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Dyad algebra and multiplication of graphs. II. Undirected graphs

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In paper I abstract vectors $|e\rangle$, their adjoints $\langle e|$, dyads such as $|e\rangle\langle e|$, and abstract linear operators were related to graphs which are in general directed. With an Hermitian operator one gets equivalence classes of undirected graphs with or without loops and multi-lines. The present paper II gives rules for the multiplication of such graphs based on their underlying dyad algebra. The results may be used in the evaluation of the outcome of successive applications of operators for observables as in the case of the powers of a one-electron Hamiltonian in the method of moments, or in using projection operators, electron density, and the like.

1. Introduction

In paper I [1] we made correspondences between abstract vectors $\{|ei\rangle\}$, their adjoints $\{\langle ei|\}$ belonging to abstract linear vector spaces V_n and V_n^+, dyads such as $\{|ei)(ej|\} \in V_n \times V_n^+$ or abstract linear operation acting on V_n, and directed graphs $\vec{G}$. Products of di-graphs were defined related to operators expressed as objects in a dyad algebra. Such multiplication of di-graphs involved "product graphs" $\vec{\mathbb{G}}_P$, which have two kinds of lines and two types of vertices [1]. A theorem indicated how the "product vertices" and one kind of lines are contracted out from $\vec{\mathbb{G}}_P$ yielding an ordinary di-graph $\vec{G}_P$ as the result of a $\vec{G} \times \vec{G}$ multiplication.

Observables in quantum mechanics correspond to Hermitian operators, such as the one-electron Hamiltonian h, or its finite version projected out in $V_n \times V_n^+$, where V_n is the finite-dimensional valency shell subspace of the full infinite dimensional one-electron space of a molecule. It is well known from matrix based graphs [2], that symmetric matrices lead to undirected or line graphs. With a dyad algebra based formulation [3,4], Hermitian operators lead to equivalence classes of undirected graphs, such as the VIFs "valency interaction formulae" of molecules, transformable within each class by pictorial VIF-rules derived from covariance principles [3–5].

The present paper (II) extends the algorithms for multiplying graphs based on their underlying dyad algebra, to undirected graphs G which in turn may be used in evaluating the outcome of successive application of operators of observables, powers or functions of Hermitian operators, powers of h (as in the method or moments [6,7]) or electron density d, projection operators on h, d, and the like.

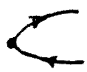
2. Definitions, dyad algebra-graph identifications

An undirected graph G is a collection of n vertices and ρ lines.

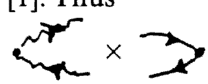
A vertex $(\bullet i)$ corresponds to the sum of a vector $|ei\rangle \in V_n$ and its adjoint $\langle ei| \in V_n^+$, or a superposition of a (directed) out-vertex (i •→–) and an in-vertex (i •←–) [1],

$$i\bullet \sim |ei\rangle + \langle ei|\,. \tag{1}$$

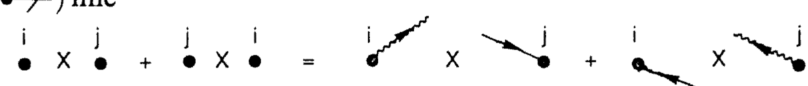
Thus vertex $(i\bullet)$ is shown in more detail as

$i\bullet \sim i$  . (2)

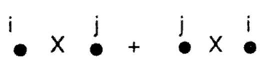
A line in G, (i •—• j) is a product of two vertices like eq. (2) multiplication being done with the left factor indicated by wiggle lines (〰〰) and the right factor by ordinary lines (——), product order being always from wiggle to ordinary lines as discussed in ref. [1]. Thus

$\bullet i \times j\bullet = i$  j, (3)

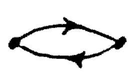
where only the terms from eqs. (1)–(3) survive if there is a net flow from a (〰>〰) to a (•→–) line

 (4)

