epsilon + 1) [E(\frac{i}{2}) \\ &+ \frac{(k' + 1)(p + q)}{4} + 1] \\ &- \left. \frac{1}{6}(p + q - 2)(p + q - 3) \right).\end{aligned}\quad (84)$$

One deduces the populations  $\tilde{\Lambda}$  of all the classes  $C_j$  ( $j = 1, \dots, k'$ ) by summing the Eqs. (59), (83) and (84), then  $\Lambda_2$  with (64) and (66) and  $\alpha = \Lambda_2 - \tilde{\Lambda}$ . The number of 3-couples present without multiplicity on  $IS$  being given by Eq. (81), it follows that:

$$\begin{aligned}\Delta_2 &= \frac{[E(\frac{i}{2}) + 1][E(\frac{i}{2}) + 2]}{2} \\ &+ \frac{k'(k' - 1)(p + q)}{48} [(2k' - 1)(p + q) + 3(2i + 5)] \\ &+ \frac{(k' - 1)}{8} [i(i + 6) - 4E(\frac{i}{2}) + 1] \\ &+ \frac{(k' - 1)}{16} [4E(\frac{i}{2}) - (p + q) + 7].\end{aligned}\quad (85)$$

One obtains  $\Delta_2$  by (22) for  $i$  odd ( $\epsilon = 1$ ). Theorem 6 is demonstrated.

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class $C_j$	$q_2$	$\mu$
$C_{k'-1}$	$E(\frac{i}{2}) + 2$	$p + q - 1 + \epsilon$
$C_{k'-1}$	$E(\frac{i}{2}) + 3$	$p + q - 3 + \epsilon$
$\vdots$	$\vdots$	$\vdots$
$C_{k'-1}$	$E(\frac{i}{2}) + \frac{p+q}{2} + 1$	$1 + \epsilon$
$C_{k'-2}$	$E(\frac{i}{2}) + \frac{p+q}{2} + 2$	$p + q - 1 + \epsilon$
$C_{k'-2}$	$E(\frac{i}{2}) + \frac{p+q}{2} + 3$	$p + q - 3 + \epsilon$
$\vdots$	$\vdots$	$\vdots$
$C_{k'-2}$	$E(\frac{i}{2}) + p + q + 1$	$1 + \epsilon$
$\vdots$	$\vdots$	$\vdots$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-3)(p+q)}{2} + 2$	$p + q - 1 + \epsilon$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-3)(p+q)}{2} + 3$	$p + q - 3 + \epsilon$
$\vdots$	$\vdots$	$\vdots$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + 1$	$1 + \epsilon$
$C_1$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + 2$	$p + q - 1 + \epsilon$
$C_1$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + 3$	$p + q - 3 + \epsilon$
$\vdots$	$\vdots$	$\vdots$
$C_1$	$E(\frac{i}{2}) + \frac{(k'-1)(p+q)}{2} + 1$	$1 + \epsilon$

Table 6: Case A. Table giving the different classes of couples with the cumulative multiplicities . If  $i$  even ( $\epsilon = 0$ ), all the cumulative multiplicity are odd; they are all even if  $i$  is odd ( $\epsilon = 1$ ).

class $C_j$	$q_2$	$\mu$
$C_{k'-1}$	$E(\frac{i}{2}) + 2$	$p + q - 1$
$C_{k'-1}$	$E(\frac{i}{2}) + 3$	$p + q - 3$
$\vdots$	$\vdots$	$\vdots$
$C_{k'-1}$	$E(\frac{i}{2}) + \frac{p+q}{2} + \frac{1}{2}$	2
$C_{k'-2}$	$E(\frac{i}{2}) + \frac{p+q}{2} + \frac{3}{2}$	$p + q$
$C_{k'-2}$	$E(\frac{i}{2}) + \frac{p+q}{2} + \frac{5}{2}$	$p + q - 2$
$\vdots$	$\vdots$	$\vdots$
$C_{k'-2}$	$E(\frac{i}{2}) + p + q + 1$	1
$\vdots$	$\vdots$	$\vdots$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-3)(p+q)}{2} + \frac{3}{2}$	$p + q$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-3)(p+q)}{2} + \frac{5}{2}$	$p + q - 2$
$\vdots$	$\vdots$	$\vdots$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + 1$	1
$C_1$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + 2$	$p + q - 1$
$C_1$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + 3$	$p + q - 3$
$\vdots$	$\vdots$	$\vdots$
$C_1$	$E(\frac{i}{2}) + \frac{(k'-1)(p+q)}{2} + \frac{1}{2}$	2

