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NUMERICAL SOLUTION OF A FIRST KIND FREDHOLM INTEGRAL EQUATION ARISING IN ELECTRON-ATOM SCATTERING

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The regularization method of Phillips and Tihonov is applied to a first kind Fredholm integral equation arising in the field of electron-atom scattering.

{This paper is in final form and no version of it will be submitted for publication elsewhere}

1. Introduction

Collision processes, taking place between (sub)atomic particles, are generally expressed in terms of scattering amplitudes. These functions, when squared, represent the probabilities of obtaining specific outcomes in a scattering event as to the momentum and energy transfer between colliding partners. The amplitudes themselves are functions of the projectile's incoming and outgoing momentum vector.

Titchmarsh [9] has shown that a function, which is analytic and bounded in its complex continuated variable, can be written in the form of an integral expression. Applying this theorem to the scattering amplitude for forward elastic scattering of electrons on noble gas atoms yields the so-called dispersion relation [3]

$$(1.1) \qquad \mathrm{Re}\ f(E) = f_B - g_B(E) + \pi^{-1} P \int_0^{\infty} \frac{\mathrm{Im}\ f(E')}{E'-E}\, dE' \ .$$

Here, E is the projectile electron's impact energy and P the principal value integral. Since electrons are indistinguishable, the amplitude consists of a direct and an exchange part; the latter accounts for the interchange of the projectile electron and one of the atomic electrons. The subscript B denotes the first Born approximations to these two parts respectively. The real and imaginary parts are related to the differential and total cross sections respectively, which are both in principle measurable quantities.

It remains, however, to prove the analytical behaviour of the amplitude for this relation to be valid. Recent investigations [1,2] have shown that (1.1) has to be modified: an extra term, the "discrepancy function" $\Delta(E)$, is added to the right-hand side due to a cut along the part of the negative real energy axis, where the exchange amplitude appeared to be non-analytic.

$$(1.2) \qquad \Delta(E) = \pi^{-1} \int_a^{\infty} \frac{\rho(E')}{E + E'}\, dE' , \quad c \le E \le d,$$

where $\rho(E')$ is the discontinuity of the non-Born part of the exchange amplitude across this cut. Sofar, direct computation of $\rho(E')$ has not been possible yet, not even for the simplest system of electron-atomic hydrogen scattering [2]. On the other hand, a recent experimental study [10] has addressed the magnitude of $\Delta(E)$ at various impact energies, where helium was used as target.

By inverting (1.2), it is hoped then to gain more insight into the behaviour of $\rho(E')$, in particular with respect to the possible existence of isolated singularities.

The discrepancy function $\Delta(E)$ is measured in a set of 23 non-equidistant points E_i, $i = 1,2,\dots,23$, in the interval $[1,300]$, with a relative error which varies between 1 and 5%. For $E > 500$, $\Delta(E)$ may be assumed to vanish.

With respect to the unknown function $\rho(E')$ in (1.2), we may assume that it tends to zero, as $E' \to \infty$, at least as fast as $(E')^{-\frac{1}{2}}$. Under this assumption we replace the infinite upperbound in (1.2) by a finite number b. The neglected part $_b\int^{\infty}$ can then be estimated as follows:

$$(1.3) \qquad \left|\frac{1}{\pi} \int_b^{\infty} (E+E')^{-1}\rho(E')dE'\right| < \frac{1}{\pi} \int_b^{\infty} (E+E')^{-1}(E')^{-\frac{1}{2}}dE' < \frac{1}{\pi}\int_b^{\infty} (E')^{-3/2}dE'.$$

The last term equals $2\pi^{-1}b^{-\frac{1}{2}}$. Hence, by taking b large enough, the neglected part can be made small, compared with the error in $\Delta(E)$ (cf. section 4).

Equation (1.2) is a special case of a Fredholm integral equation of the first kind:

$$(1.2') \qquad \Delta(E) = \int_a^b K(E,E')\rho(E')dE', \qquad c \le E \le d.$$

This type of integral equation arises in the mathematical analysis of problems from many branches of physics, chemistry and biology [5]. Also various classical mathematical problems, like the problem of harmonic continuation, numerical inversion of the Laplace transform, the backwards heat equation and numerical differentiation, can be formulated in terms of equations of the form (1.2').