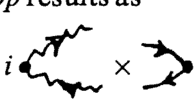
corresponding to

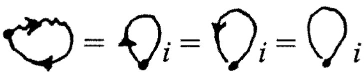
 $\sim |e_i\rangle\langle e_j| + |e_j\rangle\langle e_i|\,.$ (5)

Thus

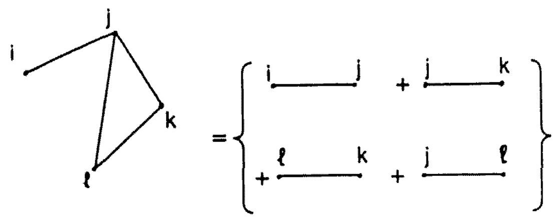
$i_\bullet \times j_\bullet = i$  $j = i$  $j\,.$ (6)

A *loop* results as

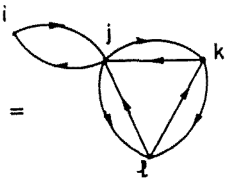
i  $i \sim [|e_i\rangle + \langle e_i|] \times [|ei\rangle + \langle ei|]$ (7)

i  $_i \sim |e_i\rangle\langle e_i|\,.$

A no-loop standard (*std*) *graph* G is a superposition of lines and corresponds to a sum of symmetrized dyads A_{ij},

$G =$  (8)

or

$G =$  $\sim A_{ij} + A_{jk} + A_{lk} + A_{jl}$,

where, e.g.,

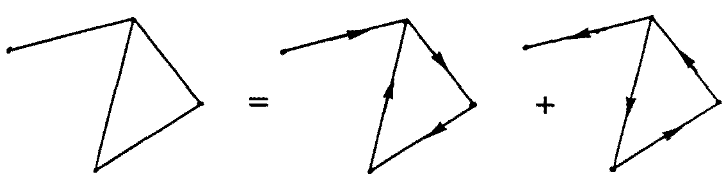
$$A_{ij} = B_{ij} + B_{ij} \tag{9}$$

with $B_{ij} = |e_i\rangle\langle e_j| \sim (i \bullet\!\!\rightarrow\!\!- j)$,
or

$$A_{ij} = [|e_i\rangle, \langle e_j|]_+ = |ei\rangle\langle ej| + |ej\rangle\langle ei|\,, \tag{10}$$

the anti-commutator $[\ ,\ ]_+$ of a vector with its adjoint.

A graph G_n on n vertices with no loops is the sum of any of its directed $\vec{G}_n$ and that $\vec{G}_n$'s reverse $\overleftarrow{G}_n$. The $\overleftarrow{G}_n$ is the $\vec{G}_n$ with all line directions reversed, e.g.,

 (11)

as seen from eq. (8).

If there are loops it is simplest to leave them on either $\vec{G}$ or its $\overleftarrow{G}$ since a directed and undirected loop are the same, eq. (7).

LEMMA 1

A graph G_n on n vertices with ρ lines has 2^ρ directed G_n's. Therefore G_n can be drawn in $2^{\rho-1}$ ways as $\vec{G}_n + \overleftarrow{G}_n$.

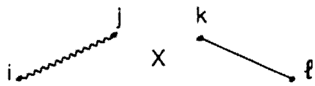
Proof

Each line in G_n can be drawn with one or the other direction, thus giving 2^ρ distinct $\vec{G}_n$. Each $\vec{G}_n$ has its unique reverse $\overleftarrow{G}_n$ with all lines reversed. Thus there are $2^\rho/2$ distinct ways to write $\vec{G}_n + \overleftarrow{G}_n$.

3. Product of two lines

As in ref. [1], in a product $G_C \times G_D$ we shall write the left factor with wiggle lines, the right with ordinary lines. Product is defined always from wiggle to ordinary lines.

