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# Linear Representation of Graphs: Applications to Molecular Graphs

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We dedicate this article to the memory of our colleague Professor Ali Reza Ashrafi who died tragically. In memory of this great kindness as well as his exceptional scientific qualities.

## Abstract

In this article we build a linear representation starting from a multigraph; this allows us to give an algebraic view of the multigraph we are studying. We show that two isomorphic multigraphs give equivalent representations ; conversely two equivalent representations give isomorphic multigraphs. For the clarity of the article we give at the beginning, classical results on representations, nevertheless these are specific to our graph representation.

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# 1 Basic Definitions and Results

This article introduces a particular representation of a group which is associated with a multigraph. The main results are that two isomorphic multigraphs generate isomorphic  $R$ -modules and conversely two  $R$ -modules associated with given multigraphs give isomorphic multigraphs. Throughout this paper we are interested in multigraphs.

Let  $\mathbb{F}_2$  be the Galois field with 2 elements. For  $r \geq 1$  we fix a set  $\mathcal{E}$  of cardinality  $r$ , and denote  $\mathbb{E} = \mathbb{F}_2[\mathcal{E}]$  the  $\mathbb{F}_2$ -algebra constructed on  $\mathcal{E}$ .

This is a  $\mathbb{F}_2$ -vector space of dimension  $r$ , and an abelian group isomorphic to  $(\mathbb{Z}/2\mathbb{Z})^r$  with exponent  $u = 2$ . It is convenient to denote the addition by  $\oplus$ , and the zero element by “ $\emptyset$ ”; an element of  $\mathbb{E}$  can be written as  $a = \oplus_{e \in \mathcal{E}} a_e e$ , where  $a_e \in \mathbb{F}_2$ . The **support** of  $a$  is defined by  $\sigma(a) = \{e \mid a_e \neq 0\}$ ,

It is well known that any abelian group of exponent  $u$  is isomorphic to its dual  $X(G) = \text{Hom}(G, C_u)$ , where  $C_u$  is a cyclic group with  $u$  elements (cf [9][p. 50]). In our case,  $G = \mathbb{E}$  and  $u = 2$ . Choose  $C_2 = \{\pm 1\}$  the multiplicative group with 2 elements.

There is an explicit isomorphism between the group  $X(\mathbb{E})$ (characters) and  $\mathbb{E}$ . In an exact phrase, the mapping  $\varphi : X(\mathbb{E}) \rightarrow \mathbb{E}$  given by  $\varphi(\chi) = \oplus_{\chi(e)=-1} e$  is an isomorphism. The converse isomorphism  $\varphi^{-1}$  is given by  $\varphi^{-1}(a) = \chi_a$ , where  $\chi_a(e) = (-1)^{a_e}$  and  $a = \oplus_{e \in \mathbb{E}} a_e e$ . For all  $b = \oplus_e b_e e \in \mathbb{E}$ , we have  $\chi_a(b) = \prod_e \chi_a(e)^{b_e} = \prod_{e \in \sigma(b)} \chi_a(e) = \prod_{e \in \sigma(b)} (-1)^{a_e} :$

$$\chi_a(b) = (-1)^{|\sigma(a) \cap \sigma(b)|}. \quad (1)$$

Suppose  $G$  is a finite group and  $V$  is a finite-dimensional vector space over a field  $k$ . A **linear representation** of  $G$  on  $V$  is a group homomorphism

$$\rho : G \rightarrow GL(V)$$

$GL(V)$  is the general linear group on  $V$ . The vector space  $V$  is also called a  $k$ -representation of  $G$ ; the dimension of  $V$  is the **degree** of the representation.

Let us recall what the **group algebra**  $k[G]$  is : it is the group-algebra

with a basis  $(a_g)_{g \in G}$  such that  $a_g a_{g'} = a_{gg'}$ , if  $g, g' \in G$ . In practice,  $a_g$  is identified to  $g$ , and the elements of  $k[G]$  are written as

$$\sum_{g \in G} a_g g$$

where  $a_g \in k$ . If  $\rho$  is a representation of  $G$ , the action  $G \times V \rightarrow V$  given by  $g.v = \rho(g)(v)$  can be extended by linearity to an action of  $k[G]$ , so that  $V$  becomes a  $k[G]$ -left module. Conversely, every  $k[G]$ -module which is of finite dimension over  $k$  defines a linear representation of  $G$ . This will allow to use at will, either the  $G$ -representation language, or the  $k[G]$ -module one.