First kind Fredholm equations belong to the class of ill-posed problems [4]. In particular, this means that (i) there may be no solution, (ii) a solution may not be unique and (iii) if we perturb the given function Δ with a small amount, the solution of the perturbed problem (if it exists) may differ from the original solution with a very large amount. Therefore, great care must be exercised when we solve (1.2) numerically, in particular, in view of the inexact data function Δ.

In this paper we present the results of experiments with the well-known regularization method of Phillips and Tihonov [6,8] for numerically solving (1.2'). The results show that it is possible to obtain satisfactory results with the regularization method at least in a qualitative sense, for problems (1.2') with highly inexact data.

2. The regularization method of Phillips and Tihonov

The regularization method of Phillips and Tihonov essentially amounts to the replacement of (1.2') by the well-posed problem

(2.1) Minimize the quadratic functional $\Phi_\alpha(\rho)$, defined by

$$\Phi_\alpha(\rho) := \|K\rho - \Delta\|^2 + \alpha\|L\rho\|^2$$

over all functions in the compact set $\{\rho : \|K\rho - \Delta\| \le \varepsilon\}$.

Here, $K : F \to G$ is a linear operator defined by $(K\rho)(E) := \int_a^b K(E,E')\rho(E')dE'$, where F and G are certain linear spaces and $\|\cdot\|$ is some norm in F and G.

L is a linear operator ($L : F \to F$) and α is a fixed positive number, to be chosen a priori. For later use, we write: $L\rho = a_0(\rho-\hat{\rho}) + a_1 d\rho/dE + a_2 d^2\rho/dE^2$, where $a_i = 0$ or 1 and $\hat{\rho} = \hat{\rho}(E)$ is an a priori known approximation to ρ. The number ε in (2.1) reflects the presence of error in the data function Δ; if Δ were known exactly, we would look for ρ such that $K\rho = \Delta$; since, however, Δ is known only approximately, we (have to) content ourselves with finding ρ such that $\|K\rho - \Delta\| \leq \varepsilon$.

Under certain, mild conditions (which we assume to be fulfilled), (2.1) has a unique solution, which we denote by ρ_α.

The proper choice of α and L in (2.1) is of crucial importance. Unfortunately, no general rule for choosing α and L is known. The following heuristics may be helpful. As is well-known, the presence of α in (2.1) provides a balance between, on one hand, minimization of $\|K\rho - \Delta\|$, i.e., solving $K\rho = \Delta$ ($\alpha=0$) and, on the other hand, minimization of the "penalty" term $\|L\rho\|$ (α large). Therefore, it seems reasonable to choose α in such a way that the solution ρ_α of (2.1) satisfies $\|K\rho_\alpha - \Delta\| \approx \varepsilon$, where ε is the (average) error in Δ. Another possibility is to let α be approximately equal to ε^2. This choice is motivated by the fact that, under certain conditions, the solution ρ_α of (2.1) tends to the solution of $K\rho = \Delta$ (if it exists) if $\varepsilon \to 0$ and if α satisfies $C_1\varepsilon^2 < \alpha < C_2\varepsilon^2$, $C_1, C_2 > 0$.

3. Numerical solution of (2.1)

In [7], a subroutine for numerically solving first kind Fredholm integral equations (1.2') via the minimization problem (2.1) of Phillips and Tihonov has been described and documented. In this subroutine, a linear system of equations is solved which results from discretization of the continuous problem (2.1). Here, we only give the linear system and for its derivation we refer to [7].

Suppose that $\Delta(E)$ is given in N points $E=E_i$, $i=1,2,\ldots,N$ ($c \leq E_1 < \ldots < E_N \leq d$) with $\Delta(E_i) =: \Delta_i$; moreover, let the integration interval $[a,b]$ be subdivided by the N+1 points $E'=E'_j$, $j=0,1,\ldots,N$ ($a=E'_0 < E'_1 < \ldots < E'_N=b$). The points E_i and E'_j need not be equidistant. Discretization of (2.1) (where the integrals over $[E'_j, E'_{j+1}]$ are approximated by using the mid-point rule) leads to the following linear system:

$$(3.1)\qquad \{K^TK + \alpha(a_0H_0 + a_1H_1 + a_2H_2)\}\vec{\rho} = K^T\vec{\Delta} + \alpha a_0\vec{\hat{\rho}}\ .$$

