A Deconvolution Method for Evaluating Small-Angle X-ray Scattering from Lamellar Structures

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(Received 3 November 1977; accepted 15 May 1978)

An iterative deconvolution method is presented which is suitable for evaluating scattering diagrams of lamellar structures with a centrosymmetric unit cell. The analysis of the scattering intensity via the \( Q \) function of Hosemann and Bagchi requires the deconvolution of the generalized Patterson function of the unit cell, the \( Q_0 \) function. Using a Gaussian representation for the electron density distribution of the unit cell \( q_0(x,y,z) \), the deconvolution of the corresponding \( Q_0 \) function is performed by a least-squares refinement of the Gaussian parameters, employing the nonlinear least-squares method of Marquardt [J. Soc. Ind. Appl. Math. (1963), 11, 431-441]. The advantages of the method are: (i) the number of parameters describing the structure \( q_0 \) can be held to a minimum; (ii) the method is also well suitable for the deconvolution of distorted \( Q_0 \) functions; (iii) the complete computing time is very short. The method has been successfully tested on a series of model functions and has been applied to an experimental function derived from the small-angle scattering data of wet erythrocyte ghost membranes. The way to estimate a first approximation of the solution is described and the limits of the method are discussed.

I. Introduction

The evaluation of small-angle X-ray scattering diagrams from lamellar systems by analyzing the Fourier transform of the scattered intensity, i.e. the generalized Patterson function or \( Q \) function (Hosemann & Bagchi, 1962) has two advantages:

1. the content of information regarding the 'lattice' can be better separated from that relating to the unit-cell structure;
2. the details of the experimental and the calculated \( Q \) function can be more easily interpreted in terms of the model being considered.

We describe a method to determine electron density distributions of layered structures, where these distributions represent the projected electron density distributions of lamellar layers onto the stacking axis. A prerequisite for the application of the method is that the \( Q_0 \) function, i.e. the generalized Patterson function of the unit cell, can be separated from the complete \( Q \) function. This is possible only in two cases:

(a) The multilayer contains only a small number of unit cells. The corresponding \( Q \) function is a rapidly decreasing quasi-periodic function from which the \( Q_0 \) function can be isolated. Examples are given by Kreutz (1968, 1970) and by Lesslauer, Cain & Blasie (1971) and Lesslauer & Blasie (1972).

(b) Consecutive unit cells are separated from each other by regions of constant electron density. The level of this constant density can be considered as the level of zero relative electron density. If the extension of these regions exceeds the extension of the unit cell (double membrane), the repeating terms of \( Q(x) \), centered at the lattice points \( nL \), do not overlap each other. In such a case the \( Q_0 \) function is obtained without an additional separation procedure. Examples for evaluation are swollen nerve myelin (McIntosh & Worthington, 1974; Worthington & McIntosh, 1974) and wet erythrocyte ghosts (Pape, Klott & Kreutz, 1977).

The three-dimensional electron density \( q(x,y,z) \) is considered to be constant in \( y \) and \( z \) directions and to vary in the \( x \) direction, the stacking direction. Therefore the representation can be reduced to an one-dimensional system. A characteristic additional property of the multilayer is the regular sequence of image \( q_m \) and mirror image \( q_{-m} \) of the single layer along the stacking direction. Thus, the unit cell, which is built up by two single layers, can be considered to be centrosymmetric.

The deconvolution of \( Q_0 \) functions referred to centrosymmetric structures has an unambiguous solution \( q_0(x,y,z) \), except for the reflection about the abscissa, i.e. \( -q_0(x) \) (Hosemann & Bagchi, 1962). Several methods have been developed to deconvolute such \( Q_0 \) functions (Hosemann & Bagchi, 1962; Kreutz, 1968; Worthington, King & McIntosh, 1974; Pape, 1974; Moody, 1974), but all these methods are limited in their application to undistorted \( Q_0 \) functions. The iterative Gaussian deconvolution method outlined below is especially suitable in the case of lattice distortions, i.e. if the distance between the two single layers building up the unit cell varies according to a statistical distance distribution.

II. Description of the one-dimensional system using convolution operations

The system consists of multilayers composed of stacked and flattened hollow vesicles (see Fig. 1). Let \( q_0(x) \) represent the projected electron density distribution of the shell of the vesicle (the single membrane) onto the stacking axis \( x \). \( q_0(x) \) denotes the density profile of the unit cell, a double membrane. This consists of the density distribution \( q_{ml}(x) \) and the density distribution of its mirror image \( q_{ml}(-x) = q_{ml}(x) \) in a spacing \( l_1 \):

\[
q_0(x) = q_{ml}(x) + q_{ml}(x) * \delta(x - l_1),
\]

where

* = convolution symbol, defined by \( f * g = \int_{-\infty}^{\infty} f(t) g(x-t) dt \)

\( \delta \) = Dirac delta function.

According to Fig. 1, we distinguish between \( l_1 \), the \text{intra-unit cell nearest-neighbor distance, and} \( l_2 \), the \text{inter-unit cell nearest-neighbor distance of adjacent single membranes. Both distances are allowed to vary and the deviation from the mean value may be governed by statistical distance distribution functions} \( H_1(x) \) and \( H_2(x) \) respectively.
With the notation:
\[ Q_m = \rho_m \ast \rho_m; \quad Q_m = \rho_m \ast \rho_m; \quad Q_m = \rho_m \ast \rho_m, \]
the \( Q_0 \) function, or generalized Patterson function of the unit cell \( Q_0 \), is given by:

(a) with lattice distortions neglected (i.e. \( l_1 \) is fixed)
\[ Q_0(x) = 2Q_m(x) + Q_m^2 \ast \delta(x - l_1), \quad x \geq 0; \tag{2} \]

(b) with lattice distortions taken into account (i.e. \( l_1 \) can vary)
\[ Q_0(x) = 2Q_m(x) + Q_m^2 \ast H_1(x - l_1). \tag{3} \]

The following deconvolution procedures are suitable to \( Q_0 \) functions, notwithstanding the method of their isolation from \( Q(x) \), the Fourier transform of the scattered intensity.

