CORRESPONDENCE BETWEEN CONTINUOUS AND DISCRETE 2-FLUX MODELS FOR REFLECTANCE AND TRANSMITTANCE OF DIFFUSING LAYERS

by

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ABSTRACT

This article provides a theoretical junction between two different mathematical models dedicated to the reflectance and the transmittance of diffusing layers. The Kubelka-Munk model proposes a continuous description of scattering and absorption for two opposite diffuse fluxes in a homogenous layer (continuous 2-flux model). On the other hand, Kubelka's layering model describes the multiple reflections and transmissions of light taking place between various superposed diffusing layers (discrete 2-flux model). The compatibility of these two models is shown. In particular, the Kubelka-Munk reflectance and transmittance expressions are retrieved, using Kubelka's layering model, with mathematical arguments using infinitely thin sublayers. A new approach to Kubelka-Munk expressions is thus obtained, giving, moreover, a kind of physical interpretation of the Kubelka-Munk theory.

INTRODUCTION

Modelization is an essential part of scientific activity. Rather often, the mathematical apparatus of a model can be as important as, for example, the physical properties it sustains. Indeed, the core of the mathematical part can convey by itself a large part of the general meaning of the model. Such will be the case, in this article, for the exponential of a matrix, that gives a key for understanding the relationship beetween continuous and discrete 2-flux models, a role that has not been noticed till now.

The continuous 2-flux model is issued from the well-known Kubelka–Munk theory, introduced by their authors in (Kubelka-Munk, 1931) and (Kubelka, 1948) and used in an extremely wide range of applications. The discrete 2-flux model was introduced by (Kubelka, 1954). Both continuous and discrete 2-flux models describe the evolution of two oppositely directed light fluxes, assumed perfectly diffused, as functions of their depth within the diffusing medium. They indirectly encapsulate into equations the three complementary phenomena taking place in elementary layers of the medium, i.e. reflection (also called backscattering), transmission and/or absorption. Their main difference lies in the assumptions made on the diffusing medium. The continuous model requires a homogeneous scattering medium, i.e. with same scattering and absorption properties whatever the depth. Selecting an infinitesimally thin sublayer located at an arbitrary depth, the variation of the upward flux and of the downward flux is described by the famous Kubelka-Munk differential equation system (3). The solutions of this system are analytical expressions for the reflectance and the transmittance of a layer as functions of its thickness. In the discrete model, the medium is assimilated to superposed diffusing layers, without concern about their thickness or their homogeneity in depth. The superposed layers may be different, with their own reflectance and transmittance at their upper and lower sides. The upward and the downward fluxes are determined by an analysis of the multiple reflections and transmissions taking place between the layers. Therefore, choosing between Kubelka-Munk and Kubelka models fundamentally depends on the nature of the considered specimen. Due to their simplicity, the 2-flux models should be restricted to highly scattering media (Vargas, 1997). Moreover, since they describe the variation of fluxes along a single depth axis, they ignore the lateral propagation of light into the medium and thereby underestimate absorption. Various attempts have been made recently to improve the Kubalka-Munk model with lateral propagation of light. They rely on extended continuous models (Mourad et al, 2002), (Yang, 2004) and/or use discrete approaches such as random walks (Vöge–Simon, 2007), Markov chains (Hébert–Hersch–Becker, 2007), etc. In this context, studying the interconnection of the classical 2-flux models may be helpful.

Our study is concentrated on homogeneous diffusing layers, satisfying the applicability conditions of both the Kubelka-Munk and the Kubelka models. On the one side, the Kubelka-Munk model gives directly analytical expressions for the layers reflectance and transmittance, being given the scattering and absorption coefficients. On the other side, there exists a relationship between these scattering and absorption coefficients and the reflectance and transmittance of infinitely thin sublayers. Then, a thick layer is modeled as a pile of these sublayers. Its reflectance and transmittance are given by Kubelka's model. Our aim is to show that they are identical to those given by the Kubelka-Munk model. For this purpose, a new matrix formalism will be introduced.

The present paper is structured as follows. The Kubelka-Munk model and the Kubelka model are first recalled in Sections 2 and 3 respectively. Then, the equations characterizing the decomposition of a layer into sublayers (Section 4) are developed; it is then shown how the Kubelka-Munk expressions for reflectance and transmittance may be derived from the Kubelka model (Section 5). Section 6 deals specifically with reflectance, for which the Kubelka-Munk expressions may be obtained using continued fractions. As a matter of conclusion, in Section 7, the proposed mathematical developments are given a physical interpretation.