Return now to  $G = \mathbb{E}$ , and choose  $k = \mathbb{F}_p$ , where  $p$  is an odd prime ; choose also for  $C_2$  the subgroup  $\{\pm 1\}$  of  $\mathbb{F}_p^\times$ . By MASCHKE's theorem [14, p. 51], since  $p \nmid |\mathbb{E}| = 2^r$ , then every finite dimensional representation of  $\mathbb{E}$  is a sum of irreducible representations, and by [14, p. 42]  $\mathbb{F}_p$  is **good** for  $\mathbb{E}$ , that is  $p \nmid |\mathbb{E}|$  and  $X^u - 1 = 0$  has  $u$  distinct roots in  $\mathbb{F}_p$ . Here,  $u = 2$  being the exponent of  $\mathbb{E}$ . So by [14, p. 53], every irreducible  $\mathbb{F}_p$ -representation is 1-dimensional.

If  $W$  is an irreducible  $\mathbb{F}_p$ -module, then  $W = \mathbb{F}_p w$ , and its character  $\chi_W$  is a homomorphism from  $\mathbb{E}$  to  $\mathbb{F}_p^\times$ . Since  $a \oplus a = \emptyset$ ,  $\chi_W(a) = \pm 1$ . Moreover, it is easy to see that two  $\mathbb{F}_p$ -modules  $W$  and  $W'$  are isomorphic if and only if  $\chi_W = \chi_{W'}$ .

The set of all irreducible characters (characters of irreducible representations) of  $\mathbb{E}$  is denoted by  $Irr(\mathbb{E})$ .

**Lemma 1.**  $Irr(\mathbb{E}) = X(\mathbb{E})$ .

*Proof.* If  $\chi \in Irr(\mathbb{E})$  is arbitrary, then  $\chi : \mathbb{E} \rightarrow C_2 \subset \mathbb{F}_p^\times$  is a morphism. This shows that  $Irr(\mathbb{E}) \subset X(\mathbb{E})$ . Conversely, if  $\chi \in X(\mathbb{E})$ , then we define  $\rho : \mathbb{E} \rightarrow Aut_{\mathbb{F}_p} x$  by  $\rho(a)(x) = \chi(a)x$ . This gives a 1-dimensional representation whose character is  $\chi$ , and so  $Irr(\mathbb{E}) \subset X(\mathbb{E})$ . Therefore,  $Irr(\mathbb{E}) = X(\mathbb{E})$ . ■

Consequently,  $Irr(\mathbb{E})$  is completely described as  $\{\chi_a, a \in \mathbb{E}\}$  of cardinal  $|\mathbb{E}| = 2^m$ . In particular, the constant function  $\chi_\emptyset = 1$  is the character of the trivial representation.

Let  $W$  be a finite dimensional representation. According to MASCHKE'S theorem [14, p. 51],  $W$  is a sum of irreducible representations, which are 1-dimensional [14, p. 53]. They are the  $2^m$  preceding representations  $W_a = \mathbb{F}_p x_a$ , (where  $\langle x_a \rangle = W_a$ ) of characters  $\chi_a$ ; regrouping in this decomposition the isomorphic components we obtain the first canonical decomposition

$$W \simeq \bigoplus_{a \in \mathbb{E}} m_a W_a, \quad m_a \geq 0, \quad m_a \in \mathbb{N} \quad (2)$$

Here,  $m_a W_a$  is called an **isotypical** representation. We have  $\chi_W = \sum_{a \in \mathbb{E}} m_a \chi_a$ .

