

On the Solution of an Ill-Posed Non-Linear Fredholm Integral Equation Connected with an Inverse Problem of Thin Film Optics

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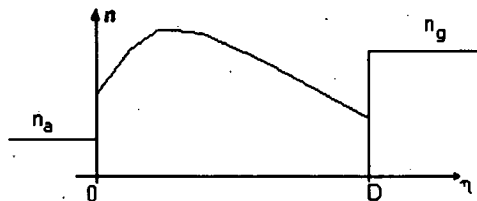
We carry out a theoretical analysis of the simultaneous identification of geometrical thickness and refractive index profile for inhomogeneous single layer systems from indirect measurements. The problem leads to a non-linear integral equation of the first kind with smooth kernel. We present a uniqueness theorem for monotone solutions referring to the Hausdorff moment problem.

Key words: *Non-linear integral equations, optics*

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1. Introduction

The identification of stratified media (for the mathematical and physical background see, e.g., [5]), that means, the determination of structure parameters from indirect measurements, is the aim of many papers (see, e.g., [2]). Questions for existence, uniqueness, and stability of solutions are often not sufficiently noted although ill-posedness must taken into account solving problems of this type. Especially, we will consider these qualities of solutions for the so-called WKB-(Webster-Kramer-Brillon)-Method, which is very important for the simultaneous identification of thickness and refractive index profile for inhomogeneous thin films from photometric



measurements [9, p. 109].

In [9, p. 111] it is shown that the optical thickness D and the Fresnel coefficients $(n_a - n(0))/(n_a + n(0))$ and $(n(D) - n_g)/(n(D) + n_g)$ describe the spectral properties of any inhomogeneous single layer system in the range of large wavelengths (WBK-range) uniquely. The refractive index profile $n = n(\eta)$ has no influence of this behavior. Therefore the inverse problem "compute the thickness and the refractive index profile from WBK-range photometric measurements" is not decidable from the mathematical point of view only (see also [1, p. 489]).

But from the physical point of view, more information about the optical parameters can be won, if the angle of incidence θ is taken in account, because the refractive index values $n(0)$, $n(d)$ and the optical thickness D are well-known functions of θ (Snellius' law; [5, p. 533]). The connection between D , the refractive index profile n as a function of the geometrical path, and

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the geometrical thickness d is given by

$$D(\theta) = \int_0^d \sqrt{(n(z))^2 - n_a^2 \sin^2 \theta} dz \quad (0 \leq z \leq d, 0 \leq \theta \leq \pi/2). \quad (1)$$

In the sequel let $n_a = 1$ for simplicity (refractive index of air). Using the transformations $t := \frac{z}{d}$, $x(t) := n(td)$, $s := \sin^2 \theta$ and $y(s) := D(\theta)$ formula (1) leads to the non-linear Fredholm integral equation

$$y(s) = d \int_0^1 \sqrt{(x(t))^2 - s} dt \quad (0 \leq s \leq 1). \quad (2)$$

Our problem requires to identify the positive parameter d and the profile $x = x(t)$ ($0 \leq t \leq 1$) simultaneously from the data $y = y(s)$ ($0 \leq s \leq 1$). Consequently, we consider

$$F(x, d) = y \quad (3)$$

with

$$F : \text{Dom}(F) \subseteq C[0, 1] \times \mathbb{R} \rightarrow C[0, 1]$$

defined by

$$[F(x, d)](s) = d \int_0^1 \sqrt{(x(t))^2 - s} dt \quad (4)$$

on the domain

$$\text{Dom}(F) = \{(x, d) \in C[0, 1] \times \mathbb{R} : x(t) \geq \epsilon > 1 \quad (0 \leq t \leq 1), d > 0\}. \quad (5)$$

In general the problem under consideration can be formulated as follows:

(P1) For given data $y \in C[0, 1]$ find $(x, d) \in \text{Dom}(F)$ satisfying $F(x, d) = y$.