With two lines $(ij) \times (kl)$ we have



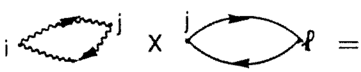
$= 0 \quad \text{if} \quad i,j \neq k,l\,.$ (12)

LEMMA 2

(13)

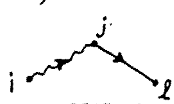
Proof

The product is



(14a)

As in ref. [1] a preliminary product graph $\mathbb{G}_P$ is obtained by superposing the two factors, resulting in a graph of two kinds of lines and two types of vertices (cf. ref. [1]). Only net flows from wiggle to ordinary lines at a vertex yield non-zero terms. Thus eq. (14a) becomes

$(ij) \times (jl) =$  only. (14b)

Then by the theorem of [1], the common vertex (i) contracts out yielding

$(ij) \times (jl) = i$  l (14c)

(This proof can be done alternatively with the dyads algebraically

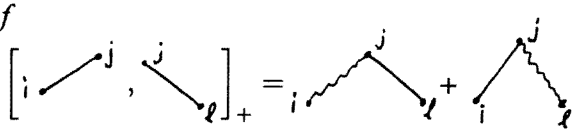
$B_{ij}B_{jl} = B_{il}\,.)$ (14d)

Since the other terms in eq. (14a) give zero, we have also $A_{ij}A_{jl} = B_{il}$.

LEMMA 3

The anti-commutator of two lines having one vertex label in common contracts out that common vertex and yields a single (undirected) line.

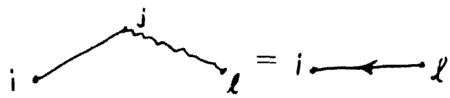
Proof



(15a)

but by eqs. (14)

and



(15b)

with their sum being (*i* •——•*l*).

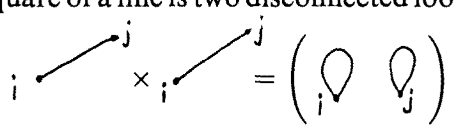
(Or with dyads:

$$[A_{ij}, A_{jl}]_+ = A_{il})$$ (15c)

4. Square of a line

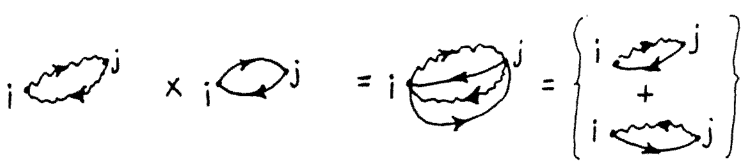
LEMMA 4

The square of a line is two disconnected loops.



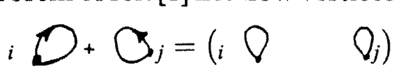
(16a)

Proof



(16b)

and by the theorem of ref. [1] net flow vertices are contracted out. Thus

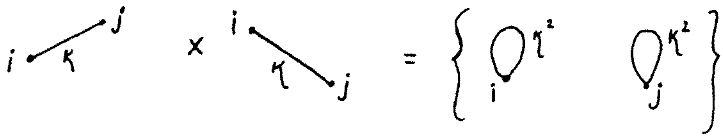
(16b) =  . (16c)

(Algebraically:

$$A_{ij}^2 = A_{ij}A_{ij} = A_{ij}A_{ji} = A_{ji}A_{ij}$$
$$A_{ij}^2 = A_{ii} + A_{jj} \,.)$$

COROLLARY

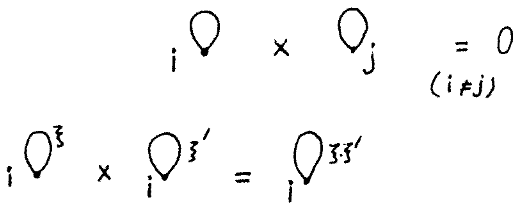
If there are non-standard (non-unity) strengths $\{\kappa \neq 1\}$ on the lines, we get



loops each with strength κ^2.

5. Products involving lines and loops

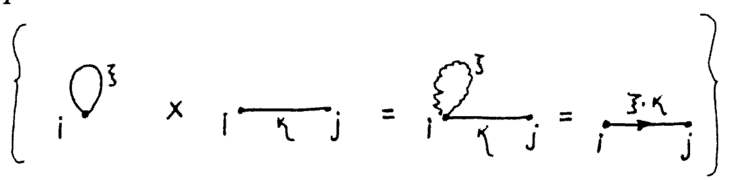
Two loops:



(17)

where ξ, ξ' are strengths $\neq 0$.

