may be looked up under the corresponding entry in Table 2.* The order of the coefficients corresponds exactly to the order of assignment of independency, *i.e.* in the case of linear relationships the independent parameters always enter on the left-hand side of the dependent ones. It is worth noting that three of the non-centrosymmetric groups have null third-rank tensors but one free coefficient as some higher level (rank 5 for 422, rank 7 for 622, rank 9 for 432).

It should also be remembered that, in a least-squares refinement of a non-centrosymmetric structure, one parameter corresponding to a non-zero entry for the point group has to be kept fixed (Hazell & Willis, 1978).

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* The tables containing the symmetry restrictions of the seventh- and eighth-rank tensors have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38913 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

BRENDEL, R. (1979). *Acta Cryst.* A**35**, 525–533.

CHUNG, D. Y. & LI, Y. (1974). *Acta Cryst.* A**30**, 1–13.

FUMI, F. G. & RIPAMONTI, C. (1983). *Acta Cryst.* A**39**, 245–251.

HAZELL, R. G. & WILLIS, B. T. M. (1978). *Acta Cryst.* A**34**, 809–811.

HUTTON, J. & NELMES, R. J. (1981). *J. Phys. C*, **14**, 1713–1736.

International Tables for X-ray Crystallography (1952). Vol. 1. Birmingham: Kynoch Press.

JOHNSON, C. K. & LEVY, H. A. (1974). *International Tables for X-ray Crystallography*, Vol. IV, pp. 311–336. Birmingham: Kynoch Press.

KUHS, W. F. (1983). *Acta Cryst.* A**39**, 148–158.

PERENTHALER, E. & SCHULZ, H. (1981). *Solid State Ionics*, **1**, 335–365.

SCHULZ, H., PERENTHALER, E. & ZUCKER, U. H. (1982). *Acta Cryst.* A**38**, 729–733.

SIROTIN, Y. I. (1960). *Sov. Phys. Crystallogr.* **5**, 157–165.

ZUCKER, U. H., PERENTHALER, E., KUHS, W. F., BACHMANN, R. & SCHULZ, H. (1983). *PROMETHEUS. Program System for Structure Refinements. J. Appl. Cryst.* **16**, 358.

ZUCKER, U. H. & SCHULZ, H. (1982). *Acta Cryst.* A**38**, 568–576.

Acta Cryst. (1984). A**40**, 137–142

The Solution of the One-Dimensional Sign Problem for Fourier Transforms

BY D. I. SVERGUN AND L. A. FEIGIN

Institute of Crystallography, Academy of Sciences of the USSR, Leninsky prospekt 59, *Moscow* 117333, *USSR*

AND B. M. SCHEDRIN

Computing Mathematics and Cybernetics Department, Moscow State University, Moscow 117234, *USSR*

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Abstract

An iterative procedure for the determination of the signs of scattering amplitudes is considered. It is assumed that the scattering density is a one-dimensional antisymmetric function with a limited range of definition. The convergence of the method to a rigorous solution is proved. The stability of the procedure with respect to various experimental errors is shown in model examples. The proof can be generalized for a one-dimensional phase determination of a continuous intensity distribution.

Introduction

When non-crystalline objects are investigated by diffraction methods, the intensity of coherent scattering $I(\mathbf{s})$ can often be measured as a continuous function of scattering vector $\mathbf{s}$ (for instance, intensity distribution along layer lines for one-dimensionally periodic structures, intensity of small-angle scattering). The restoration of the scattering density distribution frequently requires the solution of the phase problem. The latter is analogous to the phase problem in crystal-structure analysis and lies in finding the phases of scattering amplitudes $A(\mathbf{s})$ when their moduli are known from the experimental intensities. In the present paper the case will be considered when the scattering density is a one-dimensional antisymmetric function, so that its connection with the scattering amplitude is given by the sine–Fourier transform

$$A(s) = \mathcal{F}_s[\rho(r)] = \int_0^\infty \rho(r) \sin sr \, dr \qquad (1)$$

and $A(s)$ is a real function.

