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On the Number of Rumer Diagrams

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Abstract

In this paper we review the famous article "Eine für die Valenztheorie geeignete Basis der binären Vektorinvarianten" of G. Rumer, E. Teller, and H. Weyl on Rumer diagrams and use a powerful old result from algebraic geometry to enumerate these diagrams with given numbers of atoms and valence bonds.

1 Introduction and notation

"In the literature there are a number of attempts to deal with the matter of skeletal isomerism. The two papers of widest scope are those of Sylvester, [12], and of Gordan and Alexejeff, [4], in both of which the parallelism between the chemical theory of molecular structure and the algebraic theory of invariants is stressed. It seems probable that interesting and important results might be attained by exhaustively pursuing this line of attack, but chemists have never devoted to these papers the attention which they deserve". (A. C. Lunn, J. K. Senior, 1929, [8], p. 1039.)

The paper is devoted to presenting the number of Rumer diagrams with n atoms which form a molecule with m valence bonds. We follow the classical article [11] where

the atoms are represented by vectors

$$x^{(1)} = \begin{pmatrix} x_1^{(1)} \\ x_2^{(1)} \end{pmatrix}, \dots, x^{(n)} = \begin{pmatrix} x_1^{(n)} \\ x_2^{(n)} \end{pmatrix},$$
(1)

in the complex plane \mathbb{C}^2 . When $n \ge 2$ each valence bond between two of them, $x^{(i)}$ and $x^{(j)}$, is modeled by the determinant

$$[x^{(i)}, x^{(j)}] = \begin{vmatrix} x_1^{(i)} & x_1^{(j)} \\ x_2^{(i)} & x_2^{(j)} \end{vmatrix},$$
(2)

viewed as a polynomial in the four variables $x_1^{(i)}, x_2^{(i)}, x_1^{(j)}, x_2^{(j)}$. These determinants, called *brackets*, considered as complex-valued functions in two vector arguments $x^{(i)}, x^{(j)}$, defined on the plane \mathbb{C}^2 , are the building blocks of the set of all such functions $f(x^{(1)}, \ldots, x^{(n)})$ which have the same value (are *invariant*) when changing the coordinate system in \mathbb{C}^2 via transformations with determinant 1. All such transformations of \mathbb{C}^2 form a group called *special linear group* and denoted $\mathrm{SL}(\mathbb{C}^2)$, or, simply $\mathrm{SL}(2)$. More precisely, in accord with the first main theorem on invariants, homogeneous degree k invariant under the group $\mathrm{SL}(2)$ polynomial f in $x_1^{(1)}, x_2^{(1)}, \ldots, x_1^{(n)}, x_2^{(n)}$ exists exactly when k is even, k = 2m, and in this case f is a linear combinations of products (called *bracket monomials*) of the form

$$[x^{(i_1)}, x^{(j_1)}] \dots [x^{(i_m)}, x^{(j_m)}], \ 1 \le i_s < j_s \le n, \ s \in [1, m].$$

$$(3)$$

The expression of any bracket monomial (3) produces a graph G on n vertices $1, \ldots, n$ and m edges $(i_1, j_1), \ldots, (i_m, j_m)$ without loops, where the vertices are placed clockwise on a circle in this order and any edge (i_s, j_s) is represented by the segment with end points i_s and j_s . Conversely, each bracket monomial's expression (3) can be restituted from its graph G which thus is called its *valence scheme*. In case there are no intersecting edges, the valence scheme G is said to be *Rumer diagram*. In quantum chemistry, each Rumer diagram, or, what is the same, bracket monomial, represents a pure valence state of a molecule with atoms $1, \ldots, n$ and any invariant (linear combination of bracket monomials) represents a valence state (mixture of pure valence states).

This idea goes back to the providential paper [12] of J. J. Sylvester, where he, in particular, wrote: "An invariant of a form or system of algebraic forms must thus represent a saturated system of atoms in which the rays of all the atoms are connected into bonds." A meticulous historic analysis of Sylvester's contributions, written in a modern language, can be found in [6]. The analogy between invariant theory and chemistry was completely ignored by the chemists till the end of 19-th century and was galvanized by the physicist G. Rumer in his pioneering paper [10] and in its popular continuation [11]. In order for the exposition to be self-contained, in section 2 we gather the necessary definitions and results from different mathematical disciplines in three subsections: Algebra, Invariant theory, and Algebraic geometry. From the content of the first subsection we note the introduction of a special grading (via graphical multidegree) of a polynomial ring used later. In the last two subsections we discuss the isomorphism between the graded ring consisting of SL(2)-invariant polynomials in $x_1^{(1)}, x_2^{(1)}, \ldots, x_1^{(n)}, x_2^{(n)}$ and the graded homogeneous coordinate ring of the Grassmannian G(n, 2). As a consequence, we use the famous postulation formula of W. V. D. Hodge and J. E. Littlewood in order to find the dimensions of the homogeneous components of the graded ring of invariants in Theorem 2.

Section 3 is devoted to meticulous proofs of the three theorems from [11] and to the enumeration of Rumer diagrams with given numbers of atoms and valence bonds presented in Theorem 10.

Below we introduce some notation.

 $\mathbb{N}:$ The set of positive integers.

 \mathbb{N}_+ : The set of nonnegative integers.