### 1.1 The ring $R = \mathbb{F}_p[\mathbb{E}]$

The  $\mathbb{F}_p$ -algebra  $R = \mathbb{F}_p[\mathbb{E}]$  is firstly a  $\mathbb{F}_p$ -vector space of dimension  $2^m$ , with basis  $\mathbb{E}$ . An element  $\xi \in R$  is written as  $\xi = \sum_{a \in \mathbb{E}} \lambda_a a$ ,  $\lambda_a \in \mathbb{F}_p$  and the zero of  $R$  is denoted by  $0 = \sum_{a \in \mathbb{E}} 0a$ . The (additive) law  $\oplus$  of  $\mathbb{E}$  can be extend to a "multiplication" on  $R$  by

$$\left( \sum_{a \in \mathbb{E}} \lambda_a a \right) \oplus \left( \sum_{a \in \mathbb{E}} \mu_a a \right) = \sum_{a \in \mathbb{E}} \sum_{b \in \mathbb{E}} \lambda_a \mu_b a \oplus b = \sum_{c \in \mathbb{E}} \left( \sum_{a \oplus b = c} \lambda_a \mu_b \right) c.$$

In this way  $R$  is a commutative ring with unity  $\emptyset$ ,  $(\sum \lambda_a a) \oplus \emptyset = \sum \lambda_a a \oplus \emptyset = \sum \lambda_a a$  and  $R$  is of a ring of characteristic  $p$  with  $p^{2^m}$  elements.

Each representation  $\rho : \mathbb{E} \rightarrow GL(W)$  gives the structure of  $R$ -module on  $W$  by the external law  $a.w = \rho_a(w)$  extended to  $R$  by linearity.

In particular, to the irreducible representation of character  $\chi_a$ ,  $a \in \mathbb{E}$ , corresponds the principal ideal  $(\xi_a) = \xi_a \oplus R$ , where

$$\xi_a = \sum_{u \in \mathbb{E}} \chi_a(u) u$$

indeed for each  $b \in \mathbb{E}$ ,  $\xi_a \oplus b = \sum_u \chi_a(u) u \oplus b$ ; by setting  $v = u \oplus b$ , we

have

$$\begin{aligned}\xi_a \oplus b &= \sum_u \chi_a(u)u \oplus b = \sum_v \chi_a(b \oplus v)v \\ &= \sum_v \chi_a(b)\chi_a(v)v = \chi_a(b) \sum_v \chi_a(v)v \\ &= \chi_a(b)\xi_a.\end{aligned}$$

More generally if one extends  $\chi_a$  to  $R$  defining, for  $r = \sum_{b \in \mathbb{E}} r_b b$ ,  $\chi_a(r) := \sum_b r_b \chi_a(b) \in \mathbb{F}_p$ , it is easy to see that  $\xi_a \oplus r = \chi_a(r)\xi_a$ .

Hence,  $(\xi_a) = \xi_a \oplus R = \mathbb{F}_p \xi_a$ .

*Remark.* The  $(\xi_a)$  are distinct since the  $\chi_a$  are.

This ideal is clearly minimal since  $\dim_{\mathbb{F}_p} \mathbb{F}_p \xi_a = 1$ . Note that  $a = \emptyset$  gives  $\chi_a = 1$  (constant function) so  $\xi_\emptyset = \sum_{u \in \mathbb{E}} u$  and the trivial representation corresponds to the minimal ideal  $\xi_\emptyset \oplus R$ .

Recall also the **regular representation** : it is the mapping  $\rho_{\mathbb{E}} : \mathbb{E} \rightarrow \text{Aut}R$  given by  $\rho_{\mathbb{E}}(a) = \theta_a$  such that

$$\begin{aligned}\rho_{\mathbb{E}} &: \mathbb{E} \longrightarrow \text{Aut}R \\ a &\longmapsto \theta_a : r \mapsto a \oplus r\end{aligned}$$

therefore the corresponding  $R$ -module is the ring  $R$ .

If  $r_{\mathbb{E}}$  denotes the character of  $\rho_{\mathbb{E}}$ , then, as is well-known,  $r_{\mathbb{E}}(u) = 0$  if  $u \neq \emptyset$ ; and  $r_{\mathbb{E}}(u) = 2^m$  if  $u = \emptyset$ . Moreover, each irreducible representation of  $\mathbb{E}$  appears exactly one time in  $\rho_{\mathbb{E}}$ . Then the canonical decomposition of  $\rho_{\mathbb{E}}$  gives  $R = \bigoplus_{a \in \mathbb{E}} (\xi_a \oplus R)$ . The  $\xi_a \oplus R$  are natural examples of each irreducible representation.