Table 7: Case B. Table giving the different classes of couples with cumulative multiplicities for  $k'$  and  $i$  even.

class $C_j$	$q_2$	$\mu$
$C_{k'-1}$	$E(\frac{i}{2}) + 2$	$p + q$
$C_{k'-1}$	$E(\frac{i}{2}) + 3$	$p + q - 2$
$\vdots$	$\vdots$	$\vdots$
$C_{k'-1}$	$E(\frac{i}{2}) + \frac{p+q}{2} + \frac{3}{2}$	1
$C_{k'-2}$	$E(\frac{i}{2}) + \frac{p+q}{2} + \frac{5}{2}$	$p + q - 1$
$C_{k'-2}$	$E(\frac{i}{2}) + \frac{p+q}{2} + \frac{7}{2}$	$p + q - 3$
$\vdots$	$\vdots$	$\vdots$
$C_{k'-2}$	$E(\frac{i}{2}) + p + q + 1$	2
$\vdots$	$\vdots$	$\vdots$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-3)(p+q)}{2} + \frac{5}{2}$	$p + q - 1$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-3)(p+q)}{2} + \frac{7}{2}$	$p + q - 3$
$\vdots$	$\vdots$	$\vdots$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + 1$	2
$C_1$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + 2$	$p + q$
$C_1$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + 3$	$p + q - 2$
$\vdots$	$\vdots$	$\vdots$
$C_1$	$E(\frac{i}{2}) + \frac{(k'-1)(p+q)}{2} + \frac{3}{2}$	1

Table 8: Case B. Table giving the different classes of couples with the cumulative multiplicities for  $k'$  even and  $i$  odd.

class $C_j$	$q_2$	$\mu$
$C_{k'-1}$	$E(\frac{i}{2}) + 2$	$p + q - 1$
$C_{k'-1}$	$E(\frac{i}{2}) + 3$	$p + q - 3$
$\vdots$	$\vdots$	$\vdots$
$C_{k'-1}$	$E(\frac{i}{2}) + \frac{p+q}{2} + \frac{1}{2}$	2
$C_{k'-2}$	$E(\frac{i}{2}) + \frac{p+q}{2} + \frac{3}{2}$	$p + q$
$C_{k'-2}$	$E(\frac{i}{2}) + \frac{p+q}{2} + \frac{5}{2}$	$p + q - 2$
$\vdots$	$\vdots$	$\vdots$
$C_{k'-2}$	$E(\frac{i}{2}) + p + q + 1$	1
$\vdots$	$\vdots$	$\vdots$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-3)(p+q)}{2} + 2$	$p + q - 1$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-3)(p+q)}{2} + 3$	$p + q - 3$
$\vdots$	$\vdots$	$\vdots$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + \frac{1}{2}$	2
$C_1$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + \frac{3}{2}$	$p + q$
$C_1$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + \frac{5}{2}$	$p + q - 2$
$\vdots$	$\vdots$	$\vdots$
$C_1$	$E(\frac{i}{2}) + \frac{(k'-1)(p+q)}{2} + 1$	1

Table 9: Case  $C$ . Table giving the different classes of couples with the cumulative multiplicity for  $k'$  odd and  $i$  even.

Class $C_j$	$q_2$	$\mu$
$C_{k'-1}$	$E(\frac{i}{2}) + 2$	$p + q$
$C_{k'-1}$	$E(\frac{i}{2}) + 3$	$p + q - 2$
$\vdots$	$\vdots$	$\vdots$
$C_{k'-1}$	$E(\frac{i}{2}) + \frac{p+q}{2} + \frac{3}{2}$	1
$C_{k'-2}$	$E(\frac{i}{2}) + \frac{p+q}{2} + \frac{5}{2}$	$p + q - 1$
$C_{k'-2}$	$E(\frac{i}{2}) + \frac{p+q}{2} + \frac{7}{2}$	$p + q - 3$
$\vdots$	$\vdots$	$\vdots$
$C_{k'-2}$	$E(\frac{i}{2}) + p + q + 1$	2
$\vdots$	$\vdots$	$\vdots$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-3)(p+q)}{2} + 2$	$p + q$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-3)(p+q)}{2} + 3$	$p + q - 2$
$\vdots$	$\vdots$	$\vdots$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + \frac{3}{2}$	1
$C_1$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + \frac{5}{2}$	$p + q - 1$
$C_1$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + \frac{7}{2}$	$p + q - 3$
$\vdots$	$\vdots$	$\vdots$
$C_1$	$E(\frac{i}{2}) + \frac{(k'-1)(p+q)}{2} + 1$	2

