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A NUMERICAL SOLUTION TO A PROBLEM OF CRYSTAL ENERGY SPECTRUM DETERMINATION BY THE HEAT CAPACITY DEPENDENT ON A TEMPERATURE

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Abstract The paper consider an important practical problem of determining the phonon spectrum of a crystal by the heat capacity dependent on temperature. The problem reduces to an integral equation of the first kind solvable by the regularizing algorithm. This algorithm involves finite-dimensional approximation of the original problem and allows reducing the problem to a system of linear algebraic equations by use of the Tikhonov regularization method. The approximate solution accuracy accounting for the error of the finite-dimensional problem approximation has been estimated.

Key words: Fredholm integral equation of the first kind, module of continuity, evaluation of inaccuracy, ill-posed problem.

AMS Mathematics Subject Classification: 45Q05

1 Introduction

For applying the numerical methods we use discretization of the problem basic equations which results in an additional error while reducing. To minimize the error effect on the solution, it should be accounted for in the method. The numerical method of the integral equation solution used in the paper was suggested and proved in [1]. The method allowed solving the inverse problem of solid state physics [2],[3] as well as an accuracy estimating of the problem solution.

2 Statement of the problem

Let us consider the integral equation of the first kind

$$Au(s) = \int_a^b P(s,t)u(s)ds = f(t), \quad c \le t < d, \tag{1}$$

where operator A is injective, $P(s,t) \in C([a,b] \times [c,d)),\ \ d-$can be equal to ∞, $f(t) \in L_2[c,d)$.

Suppose that at $f(t) = f_0(t)$ there is a unique exact solution $u_0(s)$ of the equation (1), which belongs to a set M_r, where

$$M_r = \left\{ u(s)\ :\ u(s),\ u'(s) \in L_2[a,b],\ u(a) = u(b) = 0,\ \ \int_a^b [u'(s)]^2 ds \le r^2 \right\}, \tag{2}$$

and $u'(s)$ is a generalized derivative.

Let the exact value of $f_0(t)$ be unknown. Instead of it we are given $f_\delta(t) \in L_2[c,d)$ and $\delta > 0$ such that

$$\|f_\delta(t) - f_0(t)\|_{L_2} < \delta.$$

For given $f_\delta(t)$, δ and M_r, it is necessary to determine an approximate solution $u_\delta(s)$ and estimate it's deviation from the exact solution $u_0(s)$ in a space metric $L_2[a,b]$.

Let us introduce an operator B which maps of the space $L_2[a,b]$ into $L_2[a,b]$, by a formula

$$u(s) = Bv(s) = \int_a^s v(\xi)d\xi; \quad v(s), Bv(s) \in L_2[a,b]. \tag{3}$$

An operator C will be defined as

$$Cv(s) = ABv(s); \quad v(s) \in L_2[a,b], Cv(s) \in L_2[c,d). \tag{4}$$

It follows from (3) and (4) that

$$Cv(s) = \int_a^b K(s,t)v(s)ds, \tag{5}$$

where

$$K(s,t) = -\int_a^s P(\xi,t)d\xi. \tag{6}$$

For solving the equation (1) numerically let us approximate the operator C by a finite-dimensional operator C_n.

To define the operator C_n let us divide the interval $[a,b]$ into n equal parts and introduce the functions $\overline{K}_i(t)$ and $K_n(s,t)$ by the formulas

$$\overline{K}_i(t) = K(\bar{s}_i, t), \tag{7}$$

where

$$\bar{s}_i = \frac{s_i + s_{i+1}}{2}, \quad s_{i+1} = a + \frac{(i+1)(b-a)}{n}, \quad s_i = a + \frac{i(b-a)}{n}, \quad i = 0,1,...,n-1,$$

and

$$K_n(s,t) = \overline{K}_i(t); \quad s_i \le s < s_{i+1}, \quad t \in [c,d), \quad i = 0,1,...,n-1. \tag{8}$$

Applying (8) we can define the finite-dimensional operator C_n by a formula

$$C_n v(s) = \int_a^b K_n(s,t)v(s)ds; \quad t \in [c,d), \tag{9}$$

where C_n maps of the space $L_2[a,b]$ into $L_2[c,d)$.