THE KUBELKA-MUNK MODEL

Let us consider a homogenous layer with thickness h characterized by its absorption coefficient K and its scattering coefficient S. In this layer, the diffuse irradiance propagates upward and the diffuse irradiance propagates downward. Both i_r and i_t are functions of their depth x in the layer. Depth 0 corresponds to the layer's boundary receiving the incident irradiance I_0. Depth h indicates the other boundary. We consider, at an arbitrary depth x, a sublayer with infinitesimal thickness dx (see Fig. 1). It receives the downward irradiance $i_t(x)$ on one side and the upward irradiance $i_r(x+dx)$ on the other side. In the sublayer, at position x, a fraction Sdx from both irradiances $i_r(x)$ and $i_t(x)$ is backscattered, leading to an exchange of light, and a fraction Kdx is absorbed. ← *insert Fig. 1*

While crossing the sublayer, the upward irradiance $i_r(x+dx)$ loses both the absorbed irradiance $Ki_r(x)\,dx$ and the backscattered irradiance $Si_r(x)\,dx$ and gains the backscattered irradiance $Si_r(x)\,dx$. The irradiance $i_r(x)$ leaving the sublayer is therefore

$$i_r(x) = i_r(x+dx) - (K+S)\,i_r(x)\,dx + S\,i_t(x)\,dx \tag{1}$$

Similarly, the downward irradiance $i_t(x)$ loses the absorbed irradiance $Ki_t(x)dx$ and the backscattered irradiance $Si_t(x)$, and gains the backscattered irradiance $Si_t(x)$. The irradiance $Si_t(x+dx)$ leaving the sublayer is

$$i_t(x+dx) = i_t(x) - (K+S)\,i_t(x)\,dx + Si_r(x)\,dx. \tag{2}$$

The Kubelka-Munk differential equation system (Kubelka–Munk, 1931), (Kubelka, 1948) is obtained by a rearrangement of Eqs. (1) and (2)

$$\begin{cases} \dfrac{d}{dx} i_r(x) = (K+S)\,i_r(x) - S\,i_t(x) \\ \dfrac{d}{dx} i_t(x) = Si_r(x) - (K+S)\,i_t(x) \end{cases} \tag{3}$$

The solutions $i_r(x)$ and $i_t(x)$ of (3) can be easily determined using Laplace Transform (Hébert–Hersch, 2006), (Hébert, 2006). Another solving method, introduced by (Emmel, 1998), (Emmel-Hersch, 1999), uses a matrix representation $\frac{d}{dx}\mathbf{V} = \Omega\mathbf{V}$ for (3) and a matrix exponential for expressing $\mathbf{V} = exp(x\Omega).\mathbf{V_0}$.

The reflectance $r(h)$ of a layer with thickness h, corresponding to the ratio $i_r(0)/I_0$ of incident light emerging at depth 0 is (Kubelka, 1948)

$$r(h) = \frac{\sinh(bSh)}{b\cosh(bSh) + a\sinh(bSh)} \tag{4}$$

with

$$a = \frac{K+S}{S} \quad \text{and} \quad b = \sqrt{a^2 - 1} \tag{5}$$

The transmittance of a layer with thickness h corresponding to the ratio $i_t(h)/I_0$ of incident light emerging at depth h, is (Kubelka, 1948)

$$t(h) = \frac{b}{b\cosh(bSh) + a\sinh(bSh)} \tag{6}$$

KUBELKA'S LAYERING MODEL

When several layers with identical refractive indices are superposed, their global reflectance and transmittance can be computed according to Kubelka's layering model (Kubelka, 1954) and expressed as functions of the individual layers' reflectances and transmittances. Let us consider a "bilayer", formed by two layers with upper reflectance R_1, resp. R_2, with lower reflectance R'_1, resp. R'_2, with upper transmittance T_1, resp. T_2, and with lower transmittance T'_1, resp. T'_2. Fig. 2 shows the multiple reflection-transmission of light within the bilayer for a top illumination. Summing the different fractions of light emerging at the upper side, we obtain a geometric series expressing the bilayer's global reflectance

$$R = R_1 + T_1R_2T'_1 + T_1R_2R'_1R_2T'_1 + T_1R_2\left(R'_1R_2\right)^2T'_1 + \ldots = R_1 + T_1T'_1R_2\frac{1}{1-R'_1R_2} \tag{7}$$