Table 10: Case  $C$ . Table giving the different classes of couples with the cumulative multiplicities for  $k'$  and  $i$  odd.

class $C_j$	$q_3$	$\mu$
$C_{k'-1}$	$E(\frac{i}{2}) + 3$	$p + q - 1 + \epsilon$
$C_{k'-1}$	$E(\frac{i}{2}) + 4$	$p + q - 3 + \epsilon$
$\vdots$	$\vdots$	$\vdots$
$C_{k'-1}$	$E(\frac{i}{2}) + \frac{p+q}{2} + 2$	$1 + \epsilon$
$C_{k'-2}$	$E(\frac{i}{2}) + \frac{p+q}{2} + 3$	$p + q - 1 + \epsilon$
$C_{k'-2}$	$E(\frac{i}{2}) + \frac{p+q}{2} + 4$	$p + q - 3 + \epsilon$
$\vdots$	$\vdots$	$\vdots$
$C_{k'-2}$	$E(\frac{i}{2}) + p + q + 2$	$1 + \epsilon$
$\vdots$	$\vdots$	$\vdots$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-3)(p+q)}{2} + 3$	$p + q - 1 + \epsilon$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-3)(p+q)}{2} + 4$	$p + q - 3 + \epsilon$
$\vdots$	$\vdots$	$\vdots$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + 2$	$1 + \epsilon$
$C_1$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + 3$	$p + q - 1 + \epsilon$
$C_1$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + 4$	$p + q - 3 + \epsilon$
$\vdots$	$\vdots$	$\vdots$
$C_1$	$E(\frac{i}{2}) + \frac{(k'-1)(p+q)}{2} + 2$	$1 + \epsilon$

Table 11: Case A. Table giving the different classes of 3-couples as a function of  $q_3$  with the cumulative multiplicities. If  $i$  even ( $\epsilon = 0$ ), all the cumulative multiplicities are odd; they are all even if  $i$  is odd ( $\epsilon = 1$ ).

class $C_j$	$q_3$	$\mu$
$C_{k'-1}$	$E(\frac{i}{2}) + 3$	$p + q - 1$
$C_{k'-1}$	$E(\frac{i}{2}) + 4$	$p + q - 3$
$\vdots$	$\vdots$	$\vdots$
$C_{k'-1}$	$E(\frac{i}{2}) + \frac{p+q}{2} + \frac{3}{2}$	$2$
$C_{k'-2}$	$E(\frac{i}{2}) + \frac{p+q}{2} + \frac{5}{2}$	$p + q$
$C_{k'-2}$	$E(\frac{i}{2}) + \frac{p+q}{2} + \frac{7}{2}$	$p + q - 2$
$\vdots$	$\vdots$	$\vdots$
$C_{k'-2}$	$E(\frac{i}{2}) + p + q + 2$	$1$
$\vdots$	$\vdots$	$\vdots$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-3)(p+q)}{2} + \frac{5}{2}$	$p + q$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-3)(p+q)}{2} + \frac{7}{2}$	$p + q - 2$
$\vdots$	$\vdots$	$\vdots$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + 2$	$1$
$C_1$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + 3$	$p + q - 1$
$C_1$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + 4$	$p + q - 3$
$\vdots$	$\vdots$	$\vdots$
$C_1$	$E(\frac{i}{2}) + \frac{(k'-1)(p+q)}{2} + \frac{3}{2}$	$2$

Table 12: Case B. Table giving the different classes of 3-couples function of  $q_3$  with the cumulative multiplicities for  $k'$  and  $i$  even.