Here, $K=(K_{ij})$, where $K_{ij}=(E'_j-E'_{j-1})K(E_i,\bar{E}'_j)$, $\bar{E}'_j=\frac{1}{2}(E'_{j-1}+E'_j)$;

$\vec{\rho}=(\rho_1,\rho_2,\ldots,\rho_N)^T$, $\rho_j\approx\rho(\bar{E}'_j)$ is an approximation of ρ in the mid-point $\bar{E}'_j$;

$\vec{\Delta}=(\Delta_1,\Delta_2,\ldots,\Delta_N)^T$;

$\vec{\hat{\rho}}=(\hat{\rho}_1,\hat{\rho}_2,\ldots,\hat{\rho}_N)^T$, $\hat{\rho}_j$ is an approximation of ρ_j to be given a priori, if $a_0=1$;

H_0 is the N×N identity matrix,

$$H_1=\begin{bmatrix} 1 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 2 \end{bmatrix}_{N\times N} \quad H_2=\begin{bmatrix} 1 & -2 & 1 & & & & \\ -2 & 5 & -4 & 1 & & & \\ 1 & -4 & 6 & -4 & 1 & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & 1 & -4 & 6 & -4 & 1 \\ & & & 1 & -4 & 5 & -2 \\ & & & & 1 & -2 & 1 \end{bmatrix}_{N\times N}.$$

4. Numerical experiments

4.1 A problem with known solution

As a test, we first solved the equation

$$(4.1)\qquad \int_1^3 (E + E')^{-1}\rho(E')dE' = E^{-1}\ln\left(\frac{1+E/a}{1+E/b}\right),\qquad 1 \le E \le 2,$$

which has a known solution $\rho(E') = (E')^{-1}$. In table I we list the minimum number of correct digits obtained with N=8 data points, for $\alpha=10^{-i}$, i=0,1,..., 9, for $L\rho=\rho$, $L\rho=d\rho/dE$ and $L\rho=d^2\rho/dE^2$, respectively. We also list in table I the corresponding results obtained in case the data points Δ_j were perturbed with 1% random error (i.e., the exact values Δ_j were multiplied by the factor $1 + 0.01\times(2\times\gamma_j-1)$, where γ_j is a random number taken from the interval [0,1)).

In the case of exact data, the best results were obtained for α in the range (10^{-8} - 10^{-4}), whereas in the case of inexact data the best results were obtained for much larger values of α (10^{-4} - 10^{-3}).

Table I. The regularization method of Phillips and Tihonov applied to (4.1)
First entry :minimum number of correct digits in $\bar{E}'_j$, j=0,1,...,7;
second entry: $\| K\vec{\rho}-\vec{\Delta} \|$, $\| \cdot \|$ is the Euclidean vector norm; a(-b) means: $a \cdot 10^{-b}$.

	α	Lρ = ρ		Lρ = dρ/dE		Lρ = $d^2\rho/dE^2$	
Data exact	1	0.1	7(-1)	0.2	5(-3)	0.6	3(-5)
	1(-1)	0.5	2(-1)	0.2	5(-3)	0.6	3(-5)
	1(-2)	0.7	3(-2)	0.2	5(-3)	0.6	3(-5)
	1(-3)	0.7	4(-3)	0.5	3(-3)	0.6	3(-5)
	1(-4)	1.1	1(-3)	1.0	7(-4)	0.6	3(-5)
	1(-5)	1.4	2(-4)	0.9	9(-5)	0.6	3(-5)
	1(-6)	1.2	3(-5)	0.9	3(-5)	0.7	3(-5)
	1(-7)	1.4	1(-5)	1.0	2(-5)	1.4	1(-5)
	1(-8)	1.3	5(-6)	1.0	7(-6)	0.8	2(-6)
	1(-9)	1.1	8(-7)	0.7	1(-6)	0.8	4(-7)
Data inexact	1	0.1	7(-1)	0.2	9(-3)	0.8	3(-3)
(random error,	1(-1)	0.5	2(-1)	0.2	9(-3)	0.8	3(-3)
maximum 1%)	1(-2)	0.7	3(-2)	0.2	9(-3)	0.8	3(-3)
	1(-3)	0.8	8(-3)	0.7	7(-3)	0.8	3(-3)
	1(-4)	0.8	5(-3)	0.5	5(-3)	0.8	3(-3)
	1(-5)	0.3	4(-3)	0.5	5(-3)	0.8	3(-3)
	1(-6)	0.2	4(-3)	0.1	4(-3)	0.5	3(-3)
	1(-7)	-0.2	4(-3)	-1.0	4(-3)	-0.1	3(-3)
	1(-8)	-0.6	4(-3)	-1.6	2(-3)	-0.3	3(-3)
	1(-9)	-0.7	4(-3)	-1.7	2(-3)	-0.1	3(-3)

Other experiments with a problem with known solution and inexact data (maximum 3% random error) show a similar pattern of results [7].