The fractions of light emerging at the lower side also form a geometric series, expressing the bilayer's global transmittance

$$T = T_1T_2 + T_1R_2R'_1T_2 + T_1\left(R_2R'_1\right)^2T_2 + ... = T_1T_2\frac{1}{1-R'_1R_2} \tag{8}$$

← *insert Fig. 2*

Each layer may be represented by a 4×4 matrix, called a *layering matrix*, where the upper and lower reflectances and transmittances are arranged as follows

$$\mathbf{M}_k = \left(\begin{array}{cc|cc} 1 & -R'_k & 0 & 0 \\ R_k & A_k & 0 & 0 \\ \hline 0 & 0 & T_k & 0 \\ 0 & 0 & 0 & T'_k \end{array}\right) \tag{9}$$

with $A_k = T_kT'_k - R_kR'_k$. The top-leftmost term of the layering matrix is called the *weight* of the layering matrix. The bilayer represented in Fig. 2 has the following layering matrix

$$\mathbf{M} = \left(\begin{array}{cc|cc} 1 & -R' & 0 & 0 \\ R & A & 0 & 0 \\ \hline 0 & 0 & T & 0 \\ 0 & 0 & 0 & T' \end{array}\right) \tag{10}$$

where R and T are resp. the upper reflectance and transmittance of the bilayer, R' and T' are resp. its lower reflectance and transmittance, and $A = TT' - RR'$. It may be easily shown that the bilayer layering matrix $\mathbf{M}$ is the product of the individual layering matrices $\mathbf{M_1}$ and $\mathbf{M_2}$, divided by the weight $1-R'_1R_2$ of this product

$$\mathbf{M} = \frac{\mathbf{M}_1\mathbf{M}_2}{1-R'_1R_2} \tag{11}$$

Eq. (11) may be generalized to N superposed layers. The layering matrix $\mathbf{M}$ of the multilayer is given by the product of the individual layering matrices $\mathbf{M_k}$ divided by the weight w of the product matrix

$$\mathbf{M} = \frac{1}{w}\mathbf{M}_1\mathbf{M}_2\mathbf{M}_3...\mathbf{M}_N \tag{12}$$

DECOMPOSING A LAYER INTO SUBLAYERS

Let us consider a homogenous layer with thickness h. According to the Kubelka-Munk model, its reflectance is given by Eq. (4) and its transmittance by Eq. (6). Its layering matrix is therefore

$$\mathbf{M}(h) = \left(\begin{array}{cc|cc} 1 & -r(h) & 0 & 0 \\ r(h) & A(h) & 0 & 0 \\ \hline 0 & 0 & t(h) & 0 \\ 0 & 0 & 0 & t(h) \end{array}\right) \tag{13}$$

with $A(h) = t^2(h) - r^2(h)$. This layer is subdivided into n identical sublayers with the same thickness. Their reflectance $r(h/n)$ and transmittance $t(h/n)$ are also given by Eqs. (4) and (6) with h replaced by h/n. Their layering matrix $\mathbf{M}(h/n)$ is given by Eq. (13) with h replaced by h/n. According to relation (12), we have

$$\frac{1}{w}\left[\mathbf{M}(h/n)\right]^n = \mathbf{M}(h) \tag{14}$$

where w is the weight of matrix $\left[\mathbf{M}(h/n)\right]^n$. Thus

$$\mathbf{M}(h) = \frac{1}{w}\lim_{n\to\infty}\left[\mathbf{M}(h/n)\right]^n \tag{15}$$

where w is the weight of matrix $\lim_{n\to\infty}\left[\mathbf{M}(h/n)\right]^n$.

As n approaches infinity, the sublayer thickness h/n becomes infinitesimal. Therefore, Eq. (15) should remain valid when $r(h/n)$ and $t(h/n)$, given respectively by Eqs. (4) and (6), are reduced to the two first terms of their Taylor expansion. Since the Taylor expansion of (4) is

$$\frac{\sinh(bSx)}{a\sinh(bSx) + b\cosh(bSx)} = Sx + O\left(x^2\right) \tag{16}$$

where $O\left(x^2\right)$ means ”terms of degree 2 or more”, the sublayer reflectance becomes