Now let us estimate the value $\|C_n - C\|$. For this purpose, we introduce a function $N(t)$ by a formula

$$N(t) = \max_{a \le s \le b} |P(s,t)|; \quad t \in [c,d). \tag{10}$$

As $P(s,t) \in C([a,b] \times [c,d))$, then it follows from (10) that

$$N(t) \in C[c,d).$$

Suppose in addition that

$$N(t) \in L_2[c,d).$$

Using the function $N(t)$ defined in (10) we estimate the value of $\|C_n - C\|$.

Lemma 2.1. *Let* $h = \dfrac{b-a}{n}$*, while the operators* C *and* C_n *are defined by the formulas* (5) *and* (9)*. Then the following estimate is true* $\|C_n - C\| \le \sqrt{b-a} \cdot \|N(t)\|_{L_2} \cdot h$.

The proof is given in [4] p. 265, formula (1.17).
The value $\sqrt{b-a} \cdot \|N(t)\|_{L_2} \cdot h$ here in after is denoted as η_n.

3 Regularization method to the equation (1) solution

To solve the equation (1) we apply the finite-dimensional variant of the Tikhonov regularization method,

$$\inf \left\{ \|C_n v(s) - f_\delta(t)\|^2 + \alpha \|v(s)\|^2 \quad : \quad v(s) \in X_n \right\}, \quad \alpha > 0, \tag{11}$$

where X_n is a subspace of the functions being constant in the intervals $[s_i, s_{i+1})$, $\quad i = 0, 1, ..., n-1$, $X_n \subset L_2[a,b]$.

The existence and uniqueness of the solution $v_{\delta n}^{\alpha}(s)$ to the variational problem (11) follows from [5].

A value of the regularization parameter $\overline{\alpha} = \overline{\alpha}(C_n, f_\delta, \eta_n, \delta)$ of the problem (11) should be selected from the residual principle [6].

$$\|C_n v_{\delta h_n}^{\alpha}(s) - f_\delta(t)\| = r\eta_n + \delta. \tag{12}$$

It is known that if

$$\|f_\delta(t)\| > \delta + r\eta_n \tag{13}$$

there exists the unique solution $\alpha(\delta, n)$ to the equation (12).

If the condition (13) is satisfied, the problem (11), (12) is equivalent to the problem

$$\inf \{ \|v(s)\|^2 \quad : \quad v(s) \in L_2[a,b], \quad \|C_n v(s) - f_\delta(t)\| \le r\eta_n + \delta \},$$

(refer [7], theorem 1).

After denoting the solution $v_{\delta n}^{\alpha(\delta,n)}(s)$ of the problem (11), (12) by $v_{\delta n}(s)$, an approximate solution $u_{\delta n}(s)$ of the equation (1) takes the form

$$u_{\delta n}(s) = Bv_{\delta n}(s).$$

To reduce the problem (11) to a system of the linear algebraic equations, let us introduce an orthonormal basis $\{\varphi_i(s)\}$ in the space X_n by a formula

$$\varphi_i(s) = \begin{cases} \sqrt{\dfrac{n}{b-a}}; & s_i \le s < s_{i+1}, \\ 0; \quad s \notin [s_i, s_{i+1}), & i = 0, 1, ..., n-1. \end{cases}$$

Using the basis we define an isometric operator J_x which maps of R^n into X_n, by a formula

$$J_x[\overline{x}](s) = \sum_{i=0}^{n-1} x_i \varphi_i(s), \qquad \overline{x} = (x_0, x_1, ..., x_{n-1}),$$

and reduce the problem (11) to the following one

$$\inf\{\|C_n J_x[J_x^{-1} v(s)] - f_\delta(t)\|^2 + \alpha \|J_x^{-1}[v(s)]\|^2_{R^n} \quad : \quad J_x^{-1}[v(s)] \in R^n\}, \tag{14}$$

where J_x^{-1} is an operator inverse to J_x.