The kernel $k(s, t, x) = \sqrt{x^2 - s}$ of the integral equation (2) is continuous with respect to all three variables and has continuous partial derivatives. The derivation of k with respect to x is the following one: $k_x(s, t, x) = \frac{x}{\sqrt{x^2 - s}}$, the operator F is completely continuous and continuously Fréchet differentiable on $\text{Dom}(F)$. $F'(x_0, d_0)$ represents a compact linear operator for $(x_0, d_0) \in \text{Dom}(F)$ (see, e.g., [7]). Throughout this paper we use the notations

$$\|x\|_\infty = \max_{0 \leq t \leq 1} |x(t)| \quad \text{and} \quad \|x\|_p = \left(\int_0^1 |x(t)|^p dt \right)^{1/p}.$$

2. Aspects of ill-posedness of problem (P1)

Assertions of existence and uniqueness for solutions of problem (P1) are derived from properties of the associated direct problem and formulated in Lemma 1.

Lemma 1: *Let $y = F(x, d)$, $(x, d) \in \text{Dom}(F)$. Under the conditions stated above the following properties are valid:*

(i) $y \in C^\infty[0, 1]$ and $y(s) > 0$ ($0 \leq s \leq 1$).

(ii) For the k -th derivative we have $y^{(k)}(s) < 0$ ($k \in \mathbb{N}; 0 \leq s \leq 1$).

(iii) $y^{(k)}(0) = d f_k \mu_k$, where $\mu_k := \int_0^1 (x(t))^{1-2k} dt$ and $f_{k+1} := \frac{2k-1}{2} f_k$ ($f_0 := 1$) for $k \in \mathbb{N}_0$.

(iv) y admits a power series expansion

$$y(s) = d \sum_{k=0}^{\infty} \frac{f_k}{k!} \mu_k s^k \tag{6}$$

with the radius of convergence $\rho = \min_{0 \leq t \leq 1} x^2(t) \geq c^2 > 1$.

(v) The sequence of moments $v_k := \frac{\mu_k}{2k-1}$ ($k \geq 2$) is fully monotone.

Proof: The validity of the properties (i) - (iv) we have shown in [4]. To prove the full monotony it must be shown that $(-1)^m \Delta^m v_n \geq 0$ for all $n, m \in \mathbb{N}_0$, with $n > 1$. (see, e.g., [8]). The sequence of differences $\Delta^m v_n$ is defined by

$$\Delta^0 v_n = v_n, \quad \Delta^m v_n = \Delta^{m-1} v_{n+1} - \Delta^{m-1} v_n = \sum_{k=0}^m (-1)^k \binom{m}{k} v_{n+m-k};$$

the correctness of the sum rule is evident. Since

$$\Delta^m v_n = \int_0^1 \sum_{k=0}^m (-1)^k \binom{m}{k} \frac{(x(t))^{1-2(n+m-k)}}{2(n+m-k)-1} dt = \int_0^1 S_{nm}(x(t)) dt,$$

it is sufficient to show that $(-1)^m S_{nm}(x(t)) \geq 0$ for all $t \in [0, 1]$ and $n, m \in \mathbb{N}_0$ with $n \geq 1$. Let $t \in [0, 1]$, $n > 1$, and $m \in \mathbb{N}$ arbitrary (but fixed) be chosen and denote $h := x(t)$. Then

$$\begin{aligned} S_{nm}(h) &= \sum_{k=0}^{\infty} (-1)^k \binom{m}{k} \int_h^{\infty} z^{-2(n+m-k)} dz \\ &= \int_h^{\infty} \sum_{k=0}^m (-1)^k \binom{m}{k} z^{-2(n+m-k)} dz = \int_h^{\infty} z^{-2n} (z^{-2} - 1)^m dz. \end{aligned}$$

Owing to formula (5) we have $h \geq c > 1$, i.e. $z > 1$ and $z^{-2} - 1 < 0$. In this context it is evident that $S_{n0}(h) = h^{-2n+1}/(2n-1) > 0$ and $S_{nm}(h)(-1)^m \geq 0$ ■