We obtain the second form of the canonical decomposition as

$$W \simeq \bigoplus_{a \in \mathbb{E}} m_a (\xi_a \oplus R), \quad m_a \geq 0$$

*Remark.* We have two basis of the  $\mathbb{F}_p$ -vector space  $R$  :  $\{a, a \in \mathbb{E}\}$  and  $\{\xi_a, a \in \mathbb{E}\}$ . This proves that the  $\mathbb{F}_p$ -endomorphisms  $\theta_a : r \rightarrow a \oplus r$  of  $R$  are simultaneously diagonalizable, i.e.  $\theta_a(\xi_b) = \chi_b(a)\xi_b$ .

## 2 Labelled multigraphs

### 2.1 Definitions

Let  $T$  a fixed set of labels. A  $T$ -labelled multigraph is a five-uple

$$\Gamma = (V; E; T, \varepsilon, \omega)$$

where  $\varepsilon : E \longrightarrow \mathcal{P}_2(V)$  (subsets with 1 or 2 elements), and  $\omega : V \longrightarrow T$  the “label”-function.

An isomorphism

$$\Phi : \Gamma = (V; E; T, \varepsilon, \omega) \longrightarrow \Gamma' = (V'; E'; T, \varepsilon', \omega')$$

is a couple  $\Phi = (f, f^\#)$  of bijections :  $f : V \longrightarrow V'$ ,  $f^\# : E \longrightarrow E'$  such that :

- $\varepsilon' \circ f^\# = f \circ \varepsilon$
- $\omega' \circ f = \omega$ .

We denote  $Is(\Gamma, \Gamma')$  this set of isomorphisms.

### 2.2 Labelled $m$ -multigraphs

We fix a set  $\mathcal{E}$  of cardinality  $m$ , and consider the labelled multigraphs with the same  $E = \mathcal{E}$  :  $\Gamma = \Gamma_m = (V; \mathcal{E}; T, \alpha, \omega)$  ; an isomorphism  $\Phi = (f, f^\#)$  of labelled  $m$ -multigraphs is called  **$m$ -isomorphism** when  $f^\# = Id$ :

- $\varepsilon' = f \circ \varepsilon$
- $\omega' \circ f = \omega$ .

We denote  $Is_m(\Gamma_m, \Gamma'_m)$  the corresponding set of isomorphisms.

#### Proposition 1.

- a) Every  $\Gamma = (V; E; T, \varepsilon, \omega)$  with  $|E| = m$  has  $m!$  copies  $\Gamma_m$   
 b) Let  $\Gamma = (V; E; T, \varepsilon, \omega)$ ,  $\Gamma' = (V'; E'; T, \varepsilon', \omega')$  two labelled multigraphs with  $m$  edges. The following properties are equivalent :

- i)  $\Gamma \simeq \Gamma'$ ,  
 ii) there exists two  $m$ -isomorphic copies  $\Gamma_m \simeq_m \Gamma'_m$  of  $\Gamma, \Gamma'$ .

*Proof.*

a) Let  $\sigma : E \rightarrow \mathcal{E}$  be a bijection. Define  $\Gamma_m = (V; \mathcal{E}; T, \alpha, \delta)$  by  $\alpha = \varepsilon \circ \sigma^{-1}$ , and  $\delta = \omega$ . We have  $(Id, \sigma) \in Is(\Gamma, \Gamma_m)$  since  $\alpha \circ \sigma = Id \circ \varepsilon$ , and  $\omega \circ Id = \omega$ .

b)  $i) \implies ii)$ . Let  $\Phi = (f, f^\#) \in Is(\Gamma, \Gamma')$ .

Firstly choose  $\sigma : E \rightarrow \mathcal{E}$  and define  $\Gamma_m$  like in a).

After that, define  $\alpha' = f \circ \alpha$ ,  $\omega' = \omega \circ f$ , and  $\Gamma'_m = (V'; \mathcal{E}; T, \alpha', \omega')$ . So  $(f, Id) \in Is_m(\Gamma_m, \Gamma'_m) : \alpha' = f \circ \alpha$ ,  $\omega' \circ f = \omega$ .

Finally choose  $\tau = \sigma \circ f^{\#-1} : (Id, \tau) \in Is(\Gamma', \Gamma'_m) : \alpha' \circ \tau = \alpha \circ \sigma \circ f^{\#-1} = \varepsilon \circ f^{\#-1} = \varepsilon' = Id \circ \varepsilon'$ , and  $\omega' \circ Id = \omega'$ .

