MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **90** (2023) 5–18
ISSN: 0340–6253
doi: 10.46793/match.90-1.005A

Linear Representation of Graphs: Applications to Molecular Graphs

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(Received January 1, 2023)

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.

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

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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 "ø" ; 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 $X(G) = Hom(G, C_u)$, 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 mutiplicativ 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 $\varphi : X(\mathbb{E}) \longrightarrow \mathbb{E}$ given by $\varphi(\chi) = \oplus_{\chi(e)=-1} e$ is an isomorphism. The converse isomorphism φ^{-1} is given by $\varphi^{-1}(a) = \chi_a$, where $\chi_a(e) = (-1)^{\alpha_e}$ and $a = \oplus_{e \in \mathbb{E}} a_e e$. For all $b = \oplus_e b_e e \in \mathbb{E}$, we have $\chi_a(b) = \prod_e \chi_a(e)^{b_e} = \prod_{e \in \sigma(b)} \chi_a(e) = \prod_{e \in \sigma(b)} (-1)^{a_e}$:

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

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

$$\rho \; : \; G \longrightarrow GL(V)$$

$GL(V)$ 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 reprensation.
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 ρ is a representation of G, the action $G \times V \longrightarrow V$ 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 χ_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 irrecducible 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 $\chi : \mathbb{E} \longrightarrow C_2 \subset \mathbb{F}_p^\times$ is a morphism. This shows that $Irr(\mathbb{E}) \subset X(\mathbb{E})$. Conversely, if $\chi \in X(\mathbb{E})$, then we define $\rho : \mathbb{E} \longrightarrow Aut\mathbb{F}_p x$ by $\rho(a)(x) = \chi(a)x$. This gives a 1-dimensional representation whose character is χ, 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 $< x_a >= W_a$) of characters χ_a; regrouping in this decomposition the isomorphic components we obtain the first canonical decomposition

$$W \simeq \bigoplus_{a\in\mathbb{E}} m_a W_a, \;\; m_a \geq 0, \; m_a \in \mathbb{N} \tag{2}$$

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

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

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 $\rho : \mathbb{E} \longrightarrow GL(W)$ 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 generaly if one extends χ_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 (ξ_a) are distinct since the χ_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 $\rho_{\mathbb{E}} : \mathbb{E} \longrightarrow AutR$ given by $\rho_{\mathbb{E}}(a) = \theta_a$ such that

$$\begin{array}{cccc}\rho_{\mathbb{E}} : & \mathbb{E} & \longrightarrow & AutR \\ & a & \longmapsto & \theta_a : r \mapsto a \oplus r\end{array}$$

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 $\theta_a : r \longrightarrow a \oplus r$ 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* Γ_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* Γ, Γ'.

Proof.

a) Let $\sigma : E \longrightarrow \mathcal{E}$ 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) $i) \Longrightarrow ii)$. Let $\Phi = (f, f^{\#}) \in Is(\Gamma, \Gamma')$.

Firstly choose $\sigma : E \longrightarrow \mathcal{E}$ and define Γ_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

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

and for the labels :

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

$i) \Longrightarrow ii) :$ obvious.

■

3 Molecular multigraphs

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

First note:

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

- $VA = \{0, 1, 2, ..., N\}$, 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 sixtuplet $\mathcal{M} = (V; E, \omega, \varepsilon, \mathcal{A}, \mathcal{B})$ 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 bound between the atoms at vertices x, y.

An atom is described by several quantum numbers:

- the principal quantum number n = 1, 2, 3. . . 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,. . . 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 $m_l = -l, -l+1, ..., 0, 1, ... + l$, which counts the orientations of the orbital: these are the *boxes* of the orbital:

  * for $l = 0$; $m_0 = 0 \Longrightarrow$ 1 box for the orbital s;

  * for $l = 1; m_1 = -1; 0; +1 \Longrightarrow$ 3 boxes for the orbital p;

  * for $l = 2; m_2 = -2; -1; 0; +1; +2 \Longrightarrow$ 5 boxes for the orbital d;

* for $l = 3; m_3 = -3; -2; -1; 0; +1; +2; +3 \Longrightarrow$ 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 $1s, 2s, 2p, 3s, 3p, 3d, 4s, 4p, 4d, 4f, \ldots$ 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 exemples, 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:

  $$_6C : 1s^2 2s^2 2p^2;$$

  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

  $$_8 0 : 1s^2 2s^2 2p^4;$$

  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.
a) Every $\mathcal{M} = (V; E; T, \varepsilon, \omega)$ with $|E| = m$ possess $m!$ copies $\mathcal{M}_m$
b) 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 :
i) $\mathcal{M} \simeq \mathcal{M}'$,
ii) 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, particulary 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

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

$|\mathbb{E}| = 2^r$, 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

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

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

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

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 $|\sigma(\gamma(x)) \cap \sigma(x)| = deg_{\Gamma_m(a)} + |\{\omega(x)\} \cap \sigma(S)|$ and

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

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

Via ρ, $\mathbb{V}(\mathcal{M}_m)$ 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 γ 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) $\Longleftrightarrow$ *ii)* : Proposition 2.
ii) $\Longrightarrow$ *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 $f(x) \in \alpha'(e) \Longleftrightarrow f(x) \in f(\alpha(e)) \Longleftrightarrow x \in \alpha(e)$, so $\gamma'(f(x)) = \gamma(x)$.
iii) $\Longrightarrow$ *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 ξ_a are distinct); so (γ' 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 $x \in \alpha(e) \Longleftrightarrow f(x) \in \alpha'(e)$:
- $\alpha' = f \circ \alpha$
This achieves the proof. ■

Remark. Matricial interpretation of iii) : let $n = |V|$, and $\varphi : V \longrightarrow V'$ the R-isomorphism ; denote $M_\varphi \in GL_n(\mathbb{F}_p)$ be the matrix of φ 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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