It is necessary for the existence of a solution of problem (P1) to have an infinitely differentiable and fully monotone function y . Inconsistency of the problem must be expected, whenever $y \in F(Dom(F))$ is replaced by a randomly selected neighbouring element $\tilde{y} \in C[0, 1]$ of y . The whole content of information obtained by y with respect to x and d is expressed by the sequence $\{d\mu_k\}_{k=0}^{\infty}$ since the power series (6) is absolutely convergent for $0 \leq s \leq 1$. The derivatives $y^{(k)}(s)$ at $s = 0$ completely determine this sequence (see Lemma 1/(iii)). From an analytic point of view the values $y(s)$ outside of an arbitrarily small interval $0 \leq s \leq \varepsilon \ll 1$ are redundant. Nevertheless, these values get important in practice in order to filter out experimental errors in the data of y . Problem (P1) fails to be uniquely solvable. For example,

$$(x(t), d) \in Dom(F) \text{ and } (x(1-t), d) \in Dom(F), \text{ where } 0 \leq t \leq 1$$

both imply the same right-hand side y of the equation (3). The most serious aspect of the ill-posedness, however, is the discontinuous dependence of solutions upon the data (for an example see [4]).

3. Statements of uniqueness

In this paragraph the statements of uniqueness are based on the uniqueness of the solution of Hausdorff's moment problem.

Lemma 2 (see, e.g., [8, p. 193]): *The non-decreasing function $F = F(t)$ ($0 \leq t \leq a < \infty$) with $F(0) = 0$ is uniquely determined by the moments*

$$\mu_k := \int_0^a t^k dF(t) \quad (k \in \mathbb{N}_0). \tag{7}$$

The fully monotony [8, p. 193] of the moment sequence $\{\mu_k\}_{k=0}^\infty$ is necessary and sufficient for the existence of a function satisfying the conditions in Lemma 2.

Let $x : [0, 1] \rightarrow \mathbb{R}$ be a measurable function. We define its *distribution function* $\sigma_x : [0, \infty) \rightarrow [0, 1]$ by

$$\sigma_x(s) = \lambda(\{t \in [0, 1] : |x(t)| > s\}), \tag{8}$$

where λ denotes the Lebesgue measure. The *non-increasing rearrangement* $x^* : [0, \infty) \rightarrow \mathbb{R}$ of x is defined by

$$x^*(t) = \begin{cases} \inf\{s > 0 : \sigma_x(s) \leq t\} & (0 \leq t < 1) \\ 0 & (1 \leq t). \end{cases} \tag{9}$$

The fundamental relations between x , σ_x , and x^* are summarized in

Lemma 3 (cf. [6, p. 48]): *Let $x : [0, 1] \rightarrow \mathbb{R}$ be a measurable function. Then*

- (i) σ_x and x^* are non-decreasing and continuous on the right,
- (ii) x and x^* possess the same distributions, i.e. $\sigma_x = \sigma_{x^*}$,
- (iii) if $1 \leq p < \infty$, then $\|x\|_p = \|x^*\|_p = \left(\int_0^\infty ps^{p-1} \sigma_x(s) ds \right)^{1/p}$.

The application of this lemma to problem (P1) is obvious. However, it is necessary to occupy the continuity of the profile function x . This continuity is a result of practice.

Lemma 4: *Let $x : [0, 1] \rightarrow \mathbb{R}_+$ be a continuous function with $0 < m = \min_{0 \leq t \leq 1} x(t)$ and $M = \max_{0 \leq t \leq 1} x(t)$. Then*

- (i) $\sigma_x(s) = 1$ for $s \in [0, m)$,
- (ii) $\sigma_x(0) = 0$ for $s \geq M$,
- (iii) σ_x is decreasing on the interval $[m, M]$,
- (iv) x^* is continuous on the interval $[0, 1)$,
- (v) $x^*(1 - 0) = m$ and $x^*(0) = M$.

Proof: We set $A_s = \{t \in [0, 1] : x(t) > s\}$ for $s \in \mathbb{R}_+$. The properties (i) and (ii) are evident.