The following diagramms summarize the proof

$$\begin{array}{ccccccc}
 E & \dashrightarrow & & f^\# & \dashrightarrow & & E \\
 E & \xrightarrow{\sigma} & \mathcal{E} & = & \mathcal{E} & \xleftarrow{\tau} & E' \\
 \varepsilon \downarrow & & \downarrow \alpha & & \alpha' \downarrow & & \downarrow \varepsilon' \\
 \mathcal{P}_2(V) & \xrightarrow{Id} & \mathcal{P}_2(V) & \xrightarrow{f} & \mathcal{P}_2(V') & \xleftarrow{Id} & \mathcal{P}_2(V')
 \end{array}$$

and for the labels :

$$\begin{array}{ccccccc}
 V & \xrightarrow{Id} & V & \xrightarrow{f} & V' & \xleftarrow{Id} & V' \\
 \omega & \searrow \swarrow & \omega & \searrow \swarrow & \omega' & \searrow \swarrow & \omega' \\
 & & T & & T & & T
 \end{array}$$

$i) \implies ii)$  : obvious. ■

### 3 Molecular multigraphs

A molecular graph  $\mathcal{M}$  consists of the data of a set  $V$  of vertices representing atoms  $C, H, O, N, Li, Fe, \dots$  linked together with by single or multiple edges (bonds) representing the valences  $1, 2, 3, \dots$  plus single or multiple  $l$ -loops at some vertices.

First note:

- $AT = \{C, H, O, N, \dots, U\}$ , the set of possible atoms ( $U = 238$ );



- $VA = \{0, 1, 2, \dots, N\}$ , the set of valences and sizes of the possible multi-loops ( $N = 8$  is generally suitable).

The number of vertices does not exceed 100 in practice. *Lewis' representation* shows bonds (= edges) between atoms and single dashes around certain vertices; chemists represent these dashes with loops; hence, a molecular graph  $\mathcal{M}$  is a sextuplet  $\mathcal{M} = (V; E, \omega, \varepsilon, \mathcal{A}, \mathcal{B})$  such that  $\mathcal{A} \subseteq AT$ ,  $\mathcal{B} \subseteq VA$ ,  $\omega : V \longrightarrow AT$  is a mapping and  $\varepsilon : E \longrightarrow P_2(V)$  is another mapping given by  $\varepsilon(a) = [x, y]$  with  $P_2(V)$  being the set of parts of  $V$  having 1 or 2 elements and  $x, y$  being the extremities of the edge  $a$ , (we could have  $x = y$ ), where the set  $\{e \in E \mid \varepsilon(e) = [x, y]\}$  is a  $p$ -edge,  $p \in VA$  standing for the bond between the atoms at vertices  $x, y$ .

An atom is described by several quantum numbers:

- the principal quantum number  $n = 1, 2, 3, \dots$  which counts the energy levels (these levels are the K, L, M, ... layers of the old Bohr model);
- the azimuthal or secondary quantum number  $l = 0, 1, \dots, n - 1$  which counts the number of orbitals:
  - . for  $l = 0$ , (sharp) spherical orbital  $s$ ;
  - .  $l = 1$ , hourglass-shaped (main) orbital  $p$ ;
  - . for  $l = 2$ , (diffuse) orbital  $d$ ;
  - . for  $l = 3$ , (fundamental) orbital  $f$ ;
  - . g, h, i, k, l, ...;
- the magnetic quantum number  $m_l = -l, -l + 1, \dots, 0, 1, \dots, +l$ , which counts the orientations of the orbital: these are the *boxes* of the orbital:
  - \* for  $l = 0$ ;  $m_0 = 0 \implies 1$  box for the orbital  $s$ ;
  - \* for  $l = 1$ ;  $m_1 = -1; 0; +1 \implies 3$  boxes for the orbital  $p$ ;
  - \* for  $l = 2$ ;  $m_2 = -2; -1; 0; +1; +2 \implies 5$  boxes for the orbital  $d$ ;

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\* for  $l = 3; m_3 = -3; -2; -1; 0; +1; +2; +3 \implies 7$  cells for the orbital  $f$ .