4.2 Numerical solution of problem (1.2)

In view of (1.3), we replaced the infinite upperbound in (1.2) by $b = 2\times 10^6$, which adds an error to Δ whose absolute value is less than 0.0005. This is small compared with the measuring errors in the physical data $\Delta(E_i)$. These data values are given in table II (set I). The lowerbound of integration in (1.2) was given to be a=24.5. In order to work with an interval for E which has about the same length as the integration interval for E' ($[24.5, 2\times 10^6]$), we added 11 points E_i with value $\Delta(E_i)=0$ (see table II). This gave a total of N=34 data points. The points E'_j were chosen such that their distribution was similar to that of the points E_i:

$$E'_0 = 24.5,\ E'_{33} = 10^6,\ E'_{34} = 2\times 10^6,$$

(4.2)
$$E'_j = E'_0 + \frac{E_{j+1}-E_1}{E_{34}-E_1} \times (E'_{33} - E'_0),\ j = 1,2,\ldots,32.$$

With these provisions (1.2) was solved with the regularization method of Phillips and Tihonov for $\alpha = 10^{-4}$, and $L\rho = d^2\rho/dE^2$.

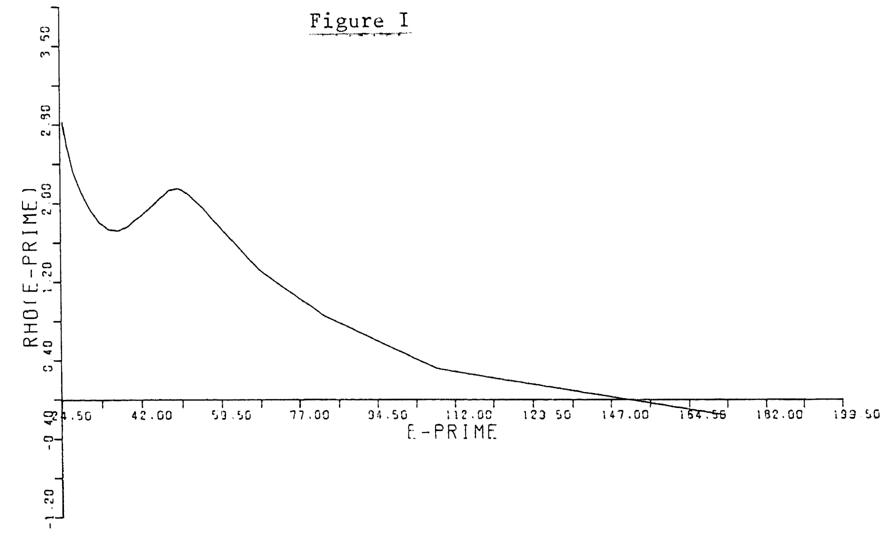
Table II. Data values $\Delta(E_i)$
(unmentioned values in the data sets II, III and IV are equal to the corresponding values in data set I)