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Then the density distribution function $\rho(r)$ can be determined by the reverse transform

$$\rho(r) = \int_0^\infty [\pm |A(s)|] \sin sr \, ds \qquad (2)$$

(the constants before the integrals are omitted for the sake of simplicity). The moduli of amplitudes $|A(s)| = [I(s)]^{1/2}$, and the problem consists of the determination of the true signs of the function $A(s)$. Such a problem must be solved, for example, in small-angle scattering when determining the radial density distribution of spherically symmetric particles (Guinier & Fournet, 1955). It should be noted, however, that the results presented below can be generalized for the case of a complex function $A(s)$.

The possibility of finding the true signs of function $A(s)$ is based on the fact that $\rho(r)$ has a finite range of definition [*i.e.* such a value R exists that $\rho(r) \equiv 0$ when $r > R$, and, therefore, R is the upper limit of integration in (1)]. This condition is fulfilled in practice, since the dimensions of any object under investigation are finite. Hosemann & Bagchi (1962) showed that the task of restoring the function $\rho(r)$ knowing $I(s)$ and R has a unique solution (except for a factor ± 1).

However, a valid method for sign determination has not yet been proposed. Many authors solved this problem by sorting out the signs of the maxima of $|A(s)|$ or simply by assigning $A(s)$ alternative signs to successive maxima of $|A(s)|$ (see, for example, Fischbach & Anderegg, 1965; Mateu, Tardieu, Luzzati, Aggerbeck & Scanu, 1972). The 'pattern recognition' technique (Luzzati, Tardieu & Taupin, 1972) sorts out all the possible combinations of signs [for a discrete function $I(s)$]. The automatic determination of the signs using explicitly the finiteness of the range of definition of $\rho(r)$ is performed in the iterative procedures (the so-called 'box-function refinement', see Makowski, 1981). Crowther (1967, 1969) has developed a general theory of such methods for non-crystallographic symmetry. These methods are simple in use and ensure reliable results. However, their convergence has not been shown rigorously elsewhere.

It is also possible in principle to restore function $\rho(r)$ without solving the sign problem, using the fact that the Fourier image of scattering intensity in the general case represents the so-called self-convolution of density distribution (Hosemann & Bagchi, 1962). To solve the one-dimensional integral equation of self-convolution using the finiteness of $\rho(r)$ a number of techniques were proposed (*e.g.* Pape, 1974; Bradaczek & Luger, 1978). These techniques, however, show a numerical instability. A method stable with respect to experimental errors was developed by Glatter (1981). Unfortunately, this method is complicated and represents the solution only as a superposition of step functions.

In this paper a simple method for restoring the true signs of scattering amplitude (1) is considered and rigorously substantiated.

The method of sign determination

The method considered below is a particular case of the general technique developed by Svergun, Feigin & Schedrin (1982) for the interpretation of small-angle scattering data. It is based on the finiteness of $\rho(r)$ and is analogous to the 'box-function refinement' technique (Makowski, 1981). The algorithm of the method consists of the iterative procedure

$$\tilde{A}_k(s) = \text{sign}\,[A_k(s)]\,|A(s)| \qquad (3)$$

$$\rho_{k+1}(r) = \tilde{\rho}_k(r) \Pi(r - R). \qquad (4)$$

Here k is the iteration number, functions $A_k(s)$ and $\rho_k(r)$, $\tilde{A}_k(s)$ and $\tilde{\rho}_k(r)$ are connected by transform (1) and the step function

$$\Pi(r - R) = \begin{cases} 1, & r \le R \\ 0, & r > R. \end{cases} \qquad (5)$$

The convergence of the process can be tested by R factors of discrepancy in reciprocal and real space:

$$R_I = \int_0^\infty [I(s) - A_k^2(s)]^2 \, ds \Big/ \int_0^\infty I^2(s) \, ds \qquad (6)$$

$$R_\rho = \int_0^R [\rho_{k+1}(r) - \rho_k(r)]^2 \, dr \Big/ \int_0^R \rho_k^2(r) \, dr. \qquad (7)$$

To substantiate the validity of process (3)–(4) the following reasoning is often given: if the set of signs determined by $A_k(s)$ is wrong, $\tilde{\rho}_k(r)$ is infinite, so transform (4) results in the change of this set. Since the true set of signs corresponds to function $\rho(r)$ having the finite support, the signs of $A_{k+1}(s)$ should be more appropriate, *etc.* Indeed, the model calculations show that the process converges uniformly over the factors R_I and R_ρ. The set of signs is restored, as a rule, almost completely and then the signs no longer change. It is obvious, however, that neither the above arguments nor model calculations can offer a rigorous proof of the convergence of the processes analogous to (3)–(4) to the true solution. Meanwhile a reliable proof of this fact would be quite important since such methods are easily applicable and are widely used in structure analysis.