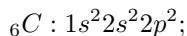
Each cell can contain 2 electrons of  $+1/2$  and  $-1/2$  spins; thus the orbital  $s$  having 1 box can contain  $2 \times 1 = 2$  electrons,  $p$  having 3 boxes can contain  $2 \times 3 = 6$  electrons, and  $d$  having 5 boxes can contain  $2 \times 5 = 10$  electrons.

A full box therefore has 2 electrons, it is a doublet; if a box has 1 electron, we say it is single. Knowing the atomic number (number of protons) we therefore have the same number of electrons, which are distributed according to the increasing levels  $1s, 2s, 2p, 3s, 3p, 3d, 4s, 4p, 4d, 4f, \dots$  respecting Hund's rule: we fill each orbital leaving the fewer empty boxes possible. Thus the orbital  $p$  has 3 boxes, which we fill in successively putting 1 electron in each box, then the  $4th$  in the first box, the  $5th$  in the second box, the  $6th$  in the last box.

We now have the electronic configuration; the electrons of the external level are the valence electrons; the valence is the number of free places on the external level. A valence of 4 means that there are 4 edges. Each doublet of the external level is represented by a loop.

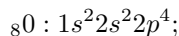
As examples, we will give the electronic configuration of Carbon, Oxygen, and Chlorine atoms.

- *Carbon*. The Carbon atom has atomic number 6 with the following electronic configuration:



4 valence electrons, valence 4, and 1 doublet at level 2. So, it has 1 loop.

- *Oxygen*. It has 8 electrons so its electronic configuration is



there are  $2 + 4 = 6$  valence electrons, its valence is 2, there is 1 doublet in the  $2s$  orbital, and 1 doublet in the  $2p$  orbital (plus 2

independent electrons). Therefore, we have 2 loops in O.

- *Chlorine.* The atomic number of Chlorine with symbol  $Cl$  is 17. It has the following electronic configuration:

$${}_{17}Cl : 1s^2 2s^2 2p^6 3s^2 3p^5;$$

7 valence electrons, valence 1, and 3 doublets at level 3. So, it has 3 loops.

We modelize now these chemical informations with the multigraph theory.

Firsly we suppose that the molecule  $\mathcal{M}$  is connected, with at least 3 vertices (in fact only the case of 2 vertices is special).

Secondly we choose  $T = AT$  for the set of labels.

For the bonds we not use of the set  $VA$ .

So we adopt the following definition : a **molecular multigraph** is a T-labelled multigraph  $\mathcal{M} = (V; E; T, \varepsilon, \omega)$ , where  $\omega : V \longrightarrow T = AT$ .

If we fix a set  $\mathcal{E}$  having m elements, we can consider the **molecular m-multigraphs**  $\mathcal{M}_m = (V; \mathcal{E}; T, \alpha, \omega)$  associated. By the Proposition 1:

**Proposition 2.**

- Every  $\mathcal{M} = (V; E; T, \varepsilon, \omega)$  with  $|E| = m$  possess  $m!$  copies  $\mathcal{M}_m$
- Let  $\mathcal{M} = (V; E; T, \varepsilon, \omega)$ ,  $\mathcal{M}' = (V'; E'; T, \varepsilon', \omega')$  be two molecular multigraphs with  $m$  edges. The following properties are equivalent :
  - $\mathcal{M} \simeq \mathcal{M}'$ ,
  - there exists two  $m$ -isomorphic copies  $\mathcal{M}_m \simeq_m \mathcal{M}'_m$  of  $\mathcal{M}, \mathcal{M}'$ .

We fix here a set  $\mathcal{E}$  having m elements, and consider the molecular m-multigraphs  $\mathcal{M}_m = (V; \mathcal{E}; T, \alpha, \omega)$  associated, particularly the  $\mathbb{F}_p$ -vector space

$$\mathbb{V}(\mathcal{M}_m) = \mathbb{F}_p[V]$$

We apply the theory of §1.1, in which we replace here the set  $\mathcal{E}$  by  $\mathcal{E} \sqcup T$ .

An element  $X \in \mathbb{E} = \mathbb{F}_2[\mathcal{E} \sqcup T]$  can be (uniquely) written

$$X = a + S, \quad a = \sum_{e \in \mathcal{E}} a_e e, \quad S = \sum_{A \in T} S_A A, \quad a_e, S_A \in \mathbb{F}_2$$

$|\mathbb{E}| = 2^r$ , where  $r = m + |T|$ .