 \mathbb{C} : The field of complex numbers.

 $[1,k] = \{1,\ldots,k\} \subset \mathbb{N}.$

 $\binom{k}{\ell}$ for $k \in \mathbb{N}, \ \ell \in \mathbb{N}_+$: The binomial coefficient.

 $n \in \mathbb{N}, n \ge 2$: The number of atoms.

 $m \in \mathbb{N}_+$: The number of valence bonds.

2 Mathematical background

Some elementary notions and statements from algebra are supposed to be known. We suggest [1] and [2] as universal references.

Algebra. By a monoid we mean a set Δ together with an associative binary operation on Δ , written additively, which has zero element 0. Examples are the set \mathbb{N}_+ with addition of integers and any Cartesian power \mathbb{N}_+^{ℓ} with componentwise addition of ℓ -tuples.

We denote by $A = \mathbb{C}[z_1, \ldots, z_r]$ the ring of polynomials in the variables z_1, \ldots, z_r over the field \mathbb{C} of complex numbers. Given a monoid Δ , we say that A is a graded of type Δ ring if there exists a family $(A_{\lambda})_{\lambda \in \Delta}$ of subgroups of the additive group A such that $A = \bigoplus_{\lambda \in \Delta} A_{\lambda}$ (any polynomial $f \in A$ can be presented uniquely as $f = \sum_{\lambda \in \Delta} f_{\lambda}$, $f_{\lambda} \in A_{\lambda}$, and only a finite number of f_{λ} are nonzero) and $A_{\lambda}A_{\mu} \subset A_{\lambda+\mu}$ for $\lambda, \mu \in \Delta$. A subring $I \subset A$ is called graded subring if $I = \bigoplus_{\lambda \in \Delta} I_{\lambda}$ where $I_{\lambda} = I \cap A_{\lambda}$ for all $\lambda \in \Delta$. nonempty subset $I \subset A$ is called *ideal* of A if difference of two polynomials in I is again in I and if the product of any polynomial with a member of I is again a member of I. The ideal I in A is said to be *homogeneous* if I is a graded subring. We note that an ideal is homogeneous if and only if it can be generated by homogeneous elements.

Any ideal I in the ring A produces a ring A/I, called *factor-ring*, in the following way: The members of the set A/I are all subsets of A of the form f + I, $f \in A$, and we have f + I = g + I if and only if $f - g \in I$. Addition and multiplication in A/I are defined naturally: (f + I) + (g + I) = f + g + I, (f + I)(g + I) = fg + I, 0 + I = I is the zero element, and 1 + I is the unit.

In general, a map from a ring (graded type Δ ring) to another ring (graded type Δ ring) is called *homomorphism* (*homogeneous homomorphism*) if it maps sums and products onto the sums and products of the corresponding images, respectively (and maps any homogeneous component into the corresponding homogeneous component). *Kernel* of this homomorphism is the ideal consisting of members of the domain which are mapped onto zero. When the homomorphism is homogeneous, then its kernel turns out to be homogeneous ideal. The map

$$c: A \to A/I, f \mapsto f + I,$$

is said to be the *canonical homomorphism* and its kernel is I. If the ring A is a graded of type Δ , $A = \bigoplus_{\lambda \in \Delta} A_{\lambda}$, and if the ideal I is homogeneous, then A/I inherits this grading via c: $A/I = \bigoplus_{\lambda \in \Delta} c(A_{\lambda})$. In this case the canonical homomorphism is homogeneous. In general, any surjective homomorphism $\varphi \colon A \to B$ of rings is, up to a unique isomorphism produced by φ , canonical: In the commutative diagram below $\overline{\varphi}$ is an isomorphism.

$$\begin{array}{c}
A & \xrightarrow{\varphi} \\
\downarrow c \\
A/I & \xrightarrow{\overline{\varphi}} & B.
\end{array}$$
(4)

Here the kernel of φ is I and commutativity means $\varphi = \overline{\varphi} \circ c$.

The natural grading of A can be defined as the grading of type \mathbb{N}_+ , where A_{λ} is the subgroup of A, consisting of all homogeneous degree λ polynomials, $\lambda \in \mathbb{N}_+$, plus the zero polynomial (which has degree $-\infty$). Since $A_0 = \mathbb{C}$, we obtain that any homogeneous component A_{λ} is a \mathbb{C} -linear space.

Let y_{ij} , $1 \leq i < j \leq n$, be $\binom{n}{2}$ in number variables, and let $\mathbb{C}[y_{ij}] = \mathbb{C}[y_{ij}, 1 \leq i < j \leq n]$ be the corresponding polynomial ring. Let us set $B = \mathbb{C}[y_{ij}]$ for short and let $B = \bigoplus_{m \in \mathbb{N}_+} B_m$ be the natural grading. For any monomial

$$g = y_{i_1 j_1} \dots y_{i_m j_m} \in B_m, \ 1 \le i_s < j_s \le n, \ s \in [1, m], \tag{5}$$

a graph G on n vertices $1, \ldots, n$ and m edges $(i_1, j_1), \ldots, (i_m, j_m)$ without loops can be constructed exactly in the same way lake the graph of a bracket monomial (3). Conversely, each such monomial g can be restituted from its graph G and the correspondence is oneto-one. We define $\deg_v(g)$ to be the degree of the vertex v of the graph $G, v \in [1, n]$.