The convergence of the method

First of all let us derive the explicit relation between the functions $A_k(s)$ and $A_{k+1}(s)$. The 'sign' function can be defined as

$$\text{sign}\,[A_k(s)] = \begin{cases} A_k(s)/|A_k(s)| & \text{if } A_k(s) \neq 0 \\ 0 & \text{if } A_k(s) = 0. \end{cases} \qquad (8)$$

Expressing $\tilde{\rho}_k(r)$ from $\tilde{A}_k(s)$ according to (2), one can

substitute it in (4) and take the sine–Fourier transform from both parts of the obtained equation. When making this it is appropriate to use the folding theorem for the sine–Fourier transforms (Sneddon, 1951): if $F_s(s)$ and $G_c(s)$ are the sine- and cosine–Fourier transforms of $f(r)$ and $g(r)$, correspondingly $F_s(s) = \mathcal{F}_s[f(r)]$, $G_c(s) = \mathcal{F}_c[g(r)]$, then

$$\mathcal{F}_s[f(r)g(r)] = F_s(s) * G_c(s) = \tfrac{1}{2}\int_0^\infty F_s(u)[G_c(|u-s|) - G_c(u+s)]\,du. \tag{9}$$

Thus, one obtains

$$A_{k+1}(s) = [\tilde{A}_k(s)] * \mathcal{F}_c[\Pi(r-R)] = \tfrac{1}{2}\int_0^\infty [A_k(u)/|A_k(u)|]|A(u)|\Pi_s(R, s, u)\,du, \tag{10}$$

where

$$\Pi_s(R, s, u) = \sin R(s-u)/(s-u) - \sin R(s+u)/(s+u). \tag{11}$$

Equations (10) and (11) provide an explicit connection between the two successive iterations. Futhermore, applying (9) to the trivial equation

$$\rho_{k+1}(r) = \rho_{k+1}(r)\Pi(r-R), \tag{12}$$

one obtains

$$A_{k+1}(s) = \tfrac{1}{2}\int_0^\infty A_{k+1}(u)\Pi_s(R, s, u)\,du. \tag{13}$$

It is obvious that all the functions which show the sine–Fourier image equal to zero beyond the finite interval $0 \le r \le R$ will obey (13).

Subtracting (13) from (10) one gets

$$\varphi(s) \equiv 0 = \tfrac{1}{2}\int_0^\infty \{[A_k(u)/|A_k(u)|] \times |A(u)| - A_{k+1}(u)\}\Pi_s(R, s, u)\,du. \tag{14}$$

It is clear that for any function $\alpha(s)$

$$\int_0^\infty \alpha(s)\varphi(s)\,ds = 0. \tag{15}$$

In particular it is valid for $\alpha(s) = A_k(s)$:

$$\tfrac{1}{2}\int_0^\infty A_k(s)\int_0^\infty \{[A_k(u)/|A_k(u)|] \times |A(u)| - A_{k+1}(u)\}\Pi_s(R, s, u)\,du\,ds = 0. \tag{16}$$

Since the integrals in (16) converge it is possible to change the order of integration:

$$\int_0^\infty \{[A_k(u)/|A_k(u)|]|A(u)| - A_{k+1}(u)\} \times \left[\tfrac{1}{2}\int_0^\infty A_k(s)\Pi_s(R, s, u)\,ds\right] du = 0. \tag{17}$$

Function $\Pi_s(R, s, u)$ is symmetrical with respect to s and u, so the inner integral in (17) is simply $A_k(u)$ [taking (13) into account]. Thus,

$$\int_0^\infty A_k(u)\{[A_k(u)/|A_k(u)|]|A(u)| - A_{k+1}(u)\}\,du = 0 \tag{18}$$

or

$$\int_0^\infty |A_k(u)A(u)|\,du = \int_0^\infty A_k(u)A_{k+1}(u)\,du. \tag{19}$$