$$r(h/n) = S\frac{h}{n} \tag{17}$$

and since the Taylor expansion of (6) is

$$\frac{b}{b\cosh(bSx)+a\sinh(bSx)} = 1 - aSx + O\left(x^2\right) \tag{18}$$

the sublayer transmittance becomes

$$t\left(h/n\right) = 1 - aS\frac{h}{n} = 1 - (K+S)\,\frac{h}{n} \tag{19}$$

Note that expressions (17) and (19) for $r(h/n)$ and $t(h/n)$ coincide with those considered in the Kubelka-Munk model. According to it, the fraction of light backscattered by a sublayer with infinitesimal thickness dx is Sdx, and the fraction of transmitted light corresponds to the fraction that is neither backscattered nor absorbed, i.e. $1 - Sdx - Kdx$. According to (13), (17) and (18), the sublayer layering matrix becomes

$$\mathbf{M}\left(h/n\right) = \left(\begin{array}{cc|cc} 1 & -sh/n & 0 & 0 \\ sh/n & A\left(h/n\right) & 0 & 0 \\ \hline 0 & 0 & 1-aSh/n & 0 \\ 0 & 0 & 0 & 1-aSh/n \end{array}\right) \tag{20}$$

with

$$A(h/n) = (1-aSh/n)^2 - (Sh/n)^2 = 1 - 2aSh/n - (bSh/n)^2 \tag{21}$$

Eq. (15) is valid when the sublayer matrix $\mathbf{M}\left(h/n\right)$ is expressed by Eq. (13), i.e. its coefficients $r(h)$ and $t(h)$ are expressed by Eqs. (4) and (6). Let us now show that it remains valid when $\mathbf{M}\left(h/n\right)$ is expressed by Eq. (20), with $r(h)$ and $t(h)$ expressed by Eqs. (17) and (19). This is the purpose of the next section.

KUBELKA-MUNK EXPRESSIONS OBTAINED FROM THE DISCRETE MODEL

Let us rearrange Eq. (20) by writing matrix $\mathbf{M}(h/n)$ as follows

$$\mathbf{M}(h/n) = \mathbf{I}_4 + \frac{1}{n}\mathbf{A} \tag{22}$$

with $\mathbf{I}_4$ the 4×4 identity matrix and

$$\mathbf{A} = \left(\begin{array}{cc|cc} 0 & -Sh & 0 & 0 \\ Sh & -2aSh + \varepsilon & 0 & 0 \\ \hline 0 & 0 & -aSh & 0 \\ 0 & 0 & 0 & -aSh \end{array}\right) \tag{23}$$

From a physical point of view, the term $\varepsilon = b^2S^2h^2/n$ in Eq. (23) accounts for the second order scattering within the sublayer, i.e. the portion of light that is scattered twice before being reflected, transmitted or absorbed. This term tends to 0 as n tends to infinity. We may conclude that the Kubelka-Munk model ignores the second order scattering and describes the behavior of light at a scale where the medium is almost nonscattering.

According to a classical limit property of the matrix exponential (Strang, 1986)

$$\lim_{n\to\infty} [\mathbf{M}(h/n)]^n = \lim_{n\to\infty} \left(\mathbf{I}_4 + \frac{1}{n}\mathbf{A}\right)^n = \exp(\mathbf{A}) \tag{24}$$

The diagonalization of matrix $\exp(\mathbf{A})$ is obtained through the diagonalization of $\mathbf{A}$ (Strang, 1986).

$$\exp(\mathbf{A}) = \mathbf{E}^{-1} \cdot \Delta \cdot \mathbf{E} \tag{25}$$

with

$$\mathbf{E}=\left(\begin{array}{cc|cc} a-b & 1 & 0 & 0 \\ a+b & 1 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{array}\right) \quad \text{and} \quad \Delta=\operatorname{diag}\left(e^{-(a+b)Sh}, e^{-(a-b)Sh}, e^{-aSh}, e^{-aSh}\right) \tag{26}$$

giving

$$\exp(\mathbf{A})=\frac{e^{-aSh}}{b}\left(\begin{array}{cc|cc} b\cosh(bSh)+a\sinh(bSh) & -\sinh(bSh) & 0 & 0 \\ \sinh(bSh) & b\cosh(bSh)-a\sinh(bSh) & 0 & 0 \\ \hline 0 & 0 & b & 0 \\ 0 & 0 & 0 & b \end{array}\right) \tag{27}$$

The weight w of matrix $\lim_{n\to\infty}(\mathbf{M}(h/n))^n$ is the top-leftmost term of $\exp(\mathbf{A})$, i.e.