Given $m, m_1, \ldots, m_n \in \mathbb{N}_+$ with $m_1 + \cdots + m_n = 2m$, we denote by B_{m_1,\ldots,m_n} the \mathbb{C} linear subspace of B_m , spanned by all monomials (5) such that $\deg_v(g) = m_v, v \in [1, n]$. The *n*-tuple m_1, \ldots, m_n is called graphical multidegree of the monomial (5).

Let us denote by Δ_2^n the monoid consisting of all *n*-tuples $(m_1, \ldots, m_n) \in \mathbb{N}_+^n$ with even sum. Thus, we obtain a finer grading of type Δ_2^n of the polynomial ring $B = \mathbb{C}[y_{ij}]$:

$$B = \bigoplus_{m \in \mathbb{N}_+} \bigoplus_{m_1 + \dots + m_n = 2m} B_{m_1, \dots, m_n},\tag{6}$$

and, moreover, for any $m \in \mathbb{N}_+$ we have

$$B_m = \bigoplus_{m_1 + \dots + m_n = 2m} B_{m_1, \dots, m_n}.$$
(7)

Invariant Theory. The vectors in \mathbb{C}^2 have the form (1) (that is, are 2×1 -matrices) and the invertible linear transformations of \mathbb{C}^2 (changes of coordinates) are 2×2 -matrices σ with det $\sigma \neq 0$. The latter form a group GL(2) (general linear group) and the special linear group SL(2) is the subgroup of GL(2), consisting of all $\sigma \in GL(2)$ with det $\sigma = 1$.

For general vectors (1) we set

$$\mathbb{C}[x^{(1)},\ldots,x^{(n)}] = \mathbb{C}[x_1^{(1)},x_2^{(1)},\ldots,x_1^{(n)},x_2^{(n)}]$$

to be the polynomial ring in 2n variables furnished with the natural grading:

$$\mathbb{C}[x^{(1)}, \dots, x^{(n)}] = \bigoplus_{k \in \mathbb{N}_+} \mathbb{C}[x^{(1)}, \dots, x^{(n)}]_k.$$
(8)

The group GL(2) (and hence SL(2)) acts on the plane \mathbb{C}^2 by matrix multiplication, called *left multiplication*: If

$$\sigma = \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix} \text{ and } x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix},$$

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then $\sigma \cdot x = \sigma x$. This action can be extended naturally on the Cartesian product $\mathbb{C}^2 \times \cdots \times \mathbb{C}^2$ (*n* times) via the rule $\sigma \cdot (x^{(1)}, \ldots, x^{(n)}) = (\sigma \cdot x^{(1)}, \ldots, \sigma \cdot x^{(n)})$. Thus, we obtain an action of the group GL(2) on the polynomial ring $\mathbb{C}[x^{(1)}, \ldots, x^{(n)}]$ via the formula

$$(\sigma \cdot f)(x^{(1)}, \dots, x^{(n)}) = f(\sigma^{-1} \cdot x^{(1)}, \dots, \sigma^{-1} \cdot x^{(n)}).$$
(9)

All of the above actions are *linear* ones: The left multiplication by a fixed $\sigma \in GL(2)$ induces an invertible linear transformation of the corresponding \mathbb{C} -linear space. In general, any linear action of a group Γ on a finite-dimensional linear space W is called *finitedimensional representation* of this group. In case W can not be represented as a direct sum of two nonzero subspaces on which this action of Γ induces actions on these subspaces, the representation W of Γ is said to be *irreducible*. When for any $\sigma \in \Gamma$, the corresponding left multiplication by σ in W is the identity linear transformation, the representation is called *identical*.

Any finite-dimensional representation of GL(2) or SL(2) can be represented as a finite direct sum of irreducible representations of this group.

In order to explain the relation of the ring $\mathbb{C}[x^{(1)}, \ldots, x^{(n)}]$ with the main statements in the classical invariant theory, we need to furnish it with a finer structure — this of a graded ring (8). The action of the group GL(2) preserves the grading: If $f \in \mathbb{C}[x^{(1)}, \ldots, x^{(n)}]_k$, then $\sigma \cdot f \in \mathbb{C}[x^{(1)}, \ldots, x^{(n)}]_k$. Moreover, let $f \neq 0$, $f = \sum_{n\geq 0} f_k$. The polynomial f is invariant if and only if each homogeneous polynomial f_k is invariant (see [3, Ch. 1, Sect. 2, Proposition 2]).