class $C_j$	$q_3$	$\mu$
$C_{k'-1}$	$E(\frac{i}{2}) + 3$	$p + q$
$C_{k'-1}$	$E(\frac{i}{2}) + 4$	$p + q - 2$
$\vdots$	$\vdots$	$\vdots$
$C_{k'-1}$	$E(\frac{i}{2}) + \frac{p+q}{2} + \frac{5}{2}$	1
$C_{k'-2}$	$E(\frac{i}{2}) + \frac{p+q}{2} + \frac{7}{2}$	$p + q - 1$
$C_{k'-2}$	$E(\frac{i}{2}) + \frac{p+q}{2} + \frac{9}{2}$	$p + q - 3$
$\vdots$	$\vdots$	$\vdots$
$C_{k'-2}$	$E(\frac{i}{2}) + p + q + 2$	2
$\vdots$	$\vdots$	$\vdots$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-3)(p+q)}{2} + \frac{7}{2}$	$p + q - 1$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-3)(p+q)}{2} + \frac{9}{2}$	$p + q - 3$
$\vdots$	$\vdots$	$\vdots$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + 2$	2
$C_1$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + 3$	$p + q$
$C_1$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + 4$	$p + q - 2$
$\vdots$	$\vdots$	$\vdots$
$C_1$	$E(\frac{i}{2}) + \frac{(k'-1)(p+q)}{2} + \frac{5}{2}$	1

Table 13: Case  $B$ . Table giving the different classes of 3-couples as a function of  $q_3$  with the cumulative multiplicities for  $k'$  even and  $i$  odd ( $\epsilon = 1$ ).

class $C_j$	$q_3$	$\mu$
$C_{k'-1}$	$E(\frac{i}{2}) + 3$	$p + q - 1$
$C_{k'-1}$	$E(\frac{i}{2}) + 4$	$p + q - 3$
$\vdots$	$\vdots$	$\vdots$
$C_{k'-1}$	$E(\frac{i}{2}) + \frac{p+q}{2} + \frac{3}{2}$	2
$C_{k'-2}$	$E(\frac{i}{2}) + \frac{p+q}{2} + \frac{5}{2}$	$p + q$
$C_{k'-2}$	$E(\frac{i}{2}) + \frac{p+q}{2} + \frac{7}{2}$	$p + q - 2$
$\vdots$	$\vdots$	$\vdots$
$C_{k'-2}$	$E(\frac{i}{2}) + p + q + 2$	1
$\vdots$	$\vdots$	$\vdots$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-3)(p+q)}{2} + 3$	$p + q - 1$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-3)(p+q)}{2} + 4$	$p + q - 3$
$\vdots$	$\vdots$	$\vdots$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + \frac{3}{2}$	2
$C_1$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + \frac{5}{2}$	$p + q$
$C_1$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + \frac{7}{2}$	$p + q - 2$
$\vdots$	$\vdots$	$\vdots$
$C_1$	$E(\frac{i}{2}) + \frac{(k'-1)(p+q)}{2} + 2$	1

Table 14: Case  $C$ . Table giving the different classes of 3-couples as a function of  $q_3$  with the cumulative multiplicities for  $k'$  odd and  $i$  even.

class $C_j$	$q_3$	$\mu$
$C_{k'-1}$	$E(\frac{i}{2}) + 3$	$p + q$
$C_{k'-1}$	$E(\frac{i}{2}) + 4$	$p + q - 2$
$\vdots$	$\vdots$	$\vdots$
$C_{k'-1}$	$E(\frac{i}{2}) + \frac{p+q}{2} + \frac{5}{2}$	1
$C_{k'-2}$	$E(\frac{i}{2}) + \frac{p+q}{2} + \frac{7}{2}$	$p + q - 1$
$C_{k'-2}$	$E(\frac{i}{2}) + \frac{p+q}{2} + \frac{9}{2}$	$p + q - 3$
$\vdots$	$\vdots$	$\vdots$
$C_{k'-2}$	$E(\frac{i}{2}) + p + q + 2$	2
$\vdots$	$\vdots$	$\vdots$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-3)(p+q)}{2} + 3$	$p + q$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-3)(p+q)}{2} + 4$	$p + q - 2$
$\vdots$	$\vdots$	$\vdots$
$C_2$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + \frac{5}{2}$	1
$C_1$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + \frac{7}{2}$	$p + q - 1$
$C_1$	$E(\frac{i}{2}) + \frac{(k'-2)(p+q)}{2} + \frac{9}{2}$	$p + q - 3$
$\vdots$	$\vdots$	$\vdots$
$C_1$	$E(\frac{i}{2}) + \frac{(k'-1)(p+q)}{2} + 2$	2

Table 15: Case  $C$ . Table giving the different classes of 3-couples as a function of  $q_3$  with the cumulative multiplicities for  $k'$  and  $i$  odd.