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High order graph formalism for multilayer structures

H. Kamal [a,b,*], E. Bernabeu [a]

[a] Optics Department, Faculty of Physics, Universidad Complutense de Madrid, Ciudad Universitaria, E-28040 Madrid, Spain
[b] Department of Physics, Faculty of Science, Ain Shams University, Cairo, Egypt

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ABSTRACT

Thin-film calculations are an important task during optical design. A new didactic and simple methodology based on flow graph theory is introduced in this article. It is proposed as an alternative way to matrix calculations as well as it is considered to be a new tool to solve lengthy graphical maps. It turned out that, this technique simplifies and reduces the calculus above all, if the impact of certain design parameter upon others is of our interest. However, the method is applied to solve multilayer dielectric structures. Furthermore, as an example to demonstrate the utility of the method, the complex refractive index of the rear surface corresponding to a 3-layer dielectric system is obtained.

1. Introduction

Multilayer optical coatings are structures of one or more layers of several thin films [1]. They are employed in many fields in optical science as well as industrial optical techniques [2]. They can be found in almost every optical device. The features of optical coatings cover high-reflectivity, spectral filtering, anti-reflectivity and beam splitting. Optical surfaces with desired reflectance, transmittance and absorption coefficients are produced by means of thin film coating [3]. Refractive indices of the film and surrounding regions, the film thickness, and the viewing angle are crucial in thin film properties. At present, in order to receive the best optical results one needs to be aware of all aspects of design and production. In this article, a new calculation methodology based on graph formalism [4] is extended to include multilayer structures so as to guarantee optimum design results.

The plan of this work is as follows: Section 2 is devoted to give a brief overview on flow-graph algebra and the basic reduction rules, followed by a résumé of Path-ordinal calculation method for high-order graph compositions. In Section 3, the path-ordinal method is applied to a multilayer structure and a general formalism is obtained. Finally in Section 4, as an example, the new high-order graph formalism is employed to calculate the complex refractive index of the rear surface corresponding to a 3-layer structure.

2. High order graphs formalism

Matrix formalism is commonly used to analyze the behavior of multilayer structures [1,6,9]. Unfortunately, matrices of high order or long composition of matrices are rather complicated to be used due to the lengthily mathematical operations. However, the extension of the graph theory to manage problems of linear algebra provides an alternative tool that simplifies the treatment of certain kind of problems [5].

Flow graphs are a graphical language for causality of linear equations. They are geometrical structures of tiny circles and lines. The circles in a graph represent variables while the line connecting two circles gives the relation between them. White and black colours of the nodes show their orientation, which is analogous to the side of the equality where they are located in traditional algebra. The black nodes represent "sources", namely the input variables one has to deal with to obtain the output variables called "sinks", which are indicated by white nodes. The line connecting two nodes is called "branch", it indicates that there exist a relation between these two nodes. The label of the branch is termed "transmittance", it gives the relation between the interconnected two variables. Furthermore, following the usual agreement, if it is not specified any value for a branch, it will be understood that it has the value 1. Branches with transmittance zero are not drawn. Fig. 1 shows some flow graph representation of linear equations.

* Corresponding author at: Universidad Complutense de Madrid, Ciudad Universitaria, Optics Department, Faculty of physics, AV Complutense Facultad De Ciencias, 28040, E-28040 Madrid, Spain. Tel.: +34 657299873.
E-mail addresses: hkamal@ucm.es, h_k_abdelhady@hotmail.com (H. Kamal).

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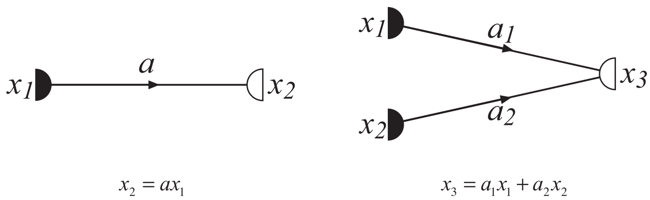

Fig. 1. Two examples of linear equations and their corresponding graphs.

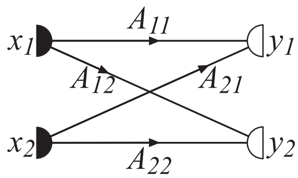

Fig. 2. A second order graph representing Eq. (2.1). The homologues of the vector parameters are the nodes and the homologues of the 2×2 matrix elements are the branches transmittance.

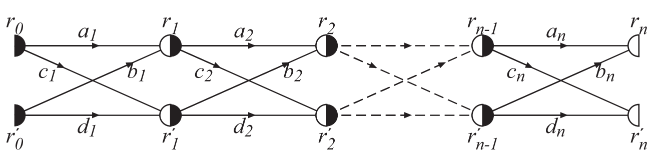

Fig. 3. A cascade graph composed of n graphs each of order two, attached side by side. Each individual graph represents a 2×2 matrix.