(iii): Let $s_0, s_2 \in [m, M]$ be arbitrary elements. We suppose that $s_0 < s_2$ and $\sigma_x(s_0) = \sigma_x(s_2)$. Set $s_1 = (s_0 + s_2)/2$ and $\varepsilon = s_2 - s_1$. Since x is continuous there are t_0, t_1 , and t_2 with $x(t_j) = s_j$ ($j = 0, 1, 2$) and $t_0 < t_2$ or $t_0 > t_2$. We can suppose that $t_0 < t_2$ and hence $t_1 \in (t_0, t_2)$.

By continuity of x there is a $\delta > 0$ such that $t_0 < t_1 - \delta$, $t_1 + \delta < t_2$, and $|x(t) - x(t_1)| < \varepsilon$ for $|t - t_1| < \delta$. Therefore $s_0 = x(t_0) < x(t) < x(t_2) = s_2$. Hence

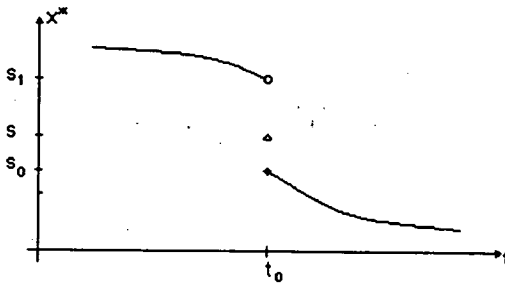
$$0 < \delta < \lambda(A_{s_0} \setminus A_{s_2}) = \lambda(A_{s_0}) - \lambda(A_{s_2}) = \sigma_x(s_0) - \sigma_x(s_2) = 0.$$

This is a contradiction.

(iv): Using Lemma 3, x^* is continuous on the right and non-increasing. This implies that the points of discontinuity are jumps. Suppose, there is an element $t_0 \in (0, 1)$ such that $x^*(t_0 - 0) > x^*(t_0 + 0) = x^*(t_0)$. Therefore, the distribution function σ_x is constant on the interval $[s_0, s_1)$, where $s_0 = x^*(t_0)$, $s_1 = x^*(t_0 - 0)$. Since σ_x is decreasing we have

$$\sigma_x(s) \leq \sigma_x(s_0) \leq t_0 \text{ for } s_0 \leq s < s_1. \tag{10}$$

It is easy to see that $s < x^*(t)$ for $t < t_0$ and therefore $\sigma_x(s) > t$ (see the sketch). This implies $\sigma_x(s) \geq t_0$. Using (10), we get $\sigma_x(s) = t_0$ for $s \in [s_0, s_1)$. This is a contradiction, since σ_x is strictly monotone.



(v): We have $x^*(0) \leq M$, by (ii). Suppose that $x^*(0) < M$, then there is an $s < M$ such that $\lambda(A_s) = 0$, i.e. A_s is an open, non-void set with measure zero. Therefore $x^*(0) = M$. Suppose that there exists a number $t < 1$ with $x^*(t) < m$. This implies the existence of an $s < m$ with $\sigma_x(s) \leq t < 1$ in contradiction to (i). Hence $x^*(1 - 0) \geq m$. Suppose that there is a number $\varepsilon > 0$ such that $x^*(t) > m + \varepsilon$ for all $t < 1$. Then we have $\sigma_x(m + \varepsilon) > t$ hence $\sigma_x(m + \varepsilon) \geq 1$. Therefore, for every $t \in [0, 1]$ we have $x(t) > m + \varepsilon$. This is a contradiction to the continuity of x . So we get $x^*(1 - 0) = m$ ■

In view of the following considerations we modify the non-increasing rearrangement introduced by (9), setting

$$x^*(1) = m := \min_{0 \leq t \leq 1} |x(t)|.$$

As a consequence of this definition, in the assertion of Lemma 3 the continuity on the right of x^* in $t = 1$ is changed, Lemma 4 is steady. The following Lemma is evident.

Lemma 5: $x \in C[0, 1]$ implies $x^* \in C[0, 1]$.

Next, we show a natural property of the non-increasing rearrangement.

Lemma 6: Let $x \in C[0, 1]$ be a non-increasing, non-negatively valued function. Then $x = x^*$.