$$w=\frac{e^{-aSh}}{b}\left(b\cosh(bSh)+a\sinh(bSh)\right)$$

Finally, according to Eq. (15), $\lim_{n\to\infty}(\mathbf{M}(h/n))^n$ divided by its weight w is the layering matrix of the layer with thickness h. As expected, Eq. (13) is retrieved with expressions (4) and (6) for $r(h)$, resp. $t(h)$

$$\frac{1}{w}\lim_{n\to\infty}(\mathbf{M}(h/n))^n=\frac{1}{w}\exp(\mathbf{A})=\mathbf{M}(h) \tag{28}$$

KUBELKA-MUNK REFLECTANCE EXPRESSED AS A CONTINUED FRACTION

Let us consider, as in Section 4, a layer with thickness h decomposed into n sublayers; let us now simply use, instead of the matrix formalism of Section 5, the reflectance formula (7). Let r_k, resp. r_{k+1}, be the reflectance of k, resp. $k+1$, superposed sublayers. According to Eq. (7), we have for every $k \geq 1$

$$r_{k+1} = r\left(h/n\right) + \frac{t^2\left(h/n\right)}{-r\left(h/n\right) + \frac{1}{r_k}} \tag{29}$$

with $r_1 = r(h/n)$. Using $n-1$ times recursion (29), we obtain a continued fraction expressing the reflectance $r_n = r(h)$ of the whole layer.

It is classically known (Yap, 2000) that every finite continued fraction

$$q_0 + \cfrac{p_1}{q_1 + \cfrac{p_2}{q_2 + \dots \atop \dots + \frac{p_k}{q_k}}} \tag{30}$$

can be reduced to a simple fraction, called a convergent of the continued fraction, whose numerator P and denominator Q are found on the second column of the following matrix product

$$\mathbf{C} = \begin{pmatrix} \dots & P \\ \dots & Q \end{pmatrix} = \begin{pmatrix} 1 & q_0 \\ 0 & 1 \end{pmatrix} \left\{ \begin{pmatrix} 0 & p_1 \\ 1 & q_1 \end{pmatrix} \begin{pmatrix} 0 & p_2 \\ 1 & q_2 \end{pmatrix} \dots \begin{pmatrix} 0 & p_k \\ 1 & q_k \end{pmatrix} \right\} \tag{31}$$

In the case at hand, it can be observed that the p_k and q_k are periodical, with period 2; thus

$$\mathbf{C}_n = \begin{pmatrix} 1 & r\left(\frac{h}{n}\right) \\ 0 & 1 \end{pmatrix} \left\{ \begin{pmatrix} 0 & t^2\left(\frac{h}{n}\right) \\ 1 & -r\left(\frac{h}{n}\right) \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & r\left(\frac{h}{n}\right) \end{pmatrix} \right\}^{n-1} \tag{32}$$

which can also be written under the form

$$\mathbf{C}_n = \begin{pmatrix} 1 & r\left(\frac{h}{n}\right) \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & t^2\left(\frac{h}{n}\right) \\ 1 & -r\left(\frac{h}{n}\right) \end{pmatrix} \left\{ \begin{pmatrix} 1 & -r \\ r & t^2\left(\frac{h}{n}\right) - r^2\left(\frac{h}{n}\right) \end{pmatrix}^{n-2} \right\} \begin{pmatrix} 0 & 1 \\ 1 & r\left(\frac{h}{n}\right) \end{pmatrix} \tag{33}$$

As n tends to infinity, $r(h/n)$ and $t(h/n)$ are reduced to expressions (17) and (19) respectively. Note that $r\left(h/n\right) = Sh/n$ tends to 0 and $t\left(h/n\right) = 1 - aSh/n$ tends to 1.

Hence, matrix $\mathbf{C}_n$ tends to

$$\mathbf{C}_\infty = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \left\{ \lim_{n\to\infty} \begin{pmatrix} 1 & -Sh/n \\ Sh/n & A(h/n) \end{pmatrix}^{n-2} \right\} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{34}$$

with $A(h/n)$ identically expressed as in Eq. (21). The matrix placed to the power $n-2$ corresponds exactly to the top-leftmost 2×2 submatrix of $\mathbf{M}(h/n)$ given by Eq. (20). Let us follow for this matrix the same reasoning line as in Section 5 for matrix $\mathbf{M}(h/n)$, noting that as n tends to infinity, exponent $n-2$ is equivalent to exponent n. As a result, the term into curly brackets in Eq. (34) is the top-leftmost 2×2 submatrix of Eq. (28). Finally, Eq. (34) becomes

$$\mathbf{C}_\infty = \begin{pmatrix} b\cosh(bSh) - a\sinh(bSh) & \sinh(bSh) \\ -\sinh(bSh) & b\cosh(bSh) + a\sinh(bSh) \end{pmatrix} \tag{35}$$

As expected, the right column of $\mathbf{C}_\infty$ gives the numerator (upper term) and the denominator (lower term) of the layer reflectance $r(h)$ expressed according to the Kubelka-Munk model.