The determinants (brackets) $p_{ij} = [x^{(i)}, x^{(j)}]$ from (2) for $1 \le i < j \le n$ are members of the polynomial ring $\mathbb{C}[x^{(1)}, \ldots, x^{(n)}]$. Let us define $p_{ij} = -p_{ji}$ for i > j. The homogeneous degree 2 polynomials p_{ij} , $1 \le i < j \le n$, satisfy the following quadratic identities:

$$p_{i_1j_1}p_{j_2j_3} - p_{i_1j_2}p_{j_1j_3} + p_{i_1j_3}p_{j_1j_2} = 0 aga{10}$$

for all subsets $\{i_1, j_1, j_2, j_3\} \subset [1, n]$, consisting of four elements. Let $\operatorname{Inv}^{(n)}$ be the subring of $\mathbb{C}[x^{(1)}, \ldots, x^{(n)}]$, generated by p_{ij} , $1 \leq i < j \leq n$. The members of the ring $\operatorname{Inv}^{(n)}$ are constructed in the following way: First, we define the map

$$\varphi \colon \mathbb{C}[y_{ij}] \to \mathbb{C}[x^{(1)}, \dots, x^{(n)}], \ f(y_{ij}) \mapsto f(p_{ij}).$$
(11)

This map is a homomorphism of rings and the ring $\operatorname{Inv}^{(n)}$ is the image of φ (that is, $\operatorname{Inv}^{(n)} = \{f(p_{ij}) \mid f \in \mathbb{C}[y_{ij}]\}$). Moreover, $\operatorname{Inv}^{(n)}$ inherits the natural structure of graded ring on the polynomial ring $\mathbb{C}[y_{ij}]$: $\operatorname{Inv}^{(n)} = \bigoplus_{m \in \mathbb{N}_+} \operatorname{Inv}^{(n)}_m$, where $\operatorname{Inv}^{(n)}_m = \varphi(\mathbb{C}[y_{ij}]_m)$. Thus, for any $m \in \mathbb{N}_+$ the \mathbb{C} -linear space $\operatorname{Inv}_m^{(n)}$ is spanned by all bracket monomials

$$p_{i_1 j_1} \dots p_{i_m j_m}, 1 \le i_s < j_s \le n, \ s \in [1, m].$$
 (12)

The first main theorem of invariants (see, for example [3, Ch. 1, Sect. 2, Proposition 3 and Ch. 2, Sect. 5, Theorem], or, [11, 1. Fundamentalsatz]) yields that the \mathbb{C} -linear space $\operatorname{Inv}_m^{(n)}$ consists of all homogeneous $\operatorname{SL}(2)$ -invariant polynomials of degree k = 2m in $\mathbb{C}[x^{(1)}, \ldots, x^{(n)}]$ and there are no homogeneous invariants in $\mathbb{C}[x^{(1)}, \ldots, x^{(n)}]_{2m+1}, m \in \mathbb{N}_+$. Thus, the subring $\operatorname{Inv}^{(n)} \subset \mathbb{C}[x^{(1)}, \ldots, x^{(n)}]$ consists of all $\operatorname{SL}(2)$ -invariant polynomials.

In case n = 1, let us denote by $\operatorname{Inv}^{(1)}$ the subring of $\mathbb{C}[x^{(1)}]$, consisting of all SL(2)invariant polynomials in two variables $x_1^{(1)}, x_2^{(1)}$. We have $\operatorname{Inv}^{(1)} = \mathbb{C}$, and, more precisely, $\operatorname{Inv}_0^{(1)} = \mathbb{C}$, $\operatorname{Inv}_m^{(1)} = 0$ for $m \in \mathbb{N}$.

Algebraic Geometry. Let us consider the homogeneous ideal Q in the polynomial ring $\mathbb{C}[y_{ij}]$, generated by the homogeneous degree 2 polynomials

$$Q_{i_1;j_1,j_2,j_3} = y_{i_1j_1}y_{j_2j_3} - y_{i_1j_2}y_{j_1j_3} + y_{i_1j_3}y_{j_1j_2}$$
(13)

for all subsets $\{i_1, j_1, j_2, j_3\} \subset [1, n]$, consisting of four elements. Because of (10) and of the second main theorem of invariants ([11, 2. Fundamentalsatz]), the kernel of the (graded) homomorphism (11) is the homogeneous ideal Q of $\mathbb{C}[y_{ij}]$. Thus, in accord with (4), the graded ring $\operatorname{Inv}^{(n)} = \bigoplus_{m \in \mathbb{N}_+} \operatorname{Inv}_m^{(n)}$ and the graded factor-ring $C = \mathbb{C}[y_{ij}]/Q$, $C = \bigoplus_{m \in \mathbb{N}_+} C_m$, are isomorphic. In particular, for any $m \in \mathbb{N}_+$ the \mathbb{C} -linear spaces $\operatorname{Inv}_m^{(n)}$ and C_m are isomorphic.

Let us consider the finer grading of the polynomial ring $\mathbb{C}[y_{ij}]$ from (6) via graphical multidegrees:

$$\mathbb{C}[y_{ij}] \oplus_{m \in \mathbb{N}_+} \oplus_{m_1 + \dots + m_n = 2m} \mathbb{C}[y_{ij}]_{m_1, \dots, m_n}.$$

Since any polynomial $Q_{i_1;j_1,j_2,j_3} \in \mathbb{C}[y_{ij}]_2$ has graphical multidegree m_1, \ldots, m_n where $m_s = 1$ for $s \in \{i_1, j_1, j_2, j_3\}$ and $m_s = 0$ otherwise, the ideal Q is also homogeneous relative to this finer grading. Therefore the factor-ring $C = \mathbb{C}[y_{ij}]/Q$ inherits also this grading. In other words, according to (7), we can write

$$C = \bigoplus_{m \in \mathbb{N}_+} \bigoplus_{m_1 + \dots + m_n = 2m} C_{m_1,\dots,m_n}, \ C_m = \bigoplus_{m_1 + \dots + m_n = 2m} C_{m_1,\dots,m_n},$$

where C_m is the image of $\mathbb{C}[y_{ij}]_m$ and C_{m_1,\dots,m_n} is the image of $\mathbb{C}[y_{ij}]_{m_1,\dots,m_n}$ via the canonical homomorphism $\mathbb{C}[y_{ij}] \to \mathbb{C}[y_{ij}]/Q$.