The linked ring is  $R = \mathbb{F}_p[\mathbb{E}]$ .

We construct a representation of the group  $\mathbb{E}$  as follow. Let

$$\begin{aligned} \gamma : V &\longrightarrow \mathbb{E} \\ x &\longmapsto \omega(x) \oplus \bigoplus_{x \in \alpha(e)} e \end{aligned}$$

To the function  $\gamma$  we associate a  $\mathbb{F}_p$ -representation of  $\mathbb{E}$ :

$$\begin{aligned} \mathbb{E} &\xrightarrow{\rho} \text{Aut} \mathbb{V} \\ X &\longmapsto \rho(X) \end{aligned}$$

where the function  $\rho(X)$  is defined on the basis  $V$  of  $\mathbb{V}$  by

$$\rho(X) = \chi_{\gamma(x)}(X)x$$

and extended by linearity to  $\mathbb{V}$ ; this is correct since  $\rho(X) \circ \rho(Y) = \rho(X + Y) = \rho(Y) \circ \rho(X)$ , and  $\rho(X)^2 = Id$ .

More precisely (1) says that  $\chi_{\gamma(x)}(X) = (-1)^{|\sigma(\gamma(x)) \cap \sigma(X)|}$ , so if  $X = a + S : \sigma(X) = \sigma(a) \sqcup \sigma(S)$ , and  $\sigma(\gamma(x)) = \{\omega(x)\} \sqcup \{e : x \in \varepsilon(e)\}$ , hence  $|\sigma(\gamma(x)) \cap \sigma(x)| = \text{deg}_{\Gamma_m(a)} + |\{\omega(x)\} \cap \sigma(S)|$  and

$$\chi_{\gamma(x)}(a + S) = (-1)^{\text{deg}_{\Gamma_m(a)} x + \mu}$$

where  $\mu = 1$  if  $\omega(x) \in \sigma(S)$ ,  $= 0$  else.

Via  $\rho$ ,  $\mathbb{V}(\mathcal{M}_m)$  becomes a  $R$ -module.

We observe that  $\mathbb{V}(\mathcal{M}_m) = \bigoplus_{x \in V} \mathbb{F}_p x$ ; each  $\mathbb{F}_p x$  is an irreducible  $R$ -module, and  $X.x = \rho(X)(x) = \chi_{\gamma(x)}(X)x$ , so that the character of  $\mathbb{F}_p x$  is

$\chi_{\gamma(x)}$ , and  $\mathbb{F}_p x \simeq \xi_{\gamma(x)} \oplus R$  (cf §1.5).

**Theorem 3.** *The canonical decomposition of  $\mathbb{V}(\mathcal{M}_m)$  is*

$$\mathbb{V}(\mathcal{M}_m) \simeq \bigoplus_{x \in V} (\xi_{\gamma(x)} \oplus R)$$

*Proof.* It is sufficient to prove that  $\gamma$  is injective : let  $x \neq y$  in  $V$  ; if  $x, y$  are not adjacent, it is clear that  $\gamma(x) \neq \gamma(y)$  ; if they are,  $\mathcal{M}_m$  being connected with at least 3 vertices, there exists an adjacent vertex to  $x$  or  $y$ , say  $z$  adjacent to  $x$  :  $\varepsilon(e) = \{x, z\}$ . Therefore  $e$  is not incident to  $y$ , and hence  $\gamma(x) \neq \gamma(y)$ . ■

Resume the hypotheses :  $\mathcal{M} = (V; E; T, \varepsilon, \omega)$  is a connected T-labelled molecular multigraph with  $m$  edges and at least 3 vertices,  $\mathcal{E}$  is a fixed set of cardinality  $m$ ,  $\mathbb{E} = \mathbb{F}_2[\mathcal{E} \sqcup T]$ ,  $R$  is the ring  $\mathbb{F}_p[\mathbb{E}]$ , and  $\mathbb{V}(\mathcal{M}_m)$  the  $R$ -module defined above. In this context :

**Theorem 4.** *The following conditions are equivalent :*

- i)  $\mathcal{M} \simeq \mathcal{M}'$  as labelled multigraphs,*
- ii) there exist copies  $\mathcal{M}_m, \mathcal{M}'_m$  which are  $m$ -isomorphs,*
- iii) there exist copies  $\mathcal{M}_m, \mathcal{M}'_m$  such that  $\mathbb{V}(\mathcal{M}_m) \simeq \mathbb{V}(\mathcal{M}'_m)$  as  $R$ -modules.*

*Proof.*

*i)  $\iff$  ii) :* Proposition 2.