Proof: From the suppositions it follows immediately that $\sigma_x(s) = \min\{t : x(t) \leq s\}$. Using the definitions of σ_x and x^* , we get $x(t) \leq s$ hence $\sigma_x(s) \leq t$, therefore, $x^*(t) \leq s$ for $0 \leq t \leq 1$.

Especially, for $s = x(t)$ we get $x^*(t) \leq x(t)$. In an analogous way we conclude from $x^*(t) \leq s$ that $x^*(t) \geq x(t)$, i.e. $x^*(t) = x(t)$ for $0 \leq t \leq 1$ ■

The following two lemmata give some properties of the non-increasing rearrangement.

Lemma 7a: *Let $x \in C[0, 1]$ be a function with $x \geq m > 0$. Then*

$$\left(\frac{1}{x}\right)^*(t) = \frac{1}{x^*(1-t)} \text{ for all } t \in [0, 1]$$

Proof: At first, we show that the functions $\frac{1}{x}(\cdot)$ and $\frac{1}{x^*}(1-\cdot)$ have the same distribution functions:

$$\begin{aligned} \sigma_{\frac{1}{x^*}(1-\cdot)}(s) &= \lambda \left\{ t \in [0, 1] : \frac{1}{x^*}(1-t) > s \right\} \\ &= \lambda \left\{ t \in [0, 1] : x^*(t) < \frac{1}{s} \right\} = 1 - \lambda \left\{ t \in [0, 1] : x^*(t) \geq \frac{1}{s} \right\}. \end{aligned} \quad (11)$$

Let $\{t_n\}$ be an arbitrary sequence with $t_n \uparrow 1/s$. If we set $A_n^* = \{t \in [0, 1] : x^*(t) > t_n\}$, then we have $A_n^* \subseteq A_m^*$ for $m < n$ hence $\{t \in [0, 1] : x^*(t) \geq 1/s\} = \bigcap_{n \in \mathbb{N}} A_n^*$. Using (11) and Lemma 3/(ii), it follows from the continuity of the Lebesgue measure that

$$\begin{aligned} \sigma_{\frac{1}{x^*}(1-\cdot)}(s) &= 1 - \lambda(\bigcap_{n \in \mathbb{N}} A_n^*) = 1 - \lim_{n \rightarrow \infty} \lambda(A_n^*) = 1 - \lim_{n \rightarrow \infty} \sigma_{x^*}(t_n) = 1 - \lim_{n \rightarrow \infty} \sigma_x(t_n) \\ &= 1 - \lambda\{t \in [0, 1] : x(t) \geq 1/s\} = \lambda \left\{ t \in [0, 1] : \frac{1}{x}(t) > s \right\} = \sigma_{\frac{1}{x}}(s). \end{aligned}$$

Now, one can deduce from the assertion of uniqueness (Lemma 6) that $\left(\frac{1}{x}\right)^*(\cdot) = \frac{1}{x^*}(1-\cdot)$, since the non-increasing rearrangements of functions are equal, if they have the same distribution functions ■

Lemma 7b: *If $n \in \mathbb{N}$, $x \in C[0, 1]$, and $x(t) \geq 0$, then $(x^*)^n = (x^n)^*$.*

Proof: Let $t \in [0, 1]$ be arbitrary chosen. Then we have

$$\begin{aligned} (x^*(t))^n &= (\inf\{s > 0 : \sigma_x(s) \leq t\})^n = \inf\{s^n > 0 : \sigma_x(s) \leq t\} \\ &= \inf\{s > 0 : \sigma_x(s^{1/n}) \leq t\} = \inf\{s > 0 : \lambda\{t' \in [0, 1] : x(t') > s^{1/n}\} \leq t\} \\ &= \inf\{s > 0 : \lambda\{t' \in [0, 1] : (x(t'))^n > s\} \leq t\} = (x^n)^*(t) \blacksquare \end{aligned}$$

Lemma 8: *If $x \in C[0, 1]$ and $0 < m \leq x(t)$ for $0 \leq t \leq 1$, then*

$$\int_0^1 (x(t))^{-n} dt = \int_0^1 (x^*(t))^{-n} dt \text{ for all } n \in \mathbb{N}.$$

The **proof** is an immediate consequence of the Lemmata 3/(iii), 7a, and 7b. We omit its carrying out ■

Let us return to the problem (P1). We get the following assertion of uniqueness.