Remark 1. Let X be the projective algebraic variety in the projective space $\mathbb{P}^{\binom{n}{2}-1}$, defined by the equations $Q_{i_1;j_1,j_2,j_3} = 0$ for all polynomials (13). The structure of X can

be recovered completely by the structure of its homogeneous coordinate ring C, that is, by the graded ring $\operatorname{Inv}^{(n)} = \bigoplus_{m \in \mathbb{N}_+} \operatorname{Inv}_m^{(n)}$ of $\operatorname{SL}(2)$ -invariants in $\mathbb{C}[x^{(1)}, \ldots, x^{(n)}]$.

On the other hand, let G(2, n) be the set of all planes in the \mathbb{C} -linear space C^n through the origin. There exists an one-to-one map between X and G(2, n) via which we can furnish the set G(2, n) with a structure of projective algebraic variety called *Grassmann* variety, or, *Grassmannian* for short. It turns out that G(2, n) is an irreducible smooth algebraic variety of dimension 2n - 4 with homogeneous coordinate ring $C = \bigoplus_{m \in \mathbb{N}_+} C_m$.

The dimension of the \mathbb{C} -linear space C_m , $m \in \mathbb{N}$, is evaluated as a polynomial of degree 2n-4 in one variable m with rational coefficients by W. V. D. Hodge and J. E. Littlewood (a particular case of their so called *postulation formula* which can be found, for example, in the book [7, vol. 2, Ch. XIV, ¶9]). Since C_m and $\operatorname{Inv}_m^{(n)}$ are isomorphic \mathbb{C} -linear spaces for all $m \in \mathbb{N}_+$, we obtain the following:

Theorem 2. For any $m \in \mathbb{N}$ one has

$$\dim(\operatorname{Inv}_{m}^{(n)}) = \begin{vmatrix} \binom{m+n-1}{n-1} & \binom{m+n-2}{n-1} \\ \binom{m+n-1}{n-2} & \binom{m+n-2}{n-2} \end{vmatrix}.$$

Corollary 3. If n = 2, then $\dim(\operatorname{Inv}_m^{(n)}) = 1$ for all $m \in \mathbb{N}$. **Corollary 4.** If $n \ge 3$, then

$$\dim(\operatorname{Inv}_{m}^{(n)}) = \frac{1}{(n-1)!(n-2)!}(m+1)(m+n-1)\prod_{\iota=2}^{n-2}(m+\iota)^{2}$$

for all $m \in \mathbb{N}$.

Remark 5. The author learned about the isomorphism between the graded ring $\text{Inv}^{(n)}$ of invariants of the special linear group SL(2) and the homogeneous coordinate ring C of the Grassmannian G(2, n) from the comments of V L. Popov to the Russian translation of [11] in the book [9].

3 Rumer diagrams

Let R(m) be the set of all Rumer diagrams produced by a fixed set (1) of n atoms connected with m valence bonds. Now, let us attach, in addition, to each atom $x^{(i)}$, $1 \in$ [1, n], the number $m_i, m_i \in \mathbb{N}_+$, of valence bonds connecting this atom. Given a sequence of non-negative integers m_1, \ldots, m_n , let $R(m_1, \ldots, m_n)$ be the set of all Rumer diagrams with these prescribed valences and let $\rho(m_1, \ldots, m_n)$ be their number. Let $\operatorname{Inv}_{m_1,\ldots,m_n}^{(n)}$ be the \mathbb{C} -linear subspace of $\operatorname{Inv}_m^{(n)}$ spanned by all bracket monomials corresponding to Rumer diagrams from $R(m_1, \ldots, m_n)$, where $m_1 + \cdots + m_n = 2m$. We have

$$R(m) = \bigcup_{m_1 + \dots + m_n = 2m} R(m_1, \dots, m_n)$$

— a union of pair-wise disjoint sets $R(m_1, \ldots, m_n)$, where for given m the sequence m_1, \ldots, m_n runs through all non-negative solutions of the Diophantine equation $m_1 + \cdots + m_n = 2m$.

In their paper [11], G. Rumer, E. Teller, and H. Weyl obtained the theorems below. For completeness, we present circumstantial versions of their proofs. Below we use the following notions from graph theory: For any two vertices i,j of a valence scheme G there are two *arcs* on the circle with these endpoints. We define *length* of an arc as the number of its internal non-isolated vertices plus one.

Theorem 6. The bracket monomials, corresponding to the Rumer diagrams from R(m)span the \mathbb{C} -linear space $\operatorname{Inv}_m^{(n)}$ for any $m \in \mathbb{N}_+$.