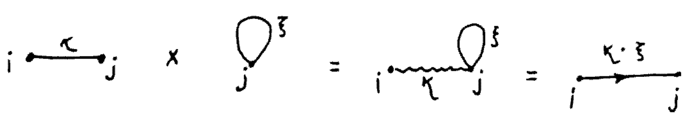
Loop × line:



(18)

(direction of final line is away from the wiggle line).

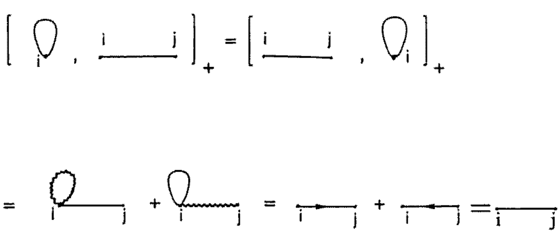
Line and loop:



(19)

(direction is away from the wiggle line).

6. Anti-commutator of line and loop



(20)

(from eqs. (18), (19) or algebraically).

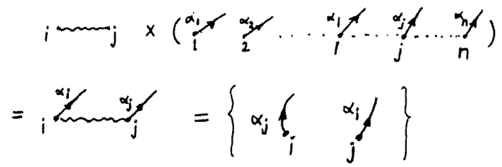
Line and free vertices

If an operator A_{ij} is acting on a vector $|u\rangle \in V_n$,

$$|u\rangle = \alpha_1|e_1\rangle + \alpha_2|e_2\rangle + \ldots \alpha + |e_n\rangle\,,$$

$$A_{ij}|u\rangle = A_{ji}|u\rangle = \alpha_j|e_i\rangle + \alpha_i|e_j\rangle\,. \tag{21a}$$

Or:

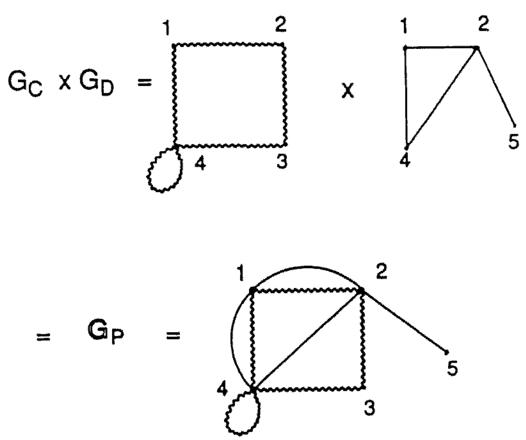


(21b)

using eq. (14), vertex contraction on each vertex.