Theorem 1: *If $(x, d) \in \text{Dom}(F)$ is a solution of the non-linear operator equation (3), then $(x^*, d) \in \text{Dom}(F)$ is a solution of (3), too. Moreover, there are not solutions $(f, d_1) \in \text{Dom}(F)$*

with $d \neq d_1$ or $(f, d) \in \text{Dom}(F)$ with $f \neq x^*$, if f is a non-increasing function.

Proof: At first, we show that (x^*, d) is a solution of (3), if this is true for $(x, d) \in \hat{D}(F)$. Using Lemma 4, we get $(x^*, d) \in D(F)$. The equations

$$\mu = \int_0^1 (x(t))^{1-2k} dt = \int_0^1 (x^*(t))^{1-2k} dt \text{ for } k \in N_0$$

follow from Lemma 3 for $k = 0$ and Lemma 8 for $k > 0$, respectively. We show the assertion of uniqueness by reference to the Hausdorff's moment problem (Lemma 2). Let $(x, d) \in \text{Dom}(F)$ and $(f, d_1) \in \text{Dom}(F)$ be solutions of the problem (P1), where $y \in C[0, 1]$ is given. Lemma 1/(iii) implies

$$y^{(k)}(0) = df_k \int_0^1 (x(t))^{1-2k} dt = d_1 f_k \int_0^1 (f(t))^{1-2k} dt \text{ for } k \in N_0.$$

Using Lemma 3, we get

$$d \int_0^1 (2k-1)s^{2k-2} \sigma_{\frac{1}{x}}(s) ds = d_1 \int_0^1 (2k-1)s^{2k-2} \sigma_{\frac{1}{f}}(s) ds \text{ for } k \in N.$$

We set $z = s^2$. Since $x(t) \geq \underline{c} > 0$ and $f(t) \geq \underline{c} > 0$ for $0 \leq t \leq 1$, it follows that

$$\int_0^{1/\underline{c}^2} z^{k-2} (d\sqrt{z}\sigma_{\frac{1}{x}}(s)) dz = \int_0^{1/\underline{c}^2} z^{k-2} (d_1\sqrt{z}\sigma_{\frac{1}{f}}(z)) dz \text{ for } k = 2, 3, \dots$$

Using Lemma 2, we have $d_1\sigma_{\frac{1}{f}} = d\sigma_{\frac{1}{x}}$. Since the distribution functions are continuous on the right in $s = 0$ and $\sigma_{\frac{1}{x}}(0) = \sigma_{\frac{1}{f}}(0) = 1$ holds, it follows that $d_1 = d$ and $\sigma_{\frac{1}{f}} = \sigma_{\frac{1}{x}}$. Therefore, $(\frac{1}{f})^* = (\frac{1}{x})^*$. The uniqueness follows from Lemma 6 taking into account that f is a non-increasing function ■

4. Conclusion Remarks

At the end we return to the physical starting point. Multiple wavelengths and multiple angle photometric measurements lead to ambiguous solution of the inverse problem if they are taken only in the WBK-range. We have shown that the geometrical thickness and the distribution function σ_x are uniquely determined by experiments of this type. Final bounds of perceptibility of optical one-film systems from its WBK-behavior can be characterized by the following

Lemma 9: Suppose that $(x, d) \in \text{Dom}(F)$ and $(\hat{x}, \hat{d}) \in \text{Dom}(F)$. The optical systems $\{n_a, x, n_s, d\}$ and $\{n_a, \hat{x}, n_s, \hat{d}\}$ are non-distinguishable in their WKB-behaviour if and only if the following holds true, simultaneously:

$$d = \hat{d}, \quad \sigma_x = \sigma_{\hat{x}}, \quad x(0)\hat{x}(1) = x(1)\hat{x}(0), \quad x(0)x(1) = \hat{x}(0)\hat{x}(1).$$

The **proof** is essentially based on the assertions of the classical WKB-method (see, e.g., [9]) and Theorem 1. We omit it since it is not difficult ■

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