*ii)  $\implies$  iii) :* Let  $\Phi = (f, Id) : \mathcal{M}_m = (V; \mathcal{E}; T, \alpha, \omega) \longrightarrow \mathcal{M}'_m = (V'; \mathcal{E}; T, \alpha', \omega')$  a  $m$ -isomorphism :  $\alpha' = f \circ \alpha$ ,  $\omega' \circ f = \omega$  ;  $f$  being bijective, by the theorem 1 it is enough to prove that  $\gamma' \circ f = \gamma$  :

$\gamma(x) = \omega(x) \oplus \bigoplus_{x \in \alpha(e)} e$  and

$\gamma'(f(x)) = \omega'(f(x)) \oplus \bigoplus_{f(x) \in \alpha'(e')} e' = \omega(x) \oplus \bigoplus_{f(x) \in \alpha'(e)} e$

(the set of edges is the same!)

we have  $f(x) \in \alpha'(e) \iff f(x) \in f(\alpha(e)) \iff x \in \alpha(e)$ , so  $\gamma'(f(x)) = \gamma(x)$ .

*iii)  $\implies$  ii) :* If  $\mathbb{V}(\mathcal{M}_m) \simeq \mathbb{V}(\mathcal{M}'_m)$ , their canonical decompositions are the same

$$\bigoplus_{x \in V} (\xi_{\gamma(x)} \oplus R) = \bigoplus_{x' \in V'} (\xi_{\gamma'(x')} \oplus R)$$

For  $x \in V$  there exists an unique  $\gamma'(x')$  such that  $\xi_{\gamma(x)} = \xi_{\gamma'(x')}$ , i.e.  $\gamma(x) = \gamma'(x')$  (recall (Remark 1) that the  $\xi_a$  are distinct); so ( $\gamma'$  injective) exists unique  $x' \in V'$  such that  $\gamma'(x') = \gamma(x)$ . Define  $f(x) = x' : \gamma(x) = \gamma'(f(x))$ .

-  $f$  is bijective, since injective : if  $x \neq y$  we have  $\gamma(x) \neq \gamma(y)$ , hence  $\gamma'(f(x)) \neq \gamma'(f(y))$  and  $f(x) \neq f(y)$ .

- from  $\gamma(x) = \gamma'(f(x))$  we deduce

$$\omega(x) \oplus \bigoplus_{x \in \alpha(e)} e = \omega'(f(x)) \oplus \bigoplus_{f(x) \in \alpha'(e)} e$$

so  $\omega(x) = \omega'(f(x))$ , and  $x \in \alpha(e) \iff f(x) \in \alpha'(e) :$

-  $\alpha' = f \circ \alpha$

This achieves the proof. ■

*Remark.* Matricial interpretation of iii) : let  $n = |V|$ , and  $\varphi : V \rightarrow V'$  the R-isomorphism ; denote  $M_\varphi \in GL_n(\mathbb{F}_p)$  be the matrix of  $\varphi$  in the bases  $V, V'$ ,  $M_{\rho(X)} \in GL_n(\mathbb{F}_p)$  the matrix of multiplication by  $X$  in  $\mathbb{V}(\Gamma_m)$  in the basis  $V$  of  $\mathbb{V}(\Gamma_m)$ , and  $M_{\rho'(X)} \in GL_n(\mathbb{F}_p)$  the matrix of multiplication by  $X$  in  $\mathbb{V}(\Gamma'_m)$  in the basis  $V'$  of  $\mathbb{V}(\Gamma'_m)$ . Then for all X :  $M_\varphi M_{\rho(X)} = M_{\rho'(X)} M_\varphi$ , i.e.

$$M_\varphi M_{\rho(X)} M_\varphi^{-1} = M_{\rho'(X)}$$

**Corollary.** *Testing if  $\mathcal{M}_m, \mathcal{M}'_m$  are  $m$ -isomorphic can be done in polynomial time.*

*Proof.* The proof follows from the fact that isomorphism problem of R-modules is done in polynomial time, [3–5, 12]. ■

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