Rewriting (10) and (13) for $A_k(s)$ and making the calculations as in (14)–(19) one obtains

$$\int_0^\infty A_k^2(u)\,du = \int_0^\infty A_k(u)|A(u)|[A_{k-1}(u)/|A_{k-1}(u)|]\,du. \tag{20}$$

Since, for any integrable function $\alpha(s)$,

$$\int_0^\infty \alpha(s)\,ds \le \int_0^\infty |\alpha(s)|\,ds, \tag{21}$$

one has from (20)

$$\int_0^\infty A_k^2(u)\,du \le \int_0^\infty |A_k(u)A(u)|\,du. \tag{22}$$

Using (19) one gets

$$\int_0^\infty A_k^2(u)\,du \le \int_0^\infty A_k(u)A_{k+1}(u)\,du. \tag{23}$$

According to the Cauchy–Schwartz inequality (Korn & Korn, 1968), one can write

$$\left|\int_0^\infty A_k(u)A_{k+1}(u)\,du\right| \le \left[\int_0^\infty A_k^2(u)\,du \int_0^\infty A_{k+1}^2(u)\,du\right]^{1/2}. \tag{24}$$

Since both parts in (23) are positive, then, using (24), one finally arrives at

$$\int_0^\infty A_k^2(s)\,ds \le \int_0^\infty A_{k+1}^2(s)\,ds. \tag{25}$$

The integrals in (25) represent simply a squared norm of solution – according to the Parseval theorem (Korn & Korn, 1968) one has

$$\|\rho_{k+1}\|^2 = \int_0^R \rho_{k+1}^2(r)\,dr = \int_0^\infty A_{k+1}^2(s)\,ds = \|A_{k+1}\|^2. \tag{26}$$

Furthermore, it is clear [for instance from (22)] that at any step of the iterative procedure

$$\|A_k\|^2 \le \|A\|^2. \tag{27}$$

Thus the sequence of the norms $\|A_k\|^2$ is monotonic, according to (25), and restricted according to (27). As known from the mathematical analysis such a sequence has a limit (Korn & Korn, 1968). Besides, it is easy to show that if $\|A_k\|^2 = \|A_{k+1}\|^2$ these functions are identical. Indeed, let us consider

$$\int_0^\infty [A_k(s) - A_{k+1}(s)]^2 \, ds = 2\|A_k\|^2 - 2\int_0^\infty A_k(s)A_{k+1}(s)\, ds \geq 0. \quad (28)$$

Comparing (25) and (28), one can infer that only the equality sign can occur in (28), *i.e.* $A_k(s)$ coincides with $A_{k+1}(s)$ everywhere.

So we have proved that process (3)–(4) always converges to some solution. Now let us consider this solution as such.

The uniqueness of the solution

First of all it will be shown that the process will not stop until the norm of the solution reaches the value of $\|A\|^2$. Let us suppose that the process stops at the kth step, *i.e.* the conditions

$$\text{sign}\,[A_{k-1}(s)] \not\equiv \text{sign}\,[A_k(s)] \quad (29)$$

$$A_k(s) = A_{k+1}(s) \quad (30)$$

are fulfilled. Then it is possible to write

$$A_k(s) = \tfrac{1}{2}\int_0^\infty [A_{k-1}(u)/|A_{k-1}(u)|] \times |A(u)|\Pi_s(R, s, u)\, du \quad (31)$$

$$A_{k+1}(s) = A_k(s) = \tfrac{1}{2}\int_0^\infty [A_k(u)/|A_k(u)|] \times |A(u)|\Pi_s(R, s, u)\, du. \quad (32)$$

Subtracting (31) from (32) and performing the calculations as in (14)–(19) one obtains

$$\int_0^\infty |A_k(u)A(u)|\, du = \int_0^\infty |A(u)|A_k(u)[A_{k-1}(u)/|A_{k-1}(u)|]\, du. \quad (33)$$

Since (29) takes place, *i.e.* the signs of $A_{k-1}(s)$ and $A_k(s)$ cannot fully coincide, then, applying (21) for estimation of the right side of (33), it is necessary to choose the 'greater than' sign. So one arrives at

$$\int_0^\infty |A_k(u)A(u)|\, du < \int_0^\infty |A_k(u)A(u)|\, du. \quad (34)$$

This contradiction proves that if the signs change at the $(k-1)$th iteration they should change at the kth iteration, too. Clearly it is equivalent to the fact that the sequence of norms is rigorously increasing.