The problem (14) is equivalent to a system of the linear algebraic equations

$$h\sum_{i=0}^{n-1} b_{ij} v_i + \alpha v_j = q_j, \qquad j = 0, 1, ..., n-1, \tag{15}$$

where $b_{ij} = \int_c^d \overline{K}_i(t)\overline{K}_j(t)dt$ and $q_j = \sqrt{h}\int_c^d \overline{K}_j(t) f_\delta(t)dt.$

Theorem 3.1. *Let $v_{\delta n}^{\alpha}(s)$ and (v_i^{α}) be the solutions of the problems* (11) *and* (15) , *respectively. Then the solutions are connected by the relation*

$$v_{\delta n}^{\alpha}(s) = \sum_{i=0}^{n-1} v_i^{\alpha} \varphi_i(s). \tag{16}$$

The proof of the theorem is given in the theorem 2 in the paper [1].

Let us denote a solution of the system (15) by $\overline{v}^{\alpha} = (v_0^{\alpha}, v_1^{\alpha}, ..., v_{n-1}^{\alpha})$. Then by using the formula (16) we write the solution of the problem (1) as $v_{\delta n}^{\alpha}(s)$.

To select a regularization parameter, we use the equation (12)

$$\|C_n v_{\delta n}^{\alpha}(s) - f_\delta\| = r\eta_n + \delta.$$

Let us denote the solution of the equation (12) by $\alpha(\delta, n)$, and that of the problem (12), (15) by $\overline{v}^{\alpha(\delta,n)}$.

4 Error estimate of the equation (1) approximate solution $u_{\delta n}(s)$

To evaluate inaccuracy let us introduce a function

$$\omega(\tau, r) = \sup\{\|u(s)\| \ : \ u(s) = Bv(s), \|v(s)\| \le r, \ \ \|Au(s)\| \le \tau\}, \quad \tau, r > 0.$$

The theorem formulated in [8] implies

Theorem 4.1. *Let $u_{\delta n}(s)$ be the approximate solution of the equation (1) while $u_0(s)$ is its exact solution. Then*

$$\|u_{\delta n}(s) - u_0(s)\| \le 2\omega(r\eta_n + \delta, r).$$

5 A numerical solution to a problem of crystal energy spectrum determination by the heat capacity dependent on a temperature

A relation between the energy spectrum of Bose system and its heat capacity dependent on a temperature is described by an integral equation of the first kind

$$Au(s) = \int_a^b P(s,t)u(s)ds = \frac{f(t)}{t}; \quad 0 \le t < \infty, \quad b > a > 0. \tag{17}$$

where $P(s,t) = \dfrac{s^2}{2t^3 \operatorname{sh}^2\left(\dfrac{s}{2t}\right)}$, $u(s) \in L_2[a,b]$, $\dfrac{f(t)}{t} \in L_2[0,\infty)$, $u(s)-$ is a spectral density of a crystal, and $f(t)$ is its heat capacity dependent on a temperature [2].

Suppose that at $f(t) = f_0(t)$ there exists an exact solution $u_0(s)$ of the equation (17) which belongs to a set M_r, where

$$M_r = \left\{u(s) \ : \ u(s), u'(s) \in L_2[a,b], \ \ u(a) = u(b) = 0, \ \ \int_a^b [u'(s)]^2 ds \le r^2\right\},$$

The uniqueness of the solution results from the research [9].

Let the exact value of $f_0(t)$ be unknown. Instead of it we are given $f_\delta(t)$ and $\delta > 0$ such that $\dfrac{f_\delta(t)}{t} \in L_2[0,\infty)$, $\left\|\dfrac{f_\delta(t)}{t} - \dfrac{f_0(t)}{t}\right\|_{L_2} \le \delta$.

On account of $f_\delta(t), \delta$ and M_r we need to determine an approximate value of $u_\delta(s)$ and estimate its deviation from the exact solution $u_0(s)$ in a metric of space $L_2[a,b]$.

It should be noted that the uniqueness of the equation (17) solution is proved in [9].