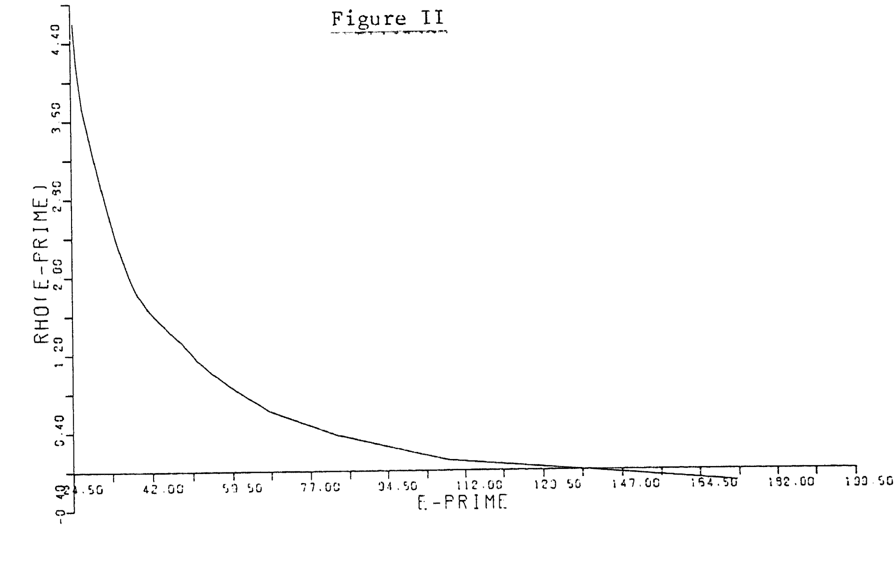
		$\Delta(E_i)=\Delta_i$			
i	E_i	I(lump in E=26)	II(lump smoothed out)	III(lump in E=20)	IV(lump in 30)
1	1.5	0.60	.	.	.
2	2.5	0.55	.	.	.
3	3.1	0.52	.	.	.
4	5.1	0.49	.	.	.
5	7.1	0.47	.	.	.
6	9.1	0.45	.	.	.
7	11.2	0.42	.	.	.
8	13.1	0.40	.	.	.
9	15.1	0.39	.	0.38	.
10	17.1	0.37	.	0.38	.
11	20.0	0.35	0.35	0.39 ←	.
12	22.0	0.35	0.34	0.37	0.34
13	24.5	0.33	0.33	0.35	0.33
14	26.0	0.36 ←	0.32	0.33	0.32
15	28.0	0.34	0.31	0.31	0.31
16	30.0	0.33	0.30	0.30	0.33 ←
17	35.0	0.29	0.28	0.28	0.31
18	40.0	0.25	.	.	0.25
19	50.0	0.17	.	.	0.19
20	70.0	0.13	.	.	0.14
21	100	0.11	.	.	.
22	200	0.06	.	.	.
23	300	0.02	.	.	.

In the data sets I, II, III and IV, 11 zero values $\Delta_{24},\ldots,\Delta_{34}$ were added, viz., for E=500, 1000, 2500, 5000, 10000, 25000, 50000, 100000, 250000, 500000 and 1000000.

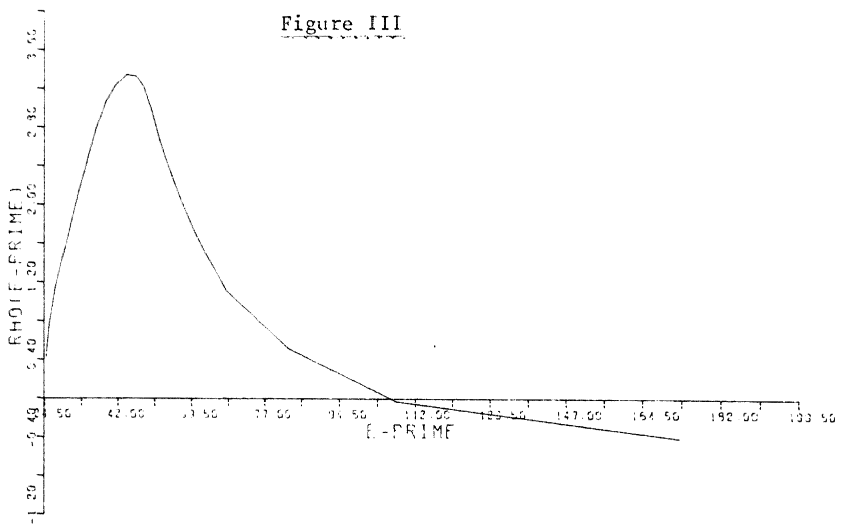
Figure I gives a graph of the numerical solution ρ_α, obtained by drawing a smooth curve through the computed values ρ_i. Figure II shows the corresponding graph obtained with the data set II given in table II. This data set was obtained from data set I by smoothing out the small lump around E=26. Data sets III and IV were obtained from data set I by moving the lump from E=26 to E=20 and to E=30, respectively. The resulting graphs are shown in figures III and IV. The curves in figures I, III and IV, although quantitatively different, show one common qualitative feature: there is one (relative) maximum. As the lump in the data is shifted towards greater values of E, this maximum decreases and moves slowly to greater values of E'. Figure II shows that this maximum in ρ_α has a one-to-one relationship with the lump in the data Δ. A final experiment with data set I was carried out as follows: the starting point E_0' of integration in (1.2) was changed from $E_0'=24.5$ to $E_0'=20$