Let us now suppose that the process converges to some solution $A_I(s)$ with the norm $\|A_I\|^2 < \|A\|^2$. It is obvious that, if one continues the process with any function $\tilde{A}_I(s)$ as the initial approximation which differs from $A_I(s)$ as little as possible and shows the same (or greater) value of the norm, the latter would increase again, so the process will not return to $A_I(s)$. It means that such a solution, if it exists, is unstable. Therefore, the inclusion of such perturbations in the procedure when the norm of the obtained solution is less than the actual value $\|A\|^2$ (it is, however, only a formal requirement, since to get an unstable solution is improbable in practice) ensures that the process will converge to the final solution with the maximal value of the norm, namely $\|A\|^2$.

Thus the squared norm of the resulting solution – function $A_s(s)$ – is equal to $\|A\|^2$. It is obvious from (22) that the only case obeying this condition is the case

$$|A_s(s)| = |A(s)| \quad \text{for all } s. \quad (35)$$

So the solution density distribution $\rho_s(r)$ given by process (3)–(4) has the same support as $\rho(r)$ and the same moduli of the sine–Fourier image. Let us consider the difference function

$$\Delta\rho(r) = \rho(r) - \rho_s(r). \quad (36)$$

Its Fourier image will be

$$\Delta A(s) = \begin{cases} 0 & \text{if } A(s)A_s(s) \geq 0 \\ 2A(s) & \text{if } A(s)A_s(s) < 0. \end{cases} \quad (37)$$

So, if the intervals existed where the signs of $A(s)$ and $A_s(s)$ were opposite [except for the case $A(s) = -A_s(s)$ and, correspondingly, $\rho(r) = -\rho_s(r)$ everywhere] then $\Delta A(s)$ would be a non-zero function equal to zero within some finite intervals. This is impossible for a function having the Fourier image with a finite support (such a function should be analytical, see Hosemann & Bagchi, 1962). Thus $\Delta A(s)$ should be either zero or $2A(s)$ everywhere, so we obtain finally

$$\rho_s(r) = \pm\rho(r). \quad (38)$$

Consequently, it has been proved that the iterative procedure (3)–(4) converges to the true solution up to a sign. It is worth noting that the result is not affected by the initial approximation (the only requirement is that the signs should change at the first iteration).

The stability of the method

The above proof, of course, deals with an ideal theoretical case – all the input parameters [function $I(s)$,

the value R] are assumed to be exactly defined. In practice they are known, as a rule, with some errors. So for practical use of the method in question its stability with respect to the experimental errors should be examined. An appropriate approach to the investigation of the stability consists of making model calculations inserting different errors in the input parameters.

The stability of the analogous algorithm was shown with a number of various model examples by Svergun, Feigin & Schedrin (1983). Here we shall present some examples to illustrate the stability of the procedure with respect to basic experimental errors.

The model calculations were carried out as follows. For a given function $\rho(r)$ the intensity curve $I(s)$ was calculated within some interval $0 \le s \le s_{max}$, then the restoration of $\rho(r)$ using procedure (3)–(4) was done for a fixed value of R. As the initial approximation the signs of the function $\cos sR$ were chosen (it can be readily shown that they are the signs of the main asymptotic trend of the functions obeying (13) when s tends to infinity). The process stopped when the R_ρ factor became less than some accuracy ε (for our calculations ε was chosen equal to 10^{-3}).

The example showing the restoration of $\rho(r)$ upon all the parameters exactly defined is given in Fig. 1 [the value of s_{max} was 0·5, *i.e.* $s_{max}R$ was equal to 50, making the termination effects in (2) negligibly small]. The process converges quite fast (it took only three iterations to get the desired accuracy) and the restored function (curve 2) coincides with the true one (curve 1) almost completely. Values

$$\mu_k = \|\rho_k\|^2 / \|\rho\|^2 \qquad (39)$$

and R_I are given in Fig. 2 as functions of the iteration number k.

