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ON THE DETERMINATION OF OPTIMAL NODES AND WEIGHT FACTORS FOR THE SOLUTION OF COMPLETELY INCOHERENT SCATTERING PROBLEM

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Abstract. For the numerical solution of the radiative transfer equation with complete redistribution of frequencies, it is necessary to select nodes and weight factors close to optimal, which provide the greatest proximity δ between the exact and approximate solutions. The issue is reduced to a discrete boundary-value problem. We prove the theorem of existence and uniqueness of solution for above discrete boundary-value problem. We show that this solution imparts minimum to the function δ. At the end of the work we give examples representing interest in radiative transfer theory of light and gamma quanta.

Keywords: nodes, weight factors, transfer equation, "shooting"method, existence of the solution, complete redistribution of frequencies.

1. The statement of problem

It is well known that the integral equation of radiative transfer of light and gamma quanta at complete redistribution of frequencies in one dimensional approximation has the form (see [1, 2]):

$$S(\tau) = g(\tau) + \int_0^\infty K(\tau - \tau')S(\tau')d\tau'. \tag{1}$$

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Here $S(\tau)$ is the desired source function, $g(\tau)$ is the free term, $K(\tau)$ is the kernel of the integral equation

$$K(\tau) = \frac{\lambda}{2} A \int_{-\infty}^{+\infty} \alpha^2(x) e^{-\alpha(x)|\tau|} dx, \tag{2}$$

λ is the quantum survival probability, A is the normalizing factor, $\alpha(x)$ is an even function and represents absorption profile, and x is the dimensionless frequency.

For numerical solution of basic integral equation (1), we divide the interval $(0, +\infty)$: $0 = x_0 < x_1 < x_2 < x_3 < \ldots < x_{n-1} < x_n < x_{n+1} = \infty$ and the kernel $K(\tau)$ replace by a kernel $\widetilde{K}$ of the form

$$\begin{aligned} K(\tau) \approx \widetilde{K}(\tau) &= \lambda A \sum_{m=0}^{n} e^{-\alpha_m |\tau|} \int_{x_m}^{x_{m+1}} \alpha^2(t) dt \\ &= \lambda A \sum_{m=0}^{n} a_m e^{-\alpha_m |\tau|} \end{aligned} \tag{3}$$

where

$$a_m = \int_{x_m}^{x_{m+1}} \alpha^2(t) dt; \quad \alpha_m = \alpha(x_m). \tag{4}$$

From (3), (4) it is easy to see that

$$\widetilde{K}(\tau) \leq K(\tau). \tag{5}$$

We also consider the integral equation with kernel $\widetilde{K}(\tau)$

$$\widetilde{S}(\tau) = g(\tau) + \int_0^{\infty} \widetilde{K}(\tau - \tau') \widetilde{S}(\tau') d\tau'. \tag{6}$$

We estimate the proximity between solutions $S(\tau)$ and $\widetilde{S}(\tau)$ in space $L_1^+(0, +\infty)$. We have

$$\| S(\tau) - \widetilde{S}(\tau) \|_{L_1^+} \leq \frac{\| g \|_{L_1^+}}{(1-\lambda)(1-\mu)} \delta, \tag{7}$$

where

$$\delta = \| K(\tau) - \widetilde{K}(\tau) \|_{L_1^+}, \tag{8}$$

$$\lambda = \int_0^{\infty} K(\tau) d\tau < 1, \quad \mu = \int_0^{\infty} \widetilde{K}(\tau) d\tau < 1. \tag{9}$$

Thus the proximity of the kernels K and $\widetilde{K}$ provides proximity of the solutions to the basic equation (1) and corresponding "reduced"equation (6). In this connection, arises the problem to determine free parameters α_m and a_m so that number δ could reach its minimum at given fixed number of n nodes. It should be noted that when the kernel permits the representation

$$K(\tau) = \int_a^b e^{-s|\tau|} d\sigma(s), \quad 0 < a < b \leq +\infty$$

(coherent scattering) the above mentioned approach for the first time was suggested in work [3].