CONCLUSION

A correspondence has been established between the Kubelka-Munk model (continuous 2-flux model) and the Kubelka layering model (discrete 2-flux model), with a mathematical equivalence achieved in the case of a homogenous diffusing layer. The transition from a discrete to a continuous model relies on a new matrix formalism and the use of a matrix exponential. The notion of layering matrix characterizes the reflectance and transmittance of layers, incorporating the limit case of infinitely thin layers. The equations of Kubelka's layering model, used to model the reflectance and the transmittance of a pile of infinitely thin layers, lead naturally to a matrix exponential, like in the work of Emmel although the "exponentialized" matrix is slightly different (Emmel-Hersch, 1999). The present contribution is a step forward in our interconnection attempt, initiated in previous works, of various classical models in the domain of color reproduction (Hebert-Hersch, 2005), (Hebert, 2006), (Hebert-Hersch-Becker, 2007).

From a physical point of view, the use of infinitesimaly thin sublayers for obtaining Kubelka-Munk expressions needs some comments. Usually, scattering is due to heterogeneities in the medium, e.g. particles, whose size cannot be assumed as infinitely small. According to the intrinsic properties of the diffusing medium, a model should be selected for the description of the scattering of light by a single particle (single scattering model (Mie, 1908) or by collections of particles (multiple scattering model). It is possible to determine first the reflectance and the transmittance of an elementary sublayer made of this diffusing medium and, afterwards, use the discrete 2-flux model to consider various superposed sublayers (Melamed, 1963). The discrete 2-flux model should be used when the sublayer behaves as a perfect diffuser, with the assumption that the medium is intensely diffusing and that the sublayer has a minimal thickness, at least the size of an average particle. The upward and downward fluxes are evaluated at discrete depths only, corresponding to multiples of the sublayer thickness. However, the equivalence that has been established between the continuous and the discrete models allows to associate to the real diffusing medium an “imaginary” medium; this medium is characterized by a scattering coefficient and an absorption coefficient such that the Kubelka-Munk model gives the same values for upward and downward fluxes at the discrete depths considered in the discrete model. At the intermediate depths, the value given by the continuous model corresponds to a mathematical interpolation.

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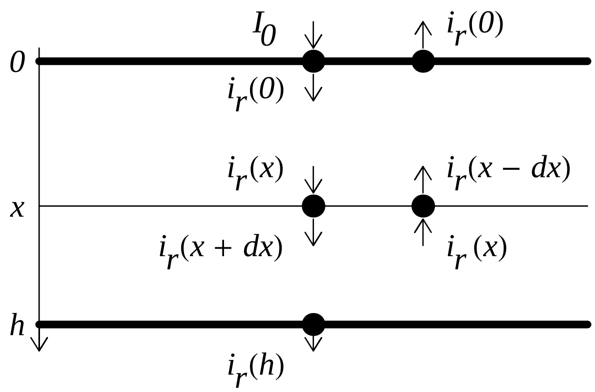

Fig. 1: *Upward and downward irradiances crossing a sublayer with thickness dx at a depth x in the diffusing layer.*

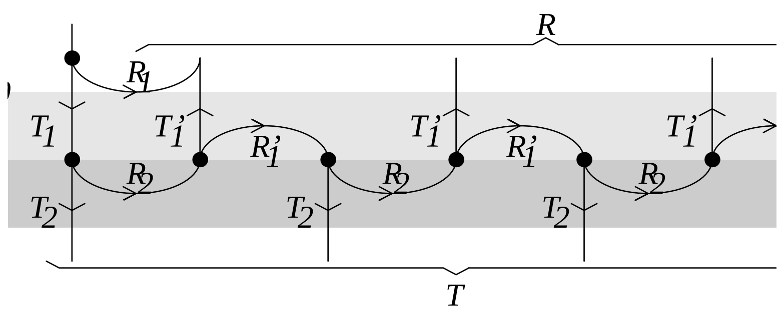

Fig. 2: *Multiple reflection-transmission of light within two superposed nonsymmetrical layers.*