Proof: The case m = 0 is trivial. We proceed by induction on $m \in \mathbb{N}$. The case m = 1 holds because the \mathbb{C} -linear space $\operatorname{Inv}_1^{(n)}$ is spanned by the brackets p_{ij} , $1 \leq i < j \leq n$, whose valence schemes are exactly the Rumer diagrams from R(1). Now, assume that the statement is true for m - 1. Let

$$p_{i_1j_1}\dots p_{i_mj_m} \tag{14}$$

be the expression of the bracket monomial with valence scheme G and without loss of generality we can assume that one of the arcs of the edge (i, j), $i = i_1$, $j = j_1$, is (one of) the arcs of G with minimal length. In case this minimal length is 1, we represent the bracket monomial $p_{i_2j_2} \dots p_{i_mj_m} \in \operatorname{Inv}_{m-1}^{(n)}$ as a linear combination of bracket monomials in $\operatorname{Inv}_{m-1}^{(n)}$, whose valence schemes G, G', \dots are Rumer diagrams from R(m-1). Multiplying the last equality by p_{ij} , we obtain that $p_{i_1j_1} \dots p_{i_mj_m}$ is a linear combination of bracket monomials in $\operatorname{Inv}_m^{(n)}$, whose valence schemes are Rumer diagrams from R(m) because the attaching the edge (i, j) to the Rumer diagrams G, G', \dots produces Rumer diagrams. Now, let this minimal length g be at least 2 and let k be an internal non-isolated point. Since there is no edge of G, which connects k to i and k to j, the edge of G that passes through k intersects (i, j). Let ℓ be the other endpoint. We can suppose $\{k, \ell\} = \{i_2, j_2\}$ and then, using the relation (10), we obtain

$$\pm p_{i_1j_1}\dots p_{i_mj_m} = p_{ij}p_{k\ell}p_{i_3j_3}\dots p_{i_mj_m} =$$

 $p_{ik}p_{j\ell}p_{i_3j_3}\ldots p_{i_mj_m}-p_{i\ell}p_{jk}p_{i_3j_3}\ldots p_{i_mj_m}.$

Thus, the bracket monomial (14) is a linear combination of two bracket monomials such that their valence schemes have arcs with length strictly less than g. By repeating this procedure a finite number of times on the summands, we finish the proof.

In the next two theorems we permit n to assume also value 1.

Theorem 7. The dimensions $N(m_1, \ldots, m_n) = \dim \operatorname{Inv}_{m_1, \ldots, m_n}^{(n)}$ satisfies the recurrence relation

$$N(m_1, \dots, m_n, m_{n+1}) = \sum_{\mu_n} N(m_1, \dots, m_{n-1}, \mu_n),$$
$$N(m_1) = \begin{cases} 1 & \text{if} \quad m_1 = 0\\ 0 & \text{if} \quad m_1 \ge 1, \end{cases}$$

where $\mu_n \in \mathbb{N}_+$ runs through those members of the sequence $m_n + m_{n+1}, m_n + m_{n+1} - 2, \ldots, |m_n - m_{n+1}|$, such that m_n, m_{n+1}, μ_n form an even triangle, that is, $\mu_n \leq m_n + m_{n+1}, m_n \leq \mu_n + m_{n+1}, m_{n+1} \leq \mu_n + m_n$, and the sum $m_n + m_{n+1} + \mu_n$ is an even number. **Proof:** The group SL(2) acts on the polynomial ring $\mathbb{C}[x^{(1)}] = \mathbb{C}[x_1^{(1)}, x_2^{(1)}]$ via the rule (9) and for any $k \in \mathbb{N}_+$ the homogeneous components $\mathbb{C}[x^{(1)}]_k$ are stable. Therefore we obtain an action of SL(2) on any \mathbb{C} -linear space $\mathbb{C}[x^{(1)}]_k$ of dimension k + 1, or, what is the same, a representation of the group SL(2). According to, for example, [5, Sec. 2, 2.3.1], the last representation is irreducible. In particular, the group SL(2) acts trivially on $\mathbb{C}[x^{(1)}]_0 = \mathbb{C}$: $\sigma \cdot \alpha = \alpha$ for all $\alpha \in \mathbb{C}$ and the corresponding representation is the identical representation.

Given $m_1, m_2 \in \mathbb{N}_+$, in accord with Clebsch-Gordan formula (see, for example, [5, Sec. 7, 7.1.4, Ex. 2]) we have

$$\mathbb{C}[x^{(1)}]_{m_1} \otimes \mathbb{C}[x^{(1)}]_{m_2} = \bigoplus_{\mu} \mathbb{C}[x^{(1)}]_{\mu},$$

where the index $\mu \in \mathbb{N}_+$ runs through all integers $m_1 + m_2, m_1 + m_2 - 2, \ldots, |m_1 - m_2|$. In other words, m_1, m_2, μ are side lengths of a triangle and, moreover, the perimeter of this triangle is an even number (*even triangle*). We denote this symmetric ternary relation by $2 \bigtriangleup (m_1, m_2, \mu)$ and can write down for short

$$\mathbb{C}[x^{(1)}]_{m_1} \otimes \mathbb{C}[x^{(1)}]_{m_2} = \bigoplus_{2 \Delta(m_1, m_2, \mu)} \mathbb{C}[x^{(1)}]_{\mu}.$$
(15)

Note that the right hand side of decomposition (15) contains the identical representation if and only if $m_1 = m_2$, and, in this case all other summands are different from it.