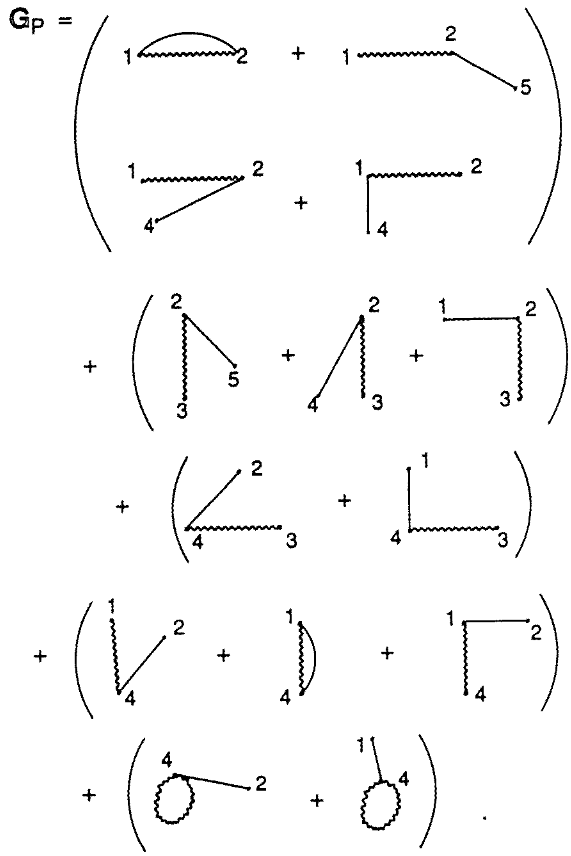
7. Product of two graphs

To calculate $G_P = G_C \times G_D$, where the factors may or may not have loops, draw the left factor with wiggle lines, than superimpose G_C and G_D to get the composite pre-product $\mathbb{G}_P$, a graph of two kinds of lines and two types of vertices as in ref. [1]. For example,



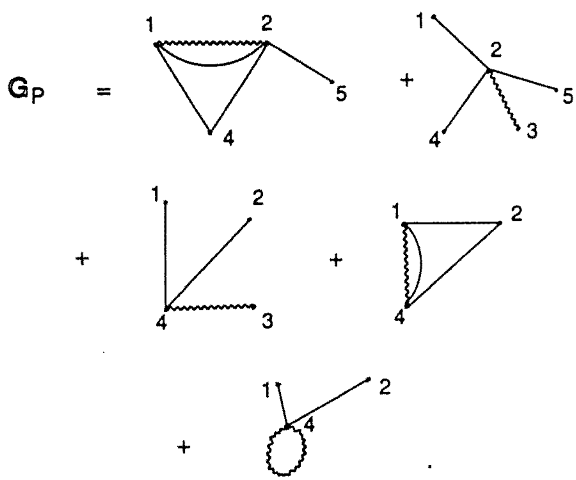
(22)

The only non-zero terms in $\mathbb{G}_P$ result when we go *from* a wiggle line *to* adjacent ordinary lines. Thus



(23)

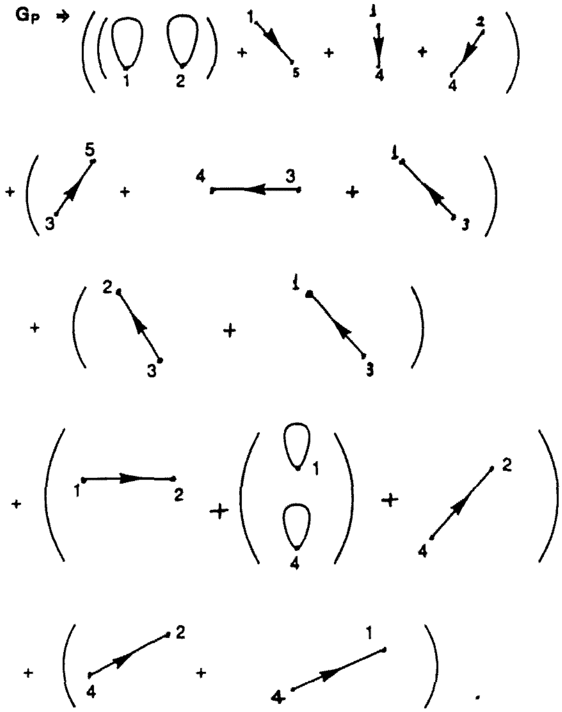
Each ( )-block in eq. (23) is for one wiggle line out of the G_C. There are five such lines in G_C, hence five blocks, each block showing its wiggle lines connected to its ordinary lines; more compactly the blocks in G_P are



(23′)

Using the vertex contractions as in the previous sections, in each term of eqs. (23), (23′) we get

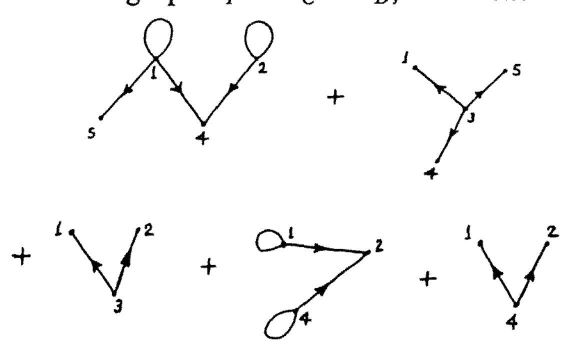
$\mathrm{G_P} \to$



(24)