As flow graphs express linear equations, similarly, it is also possible to express with graphs a linear expression between two vectors (the vector is regarded as column matrix). Considering the algebraic relation between the two dimensional vectors of Eq. (2.1), the second order graph of Fig. 2 is obtained.

$$\begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} A_{11} & A_{21} \\ A_{12} & A_{22} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \tag{2.1}$$

Now we introduce some criteria so as to describe graphs. The *order of a graph* is defined as the smallest number of sources or sinks forming such graph. Also, we define a *cascade graph* as a graphical composition of several graphs of the same order. A $m \times n$ cascade graph is referred to a graph composed of n graphs each of order m.

Many problems in physics imply multiplication of matrices of the same order which are solved through its alternative graphical representation. Fig. 3 represents a composition of n graph each of order two, the result is $2 \times n$ cascade graph,

which is equivalent to the matrix expression,

$$\begin{pmatrix} r_n \\ r'_n \end{pmatrix} = \begin{pmatrix} a_n & b_n \\ c_n & d_n \end{pmatrix} \cdots \begin{pmatrix} a_2 & b_2 \\ c_2 & d_2 \end{pmatrix} \begin{pmatrix} a_1 & b_1 \\ c_1 & d_1 \end{pmatrix} \begin{pmatrix} r_0 \\ r'_0 \end{pmatrix} \tag{2.2}$$

When a cascade flow graph has been formed, there exist two conventional ways to get the result of the graph. First, by the flow graph algebra technique and second, by Mason's rule [8]. By means of the five basic algebraic rules namely: addition, product, transmission, suck up node and self-loop elimination rules an equivalent simpler graph is obtained. Mason's rule is recommended when we are only interested in one of the output variables as a function of one of the input variables.

In this article we apply an alternative method characterized by the ordinal of the path [4]. Both the equivalent matrix as well as the residual graph of the whole system can be obtained directly from the individual element matrix of the system cascade graph. Also, the impact of certain input parameters of the problem on others could be obtained easily without solving the whole graph.

Consider a $m \times n$ cascade graph of Fig. 4, the input variables are the vector

$$\vec{x}_0 = (x_{01}, x_{02}, x_{03}, \ldots, x_{0k}, \ldots, x_{0m}),$$

While the output variables are represented by the vector

$$\vec{x}_n = (x_{n1}, x_{n2}, x_{n3}, \ldots, x_{nk}, \ldots, x_{nm}).$$

The total number of possible paths connecting the input nodes to the output ones is,

$$N_{m,n} = m^{n+1}.$$

If "i" is defined as the "path-ordinal", then for any arbitrary path $(1 \le i \le N_{m,n})$ connecting any node of the input vector with other in the output vector. There exist a characteristic "path-set" $\{\theta_{ij}\}$ that defines the trajectory of the path along the graph.

$$\{\theta_{ij}\} = \{\theta_{i0}, \theta_{i1}, \theta_{i2}, \ldots, \theta_{in}\},$$

where θ_{ij} can take any of the values, $1 \le \theta_{ij} \le m$. If $\theta_{ij} = k$, this means that the path number "i" passes through the kth node of the jth vector, x_{jk}.

According to flow graph algebra, any possible path P_i starting from a node in the input vector and ending in an output-vector-node has a "path-value" which can be considered as the product of the transmittances corresponding to each branch along the path,

$$P_i = \prod_{j=1}^{n} A_{ij}\left(\theta_{i(j-1)}, \theta_{ij}\right), \tag{2.3}$$

where A_{ij} is considered to be the transmittance of the branch in the jth graph within the path "i".

Defining a path sequence, all the paths "i" that starts from the node x_{0k} have the ordinal $i = k, k+m, k+2m, \ldots, k+nm$. Corresponding to P^{k+nm} where $1 \le k \le m$ for every $n = 0, 1, \ldots, m-1$.

As the output vector $\to x_n$ is composed of m outgoing nodes, therefore the total number of paths $N_{m,n}$ is divided into m groups each has m^n paths. The first group ends at the node x_{n1} corresponding to the ordinals $(1 \le i \le m^n)$ and the second group ends at the node x_{n2} $(1 + m^n \le i \le 2m^n)$. The paths that end at the node x_{nL} have the path ordinals within the range $(1 + (L-1)m^n \le i \le Lm^n)$.

For $m \times n$ cascade graph, there are m^{n-1} paths connecting an output node with an input one. According to the path sequence, the paths that start from an input node x_{0k} and ends at an output node x_{nL}, have the path ordinals $i = k + (L-1)m^n, k + m + (L-1)m^n, \ldots, k - m + Lm^n$. The contribution of the source x_{0k} to the sink x_{nL}, can be expressed as,

$$x_{nL} = \sum_{k=1}^{m} T^{kL} x_{0k},$$

where T^{kL} is the summation of the product of all the possible paths from k to L.

$$T^{kL} = \sum_{r=1}^{m^{n-1}} P^{kL}_{k-m+(L-1)m^n+rm}. \tag{2.4}$$

An example of the path-set and its corresponding path-value are illustrated in Fig. 5.