Tensoring the equality (15) by $\mathbb{C}[x^{(1)}]_{m_3}$, the equality thus obtained by $\mathbb{C}[x^{(1)}]_{m_4}$, etc., we obtain inductively on n that

$$\mathbb{C}[x^{(1)}]_{m_1} \otimes \cdots \otimes \mathbb{C}[x^{(1)}]_{m_n} = \bigoplus_{\mu \ge 0} N_\mu(m_1, \dots, m_n) \mathbb{C}[x^{(1)}]_\mu$$
(16)

where $N_{\mu}(m_1, \ldots, m_n) \geq 0$ and only for a finite number of indices μ we have $N_{\mu}(m_1, \ldots, m_n) > 0$. The corresponding $\mathbb{C}[x^{(1)}]_{\mu}$ are the irreducible components of the representation $\mathbb{C}[x^{(1)}]_{m_1} \otimes \cdots \otimes \mathbb{C}[x^{(1)}]_{m_n}$ and $N_{\mu}(m_1, \ldots, m_n) > 0$ are their multiplicities.

Now let $n \ge 2$, let us write down equality (16) for n-1 and tensor it by $\mathbb{C}[x^{(1)}]_{m_n}$:

$$\mathbb{C}[x^{(1)}]_{m_1} \otimes \cdots \otimes \mathbb{C}[x^{(1)}]_{m_n} = \bigoplus_{\mu \ge 0} N_\mu(m_1, \dots, m_{n-1}) \mathbb{C}[x^{(1)}]_\mu \otimes \mathbb{C}[x^{(1)}]_{m_n}.$$
(17)

The identical representation is contained in the right hand side of (17) if and only if $\mu = m_n$, and in this case we have

$$N_{m_n}(m_1, \dots, m_{n-1}) = N_0(m_1, \dots, m_n) = N(m_1, \dots, m_n)$$
(18)

for all $n \geq 2$.

Further, let us plug the equality

$$\mathbb{C}[x^{(1)}]_{\mu} \otimes \mathbb{C}[x^{(1)}]_{m_n} = \bigoplus_{2 \triangle (\mu, m_n, \kappa)} \mathbb{C}[x^{(1)}]_{\kappa}$$

in (17):

$$\mathbb{C}[x^{(1)}]_{m_1} \otimes \cdots \otimes \mathbb{C}[x^{(1)}]_{m_n} = \bigoplus_{\nu \ge 0} N_{\nu}(m_1, \dots, m_{n-1})(\bigoplus_{2 \bigtriangleup (\nu, m_n, \kappa)} \mathbb{C}[x^{(1)}]_{\kappa}).$$

Let us fix μ and set $\kappa = \mu$. Then

$$\mathbb{C}[x^{(1)}]_{m_1} \otimes \cdots \otimes \mathbb{C}[x^{(1)}]_{m_n} = \left(\sum_{2 \triangle (\nu, m_n, \mu)} N_{\nu}(m_1, \dots, m_{n-1})\right) \mathbb{C}[x^{(1)}]_{\mu} + \bigoplus_{\nu \neq \mu} \mathbb{C}[x^{(1)}]_{\nu}.$$
(19)

Comparing the equalities (16) and (19), we have

$$N_{\mu}(m_1,\ldots,m_n)=\sum_{2\triangle(m_n,\mu,\nu)}N_{\nu}(m_1,\ldots,m_{n-1}).$$

Taking into account (18), we obtain

$$N(m_1, \dots, m_n, m_{n+1}) = \sum_{2 \triangle (m_n, m_{n+1}, \mu_n)} N(m_1, \dots, m_{n-1}, \mu_n).$$

In case n = 1 we have

$$N(m_1) = \begin{cases} 1 & \text{if} & m_1 = 0\\ 0 & \text{if} & m_1 \ge 1 \end{cases}$$

The proof is done.

Remark 8. In quantum mechanics the irreducible representation of the special linear group SL(2), given by the formula

$$\operatorname{SL}(2) \to \operatorname{GL}(\mathbb{C}[x_1, x_2]_m), \ \sigma \mapsto (f(x) \mapsto f(\sigma^{-1} \cdot x)),$$

where $f \in \mathbb{C}[x_1, x_2]_m$, $x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$, models the spin momentum $\frac{m}{2}$ of the electron configuration of an atom of valence m.

Clebsch-Gordan formula

$$\mathbb{C}[x_1, x_2]_{m_1} \otimes \mathbb{C}[x_1, x_2]_{m_2} = \bigoplus_{\mu} \mathbb{C}[x_1, x_2]_{\mu},$$

where the index $\mu \geq 0$ runs through all integers $m_1 + m_2, m_1 + m_2 - 2, \ldots, |m_1 - m_2|$, reflects the following fact from quantum theory: If the electron configuration of an atom of valence m_1 interacts with the electron configuration of an atom of valence m_2 , then the resulting spin $\frac{\mu}{2}$ can assume all values between $\frac{|m_1-m_2|}{2}$ and $\frac{m_1+m_2}{2}$.

Theorem 9. (i) The function $\rho(m_1, \ldots, m_n)$ satisfies the recurrence relation from Theorem 7.

(ii) One has $\rho(m_1, \ldots, m_n) = N(m_1, \ldots, m_n)$ for all $m_1, \ldots, m_n \in \mathbb{N}_+$.