The errors in practice can appear due to the following factors: (1) the uncertainty of the R value; (2) statistical noise in $I(s)$; (3) the termination of $I(s)$ for $s > s_{max}$. Besides, a question arises whether the solution remains independent of the initial approximation under the erroneous input data. Our calculations demonstrate the stability of the procedure with respect to all these factors. In particular it should be noted that the increase of R would not alter the result (for $R' > R$ all the above formulae hold, so the increase of R can only lead to an increase of the number of iterations in order to achieve the same accuracy ε). Meanwhile the decrease of R should worsen the R_I factor of the resulting solution (see Svergun, Feigin & Schedrin, 1983). Thus, such a method can be applied for refinement of the value of R when it is approximately known.

Figs. 1 and 2 show the application of the method when the distortions are inserted into all the input parameters simultaneously: the value of $R' = 0{\cdot}9\,R$, $I(s)$ contains the normally distributed statistical noise with the standard deviation $\sigma = 20\%$, the value of $s_{max} = 0{\cdot}2$, *i.e.* $s_{max}R' = 18$ (quite a realistic case for an experiment). The initial approximation was also changed (the signs of the function $\cos 2{\cdot}5\,sR$ were taken). Nevertheless it is evident that no significant changes occur besides the increase of the number of iterations required. Analogous results were obtained for a number of other model functions. Fig. 3 gives an example of application of the procedure for the restoration of the function $\rho(r)$ containing discontinuities (namely multistep function). This is the most unfavourable case because the termination effects in (2) become quite significant. However, as one can see from Fig. 3, the restoration remains satisfactory (to reduce the termination effects we used the filter described by Rolbin, Svergun, Feigin & Schedrin, 1980).

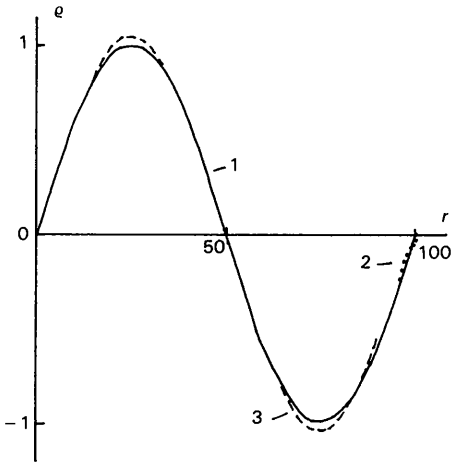

Fig. 1. The restoration of the model density distribution. (1) Function $\rho(r)$, $R = 100$; (2) function $\rho_s(r)$, $s_{max} = 0{\cdot}5$; (3) $\rho_s(r)$ when inserting the errors into all input parameters.

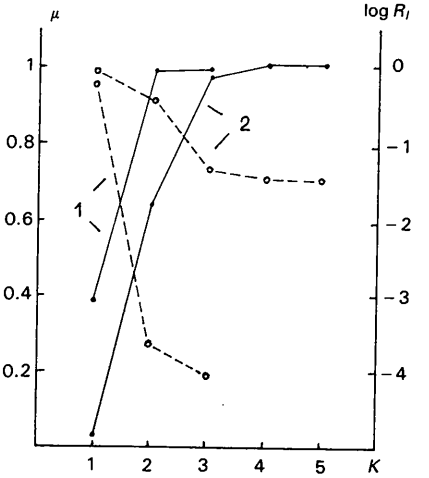

Fig. 2. The norm of the solution and R_I factor as functions of the iteration number. (1) The restoration by the exact data; (2) the restoration in the presence of errors. Solid line μ_k, dashed line R_I.

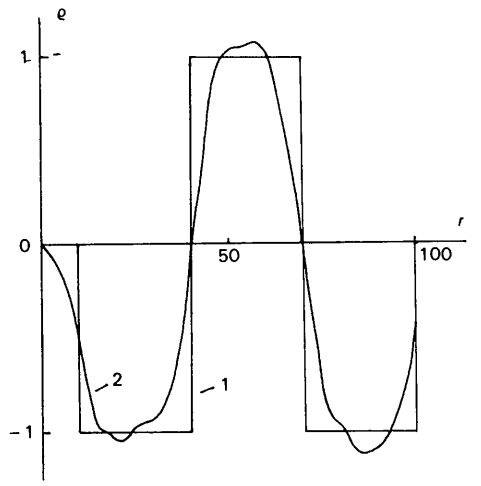

Fig. 3. The restoration of multistep distribution. (1) $\rho(r)$, $R = 100$; (2) $\rho_s(r)$, $s_{max} = 0{\cdot}5$. The result of the 5th iteration is given, $\mu = 0{\cdot}76$, $R_f = 0{\cdot}187$.