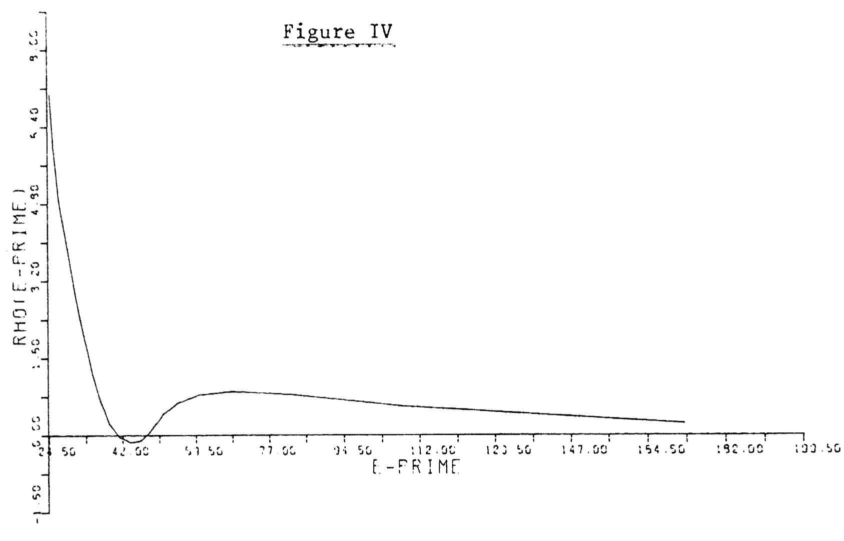
Figures I and II Numerical solutions ρ_α obtained with data sets I and II, resp.





Figures III - IV Numerical solutions ρ_α obtained with data sets III - IV,resp.





and to $E'_0=15$, respectively. The points E'_j, $j=1,2,\ldots,32$ were recomputed according to (4.2), and the system (3.1) was solved. In both cases, the resulting curves showed the same qualitative behaviour as the curve in figure I. Moreover, the following common quantitative feature was observed: the location of the relative maximum in ρ_α was approximately the same for the three experiments, viz., $E' \approx 48$.

The experiments described above were also carried out for several other values of α in the range $(10^{-5} - 10^{-3})$ and the results were very similar to the results obtained for $\alpha=10^{-4}$. In our experiments with problems with a known solution and inexact data (cf. section 4.1 and [7]), we used the same kernel $(E+E')^{-1}$ as in (1.2) and we obtained the best results also for α in the range $(10^{-5} - 10^{-3})$. Therefore, we may conclude that the numerical solution obtained for the physical problem (2.1) in figure I is reliable, at least in a qualitative sense, and that this is the best result that can be obtained, given the errors in the data function Δ, and given the mathematical model (1.2) of the physical problem.

5. References

[1] Combes, J.M. and A. Tip(1983) CNRS preprint.
[2] Dumbrajs, O. and M. Martinis(1982) J. Phys. B: Atomic and Molecular Physics 15, 961.
[3] Gerjuoy, E. and N.A. Krall(1962) Physical Review 127, 2105.
[4] Lavrentiev, M.M.(1967) Some improperly posed problems of mathematical physics, Springer Tracts in natural philosophy, vol. 11(Springer, Berlin).
[5] Nedelkov, I.P.(1972) Improper problems in computational physics, Comp. Phys. Comm. 4, 157-164.
[6] Phillips, D.L.(1962) A technique for the numerical solution of certain integral equations of the first kind, J.ACM 9, 84-97.
[7] te Riele, H.J.J.(1984) A program for solving first kind Fredholm integral equations by means of regularization, preprint, submitted for publication.
[8] Tihonov, A.N. and V.Y. Arsenin(1977) Solution of ill-posed problems (V.H. Winter and Sons, Washington D.C.).
[9] Titchmarsh, E.C.(1948) Introduction to the theory of Fourier integrals (The Clarendon Press, Oxford).
[10] Wagenaar, R.W.(1984) Small angle elastic scattering of electrons by noble gas atoms, Doctor's Thesis (Amsterdam).

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