Proof: (i) Given a valence scheme in $V(m_1, \ldots, m_n, m_{n+1})$, let $m_{n,n+1}$ be the number of valence bonds that connect n and n + 1. We construct a valence scheme in $V(m_1, \ldots, m_{n-1}, \mu_n)$, where $\mu_n = m_n + m_{n+1} - 2m_{n,n+1}$ (so $2 \bigtriangleup (m_n, m_{n+1}, \mu_n)$ holds) on the vertices $1, \ldots, a$ in the following way:

(a) Omit the valence bonds that connect n and n+1.

(b) Omit the vertex n + 1 and attach its $m_{n+1} - m_{n,n+1}$ vertices left, to the vertex n without changing their other endpoints.

Thus, we obtain a map

$$\psi: V(m_1, \ldots, m_n, m_{n+1}) \to \bigcup_{2 \triangle (m_n, m_{n+1}, \mu_n)} V(m_1, \ldots, m_{n-1}, \mu_n),$$

which turns out to be surjective.

Indeed, given a valence scheme in $V(m_1, \ldots, m_{n-1}, \mu_n)$ we can find a valence scheme in $V(m_1, \ldots, m_{n-1}, m_n, m_{n+1})$, which is mapped onto the former, in the following way:

(A) Add an additional point n + 1 to $1, \ldots, n$.

(B) Distribute the $\mu_n = m_n + m_{n+1} - 2r$ valence bonds through n where $0 \le r \le \min(m_n, m_{n+1})$ (that is, $2 \bigtriangleup (m_n, m_{n+1}, \mu_n)$) as follows: Leave $m_n - r$ in number valence bonds attached to n and attach $m_{n+1} - r$ in number valence bonds to n + 1.

(C) Add r valence bonds which connect n with n + 1.

The inverse image $\psi^{-1}(G)$ of a valence scheme $G \in V(m_1, \ldots, m_{n-1}, \mu_n)$, where $2 \bigtriangleup (m_n, m_{n+1}, \mu_n)$, contains at most $\binom{\mu_n}{m_{n+1}-r}$ valence schemes from $V(m_1, \ldots, m_n, m_{n+1})$.

Since n and n + 1 are neighbours (the arc n n + 1 has length 1), ψ maps Rumer diagrams onto Rumer diagrams (the construction in (b) does not produce intersecting edges). Now, let $G \in R(m_1, \ldots, m_{n-1}, \mu_n)$, where $2 \bigtriangleup (m_n, m_{n+1}, \mu_n)$. The intersection $\psi^{-1}(G) \cap R(m_1, \ldots, m_n, m_{n+1})$ has exactly one member which can be constructed via the distribution process from (B) as follows: Order the other endpoints of the μ_n valence bonds through n clockwise and attach the first $m_{n+1} - r$ of them to n + 1. Thus, the restriction

$$\psi \colon R(m_1,\ldots,m_n,m_{n+1}) \to \bigcup_{2 \triangle (m_n,m_{n+1},\mu_n)} R(m_1,\ldots,m_{n-1},\mu_n)$$

is a bijection, hence

$$\rho(m_1,\ldots,m_n,m_{n+1}) = \sum_{2 \triangle (m_n,m_{n+1},\mu_n)} \rho(m_1,\ldots,m_{n-1},\mu_n).$$

Moreover, we have

$$\rho(m_1) = \begin{cases} 1 & \text{if} \quad m_1 = 0\\ 0 & \text{if} \quad m_1 \in \mathbb{N}. \end{cases}$$

(ii) This follows from part (i).

Let $\rho(n, m)$ be the number of Rumer diagrams on n atoms with m valence bonds. **Theorem 10.** If $m \in \mathbb{N}$, then one has

$$\rho(n,m) = \begin{vmatrix} \binom{m+n-1}{n-1} & \binom{m+n-2}{n-1} \\ \binom{m+n-1}{n-2} & \binom{m+n-2}{n-2} \end{vmatrix}.$$

Proof: In accord with Theorem 7 and Theorem 9, we have

$$\rho(n,m) = \sum_{m_1+\dots+m_n=2m} \rho(m_1,\dots,m_n) = \sum_{m_1+\dots+m_n=2m} N(m_1,\dots,m_n) =$$
$$\sum_{m_1+\dots+m_n=2m} \dim \operatorname{Inv}_{m_1,\dots,m_n}^{(n)} = \dim \operatorname{Inv}_m^{(n)},$$

therefore

$$\rho(n,m) = \dim \operatorname{Inv}_m^{(n)} \tag{20}$$

and Theorem 2 finishes the proof.

Corollary 11. The monomials that correspond to the Rumer diagrams from R(m) form a basis for the \mathbb{C} -linear space $\operatorname{Inv}_m^{(n)}$ for any $m \in \mathbb{N}_+$. **Proof:** Because of Theorem 6, the monomials (12) that correspond to the Rumer diagrams from R(m) span the \mathbb{C} -linear space $\operatorname{Inv}_m^{(n)}$. On the other hand, (20) yields that their number is equal to the dimension of $\operatorname{Inv}_m^{(n)}$ for $m \in \mathbb{N}$. Since $\operatorname{Inv}_0^{(n)} = \mathbb{C}$ and $\rho(n, 0) = 1$, we are done.

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