We have

(10)
$$\delta(x_1, x_2, x_3, \ldots, x_n) = \int_0^\infty [K(\tau) - \widetilde{K}(\tau)] d\tau = \lambda A \left[1 - \sum_{m=0}^{n} \frac{1}{\alpha_m} \int_{x_m}^{x_{m+1}} \alpha^2(t) dt \right].$$

Minimization of the function δ $\left(\frac{\partial \delta}{\partial x_k} = 0 \right)$ yields the relation

$$-\frac{1}{\alpha_m^2} \alpha_m' \int_{x_m}^{x_{m+1}} \alpha^2(x) dx - \alpha_m + \frac{\alpha_m^2}{\alpha_{m-1}} = 0. \tag{11}$$

The boundary conditions are added to the relation (11)

$$x_0 = 0, \quad x_{n+1} = \infty. \tag{12}$$

The nodes x_k can be determined from equation

$$\int_{x_m}^{x_{m+1}} \alpha^2(x) dx = F(x_m, x_{m-1}), \tag{13}$$

where

$$F(x_m, x_{m-1}) = -\frac{\alpha_m^3}{\alpha_m'} \left(1 - \frac{\alpha_m}{\alpha_{m-1}} \right). \tag{14}$$

We assume that $x_0 = 0$, $x_1 = t$ and from the equation (13) we determine $x_1, x_2, x_3, \ldots, x_k$ for a fixed number of n, at $x_{n+1} = \infty$. Here t is the parameter.

It should be noted that right hand side integral in equation (13) is monotonously increasing over x_k. If in finding the values of x_k $(k < n)$ we fail to determine the resulting $x_{k+1}, x_{k+2}, \ldots, x_n$, i.e. equation (13) does not take place despite the increase of the integer upper limit, then the value of the parameter $x_1 = t$ should be decreased. And the contrary, if the values of x_k $(k > n)$ are found, then the values of initial parameter $x_1 = t$ should be increased. This process continues until all the nodes x_k $(k = n)$ are found.

Actually, from the boundary-value problem we proceed to a recurrent system. This approach is known as a "shooting" method, which often applied to the numerical solution of boundary-value problems (see [4]).

2. Basic result

Below we prove that nodes $\{x_k\}_{k=0}^{\infty}$ being determined from (13) are unique for given fixed n and this solution imparts minimum to the function δ.

Theorem 1. *Let* $\alpha(0) = 1, \quad \alpha(\infty) = 0, \quad \alpha'(x) < 0, \quad x > 0$. *Let for arbitrary* x_* *there exists such number* P_{x_*} *that*

$$| F(x,y) | \le P_{x_*} | x - y |, \quad 0 \le y \le x \le x_*, \tag{15}$$

where

$$F(x,y) = -\frac{\alpha^3(x)}{\alpha'(x)} \left[1 - \frac{\alpha(x)}{\alpha(y)} \right]. \tag{16}$$

Then

a) for each $n \in \mathbb{N}$ *there exists unique solution* $(x_1, x_2, x_3, \ldots, x_n)$ *satisfying the equation*

$$\int_{x_m}^{x_{m+1}} \alpha^2(x)dx = F(x_k, x_{k-1}), \quad x_0 = 0, \quad k = 0, 1, 2, \ldots, n-1, \quad x_k = x_k(x_1), \tag{17}$$

b) discrete boundary-value problem (11),(12) *has unique solution* $(x_1, x_2, x_3, \ldots, x_n)$, *which imparts minimum to the function* δ.

Proof. We designate

$$H(x) = \int_x^\infty \alpha^2(t)dt - F(x,0). \tag{18}$$

From conditions of theorem it follows that $F(0,0) = 0$. Then

$$H(0) = \int_0^\infty \alpha^2(x)dx > 0. \tag{19}$$

Two cases are possible:

$$\text{i)} \;\; H(x) > 0 \text{ for } \forall\, x > 0 \quad \text{and} \quad \text{ii)} \;\; \exists\, \widetilde{x} : \;\; H(\widetilde{x}) = 0. \tag{20}$$

First we consider case i). We select $x_1 > 0$. Since $\int_{x_1}^\infty \alpha^2(t)dt - F(x_1, 0) = H(x_1) > 0$, then there exists unique number x_2 such that

$$\int_{x_1}^{x_2} \alpha^2(t)dt = F(x_1, x_0).$$

Thus,we have found $x_1, x_2, x_3, \ldots, x_n$. Then from obvious inequalities $F(x_k, x_{k-1}) < F(x_k, 0)$ and $H(x_k) > 0$ it follows that

$$\int_{x_k}^\infty \alpha^2(x)dx > F(x_k, x_{k-1}).$$

Hence there exists unique number x_{k+1}, such that

$$\int_{x_k}^{x_{k+1}} \alpha^2(x)dx = F(x_k, x_{k-1}). \tag{21}$$

The case ii). We denote

$$x_* = min\{x : H(x) = 0\}, \quad m = \int_{x_*}^{\infty} \alpha^2(t)dt, \tag{22}$$

$$h = max\{1, \alpha^{-2}(x_*)\}, \quad p = max\{1, P_{x_*}\}. \tag{23}$$

We have

$$| x - y | \leq h \int_{y}^{x} \alpha^2(t)dt, \tag{24}$$

$$| F(x, y) | \leq p \mid x - y \mid, \quad 0 \leq y \leq x \leq x_*. \tag{25}$$

We select such a small point x_1 , so that the both inequalities take place:

$$[1 + ph + p^2h^2 + \ldots + p^{n-2}h^{n-2}]x_1 < x_*, \tag{26}$$

$$p^{n-2}h^{n-1}x_1 < m. \tag{27}$$

From (24) and (27) we have

$$F(x_1, x_0) \leq p \mid x_1 - x_0 \mid = px_1 < m. \tag{28}$$

From (26) it follows that $x_1 < x_*$. Then $\int_{x_1}^{\infty} \alpha^2(t)dt > m$ and therefore there exists x_2:

$$\int_{x_1}^{x_2} \alpha^2(t)dt = F(x_1, x_0),$$

besides,

$$| x_2 - x_1 | \leq h \int_{x_1}^{x_2} \alpha^2(t)dt = hF(x_1, x_0) \leq phx_1. \tag{29}$$

From (29) it follows that

$$x_2 \leq (1 + p)hx_1, \quad | F(x_2, x_1) \leq p \mid x_2 - x_1 \mid \leq p^2hx_1 < m. \tag{30}$$

Thus, we have found $x_1, x_2, x_3, \ldots, x_n, \quad (k \leq n - 2)$ and

$$x_k \leq [1 + ph + \ldots + (ph)^{k-1}]x_1 \ (< x_*), \tag{31}$$

$$| F(x_k, x_{k-1}) | \leq p^k h^{k-1} x_1 \ \ (< m). \tag{32}$$

Then from (31) and (32) it follows that there exists unique x_{k+1} :

$$\int_{x_k}^{x_{k+1}} \alpha^2(t)dt = F(x_k, x_{k-1}).$$

Taking into consideration (31), (32), (24), we obtain

$$x_{k+1} \leq [1 + ph + \ldots + (ph)^k]x_1 \quad (< x_*),$$
$$| F(x_{k+1}, x_k) | \leq p^{k+1}h^k x_1 \qquad (< m).$$

Thus by induction we show that if $k \le n-2$, then there exists unique x_{k+1} :

$$\int_{x_k}^{x_{k+1}} \alpha^2(t)dt = F(x_k, x_{k-1}) \tag{33}$$

and the conditions (31), (32) are fulfilled. Imposing $k = n-1$ and using (24), (25), (31), (32) we conclude that

$$\exists \ x_n : \int_{x_{n-1}}^{x_n} \alpha^2(t)dt = F(x_{n-1}, x_{n-2}).$$

The theorem is proved. □

3. Examples

It is easy to check that functions $\alpha(x) = e^{-x^2}$ (Doppler profile) and $\alpha(x) = \dfrac{1}{1+x^2}$ (Lorentz profile), representing practical interest in radiative transfer theory of light and gamma quanta (see [1]), satisfy conditions of theorem .

Lets verify the condition (15).

In the case of the Doppler profile $\alpha(x) = e^{-x^2}$, $A = \dfrac{1}{\sqrt{\pi}}$ we have

$$| F(x,y) | = \frac{e^{-2x^2}}{2x}(1-e^{-(x^2-y^2)}) \le \frac{e^{-2x^2}}{2x}(x^2-y^2) \le | x-y |, \ p=1, \ 0 \le y \le x \le x_*.$$

The relation (13) takes the form

$$\int_{x_m}^{x_{m+1}} \alpha^2(t)dt = \frac{e^{-2x_m^2}}{2x_m}\left[1 - \frac{e^{-x_m^2}}{e^{-x_{m-1}^2}}\right], \quad a_m = \frac{1}{\sqrt{\pi}} \int_{x_m}^{x_{m+1}} e^{-2t^2} dt.$$

In case of Lorentz profile $\alpha(x) = \dfrac{1}{1+x^2}$, $A = \dfrac{1}{\pi}$,

$$| F(x,y) | = \tfrac{1}{2x(1+x^2)}\left(\tfrac{x^2-y^2}{1+x^2}\right) \le \tfrac{x-y}{1+x^2} \le \tfrac{1}{2}(x-y), \quad p=1, \ 0 \le y \le x \le x_*.$$

The relation (13) takes the form.

$$\frac{x_{m+1}}{x_{m+1}^2+1} + arctg\, x_{m+1} = \frac{x_m}{x_m^2+1} + arctg\, x_m + \frac{x_m^2 - x_{m-1}^2}{x_m(x_m^2+1)^2},$$

$$a_m = \frac{1}{\pi}\left[\frac{x_{m+1}}{x_{m+1}^2+1} - \frac{x_m}{x_m^2+1} + arctg\, x_{m+1} - arctg\, x_m\right].$$

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