Conclusions

The method presented can be applied for determinations of signs of scattering amplitudes in the analysis of various non-crystalline objects. In particular it is possible to use the method in small-angle scattering for the restoration of the structure of the particles which can be described by a one-dimensional function [spherically symmetrical, rod-like (Fedorov, 1971); flattened (Lesslauer, Cain & Blasie, 1972)].

The above proof can be used also for the general case of one-dimensional Fourier transform

$$A(s) = \int_{R_1}^{R_2} \rho(r) \exp(isr)\, dr. \qquad (40)$$

In this case (3) and (8) provide the phases of $\tilde{A}_k(s)$ and the function

$$\Pi(r, R_1, R_2) = \begin{cases} 1, & R_1 \le r \le R_2 \\ 0, & r < R_1, r > R_2 \end{cases} \qquad (41)$$

should be substituted into (4) instead of $\Pi(r - R)$. The convergence of such a procedure can be proved with arguments similar to these considered above. The difference will lie in the fact that the coincidence of the moduli (35) does not ensure the uniqueness of the solution. The number of possible solutions in this case will depend on the number of complex zeros of the analytical continuation of function $A(s)$ (Walther, 1962). The iterative procedure will converge to one of these solutions depending on the initial approximation.

References

BRADACZEK, H. & LUGER, P. (1978). *Acta Cryst.* A**34**, 681–683.

CROWTHER, R. A. (1967). *Acta Cryst.* **22**, 758–764.

CROWTHER, R. A. (1969). *Acta Cryst.* B**25**, 2571–2580.

FEDOROV, B. A. (1971). *Acta Cryst.* A**27**, 35–47.

FISCHBACH, F. A. & ANDEREGG, J. W. (1965). *J. Mol. Biol.* **14**, 458–473.

GLATTER, O. (1981). *J. Appl. Cryst.* **14**, 101–108.

GUINIER, A. & FOURNET, G. (1955). *Small-Angle Scattering of X-rays*, p. 28. New York: Wiley.

HOSEMANN, R. & BAGCHI, S. N. (1962). *Direct Analysis of Diffraction by Matter*, Ch. 15. Amsterdam: North Holland.

KORN, G. & KORN, T. (1968). *Mathematical Handbook*, Ch. 4. New York: McGraw-Hill.

LESSLAUER, W., CAIN, J. E. & BLASIE, J. K. (1972). *Proc. Natl Acad. Sci. USA*, **69**, 1499–1503.

LUZZATI, V., TARDIEU, A. & TAUPIN, D. (1972). *J. Mol. Biol.* **64**, 268–286.

MAKOWSKI, L. (1981). *J. Appl. Cryst.* **14**, 160–168.

MATEU, L., TARDIEU, A., LUZZATI, V., AGGERBECK, L. & SCANU, A. M. (1972). *J. Mol. Biol.* **70**, 105–116.

PAPE, E. H. (1974). *Biophys. J.* **14**, 284–294.

ROLBIN, YU. A., SVERGUN, D. I., FEIGIN, L. A. & SCHEDRIN, B. M. (1980). *Kristallografiya*, **26**, 1125–1128 (in Russian). Engl. trans: *Sov. Phys. Crystallogr.* (1981), **26**, 645–648.

SNEDDON, I. (1951). *Fourier transforms*, Ch. 1. New York: McGraw-Hill.

SVERGUN, D. I., FEIGIN, L. A. & SCHEDRIN, B. M. (1982). *Acta Cryst.* A**38**, 827–835.

SVERGUN, D. I., FEIGIN, L. A. & SCHEDRIN, B. M. (1983). *Kristallografiya*, **28**, 252–259.

WALTHER, A. (1962). *Opt. Acta* **10**, 41–49.