Let us introduce an operator B which maps of the space $L_2[a,b]$ into $L_2[a,b]$ by a formula

$$u(s) = Bv(s) = \int_a^s v(\xi)d\xi; \quad v(s), \ Bv(s) \in L_2[a,b]$$

and an operator C

$$Cv(s) = ABv(s); \qquad v(s) \in L_2[a,b], \quad Cv(s) \in L_2[0,\infty).$$

It follows from (3)– (6) that $Cv(s) = \int_a^b K(s,t)v(s)$ where $K(s,t) = -\int_a^s P(\xi,t)d\xi.$

Now we use a construction described by the formulas (7)–(9) to replace the operator C with the finite-dimensional operator C_n.

Consequently,

$$C_n v(s) = \int_a^b K_n(s,t)v(s)ds; \qquad t \in [0,\infty),$$

where $K_n(s,t)$ is defined by a formula (8) while C_n maps of the space $L_2[a,b]$ into $L_2[0,\infty)$.

It follows from (10) and (17) that

$$N(t) \le \frac{b^2}{2t^3 \operatorname{sh}^2\left(\frac{a}{2t}\right)}. \tag{18}$$

As a result, we obtain from (18) that, as $t \to \infty$

$$\frac{b^4}{4t^6 \operatorname{sh}^4\left(\frac{a}{2t}\right)} \cong \left(\frac{b}{\sqrt{2}a}\right)^4 \frac{1}{t^2}, \tag{19}$$

while as $t \to 0$

$$\frac{b^4}{4t^6 \operatorname{sh}^4\left(\frac{a}{2t}\right)} \to 0. \tag{20}$$

It follows from (19) and (20) that

$$\frac{b^2}{2t^3 \operatorname{sh}^2\left(\frac{a}{2t}\right)} \in L_2[0,\infty). \tag{21}$$

while the lemma 2.1, (18), and (21) imply that

$$\|C_n - C\| \le \sqrt{b-a} \cdot \frac{b^2}{2}\left[\int_0^\infty \frac{dt}{t^6 \operatorname{sh}^4\left(\frac{a}{2t}\right)}\right]^{1/2} \cdot h. \tag{22}$$

Let us denote the value $\sqrt{b-a} \cdot \frac{b^2}{2}\left[\int_0^\infty \frac{dt}{t^6 \operatorname{sh}^4\left(\frac{a}{2t}\right)}\right]^{1/2} \cdot h$ as η_n.

According to the paragraph 2, let us consider a variational problem

$$\inf\left\{\|C_n v(s) - \frac{f_\delta(t)}{t}\|^2 + \alpha\int_a^b [v(s)]^2 ds \quad : \quad v(s) \in L_2[a,b]\right\}, \quad \alpha > 0. \tag{23}$$

The problem (23) has a unique solution $v^\alpha_{\delta n}(s)$. A value of the regularization parameter α in the solution $v^\alpha_{\delta n}(s)$ should be selected from the residual principle

$$\|C_n v^\alpha_{\delta n}(s) - f_\delta(t)\| = \delta + r\eta_n.$$

Applying the method described in detail in the paragraph 2 to the problem, we reduce it to a system of the linear algebraic equations (15) where the regularization parameter is to be selected from the condition (12).

The lemma 5 in the paper [10] implies that, for the equation (22) on the set M_r defined by the formula (2), the following estimate is true for a module of continuity $\omega(\sigma, r)$

$$\omega(\sigma, r) \le r\left[1 + \frac{1}{\pi}\ln^2\left(\frac{r}{4\sigma}\right)\right]^{-1/2}. \tag{24}$$

We obtain the final estimate from the theorem 4.1 and the formula (24)

$$\|u_{\delta n}(s) - u_0(s)\| \le 2r\left[1 + \frac{1}{\pi}\ln^2\left(\frac{r}{4(r\eta_n + \delta)}\right)\right]^{-1/2}.$$

6 Conclusion

The paper improves the results of the paper [10] by means of the problem discretization, and reducing the regularization method to a system of linear algebraic equations as well as accounting for the discretization error of an integral equation when selecting a regularization parameter. It is shown that no significant transformation for the physical model of problem is required to apply the numerical methods. This allows considering a priori information effectively while solving the problem. It results from the calculations presented in [10], p. 134, that the method restores the solution closely.

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