Or G_P going into the contracted graph $G_P = G_C \times G_D$, first in each block:

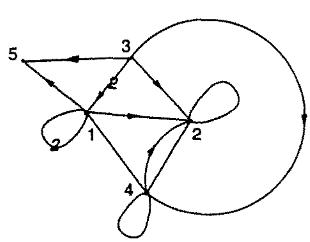
$\mathbb{G}_\mathrm{P} \to \mathrm{G_P} =$



(24′)

Adding up eq. (24′)

$\mathbb{G}_\mathrm{P} =$

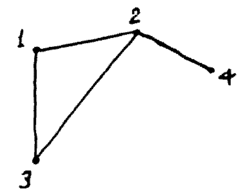


Note that $(\vec{31})$ lines superimposed gave a strength of 2 (written on the line), two loops of std strength=1 at each at vertex 1 gave a loop of strength = 2, and opposite di-lines at (14) gave an undirected line (14), and similarly at (24) which, however, has also a di-line.

8. Another example – square of a graph

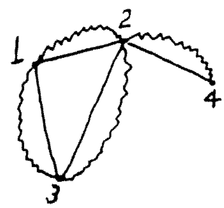
Let

G =



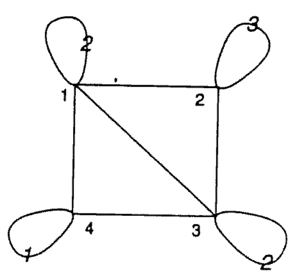
corresponding, e.g., to a one-electron Hamiltonian h. Calculate h^2.

$G^2 = G \times G = \mathbb{G}_P =$



Done as in the previous example, we get

$G_P \rightarrow G_P =$



(26)

All lines are undirected as expected from both h and therefore h^2 being Hermitian. The loops have strengths equal to the degrees ("star-value") of respective vertices in G.

Trace of a graph is given by the sum of the strengths of its loops (cf. e.g. ref. [1]). Thus for $h \sim G$, the trace of $h^2 \sim G^2 = G_P$ is

$$\mathrm{Tr}\, h^2 = \sum_{G^2} \xi_i = 2 + 3 + 2 + 1 = 8$$

which agrees with the theorem (refs. [2,6,7]) and references therein] that $\mathrm{Tr}\, h^2 = 2\rho$, where ρ is the number of lines in the unsquared $G \sim h$.

For multiple products, e.g., $G_P = G_C \times G_D \times G_F$ it is best to do the last two factors first and reduce their $\mathbb{G}'_P \rightarrow G'_P = G_D \times G_F$, then multiply the resulting $G_C \times G_{P'} = G_P$.

References

[1] O. Sinanoğlu, J. Math. Chem. 14 (1993) 185.

[2] D.M. Cvetković, M. Doob and H. Sachs, *Spectra of Graphs* (Academic Press, New York, 1980).

[3] O. Sinanoğlu, Theor. Chim. Acta 65 (1984) 233, 243, 249, 255, 261.

[4] O. Sinanoğlu, in: *Chemical Applications of Topology and Graph Theory*, ed. R.B. King (Elsevier, Amsterdam, 1983) pp. 57–74.

[5] O. Sinanoğlu, Chem. Phys. Lett. 103 (1984) 315; Int. J. Quant. Chem. 36 (1989) 545; Tetrahedron Lett. 29 (1988) 889.

[6] J.K. Burdett and S. Lee, J. Am. Chem. Soc. 107 (1985) 3050.

[7] D. Bonchev, O. Mekenyan and O.E. Polansky, in: *Graph Theory and Topology in Chemistry*, eds. R.B. King and D.H. Rouvray (Elsevier, Amsterdam, 1987) p. 209.