The relation between \( Q(x) \) and \( Q_0(x) \) is thereby given by
\[ Q(x) = Q_0(x) \ast [z(x) \ast s(x) \ast s(-x)], \tag{4} \]
where \( z(x) \) denotes a one-dimensional lattice autocorrelation function and \( s(x) \) represents the shape function of a multilayer, defined by \( s(x) = 1 \) within the multilayer, and \( s(x) = 0 \) elsewhere.

Note that both the \( Q_0 \) function and the \( Q \) function are always centrosymmetric functions according to their definitions. In equations (2) and (3), therefore, only the right halves of these functions are represented, corresponding to \( x \) values greater than or equal to zero.

### III. Iterative Gaussian least-squares deconvolution (LSD) procedure

To calculate the electron density profile \( \rho_m \) of a single membrane by a deconvolution procedure, we proceed in the following way:

We represent \( \rho_m \) by a sum of \( N_0 \) Gaussians of the same width:
\[ \rho_m = \sum_{k=1}^{N_0} A_k \exp \left[ -0.5c(x - x_k)^2 \right]. \tag{5} \]

\( N_0 \) lies between 3 and 6 in the following examples. The distance distribution function \( H_1 \) is also generated by a Gaussian function:
\[ H_1(x) = (c_1 / \pi)^{0.5} \exp \left[ -c_1(x - l_1)^2 \right]. \tag{6} \]

It is convenient to choose Gaussian functions, because the convolution of a Gaussian with a Gaussian yields a Gaussian. Thus all terms in equations (2) and (3) are easily calculated as convolution polynomials of Gaussian functions:
\[ Q_m = \sum_{i=1}^{N_0} \sum_{k=1}^{N_0} A_i A_k \exp \left[ -0.5c(x - x_i - x_k)^2 \right], \tag{7} \]
\[ Q_m = \sum_{i=1}^{N_0} \sum_{k=1}^{N_0} A_i A_k \exp \left[ -0.5c(x + x_i + x_k)^2 \right], \tag{8} \]
where \( w_Q \) is given by \( w_Q = (\pi / 2c)^{0.5} \). Additional convolution with \( H_1(x) \) leads to the second term of equation (3)
\[ Q_m = w_Q w_{H_Q} \sum_{i=1}^{N_0} \sum_{k=1}^{N_0} A_i A_k \exp \left[ -c_1 / (c_1 + 0.5c) \right] \exp \left[ -c_1(x + x_i + x_k - l_1)^2 \right], \tag{9} \]
where \( w_{H_Q} \) is given by \( w_{H_Q} = [c_1 / (c_1 + 0.5c)]^{0.5} \).

The use of Gaussians of different widths in \( \rho_m \) has no significant effect on the degree of agreement between experimentally observed and synthesized functions. In order to reduce the number of parameters, only Gaussians of equal width were used.

With an initial set of parameters \( A_i, x_i, c, c_1, l_1 \) we calculate the quantities \( Q_m, H_1 \) and \( Q_m \) and the complete expression \( Q_0(x) \) according to (3). The result is compared with the input \( Q_0 \) function, either given as a model \( Q_0 \) function (in tests) or as an experimentally obtained \( Q_0 \) function. In a subsequent least-squares refinement procedure (Marquardt, 1963), the parameters of the Gaussians describing \( \rho_m \) and \( H_1 \) are varied until the differences between \( Q_0 \), input and \( Q_0 \), recalculated are minimized. The solution \( \rho_m \) that gives the best agreement between \( Q_0 \), input and \( Q_0 \), recalculated will be considered as the correct one.

To quantify the extent of agreement, the following \( R_Q \) value is defined:
\[ R_Q = \frac{\sum_{m=1}^{m_c} \left[ Q_0 \text{, input}(x_m) - Q_0 \text{, recal}(x_m) \right]^2}{\left[ Q_0 \text{, input}(x_m) \right]^2}, \tag{10} \]
where \( m_c \) represents the number of sampled values of the \( Q_0 \) function taken on a discrete, equidistant set of points along the \( x \) axis with a \( \Delta x \) of 2 Å in all of the examples.
Proof of the Gaussian deconvolution method by another deconvolution method using Fourier series expansions

$Q_0$ functions, undisturbed by a distance distribution function $H_f(x-l_1)$ can be deconvoluted using other deconvolution methods, e.g. the Fourier analytical deconvolution (FAD) method of Pape (1974), which is particularly suitable in this case. It consists of a determination of the Fourier cosine coefficients $a_k$ of the solution $Q_0(x)$, developed within the interval $D_0$, where $D_0$ denotes the double membrane extension. This can be done in two steps: From the Fourier cosine coefficients of $Q_0(x)$, expanded within the interval $(0,D_0)$ at first the absolute values of the coefficients $a_k$ of $Q_0$ are determined, whereas the Fourier-sine-coefficients of $Q_0$ render a system of simultaneous equations, which enables the determination of the signs.

But this Fourier analytical deconvolution procedure cannot be directly applied to distorted $Q_0$ functions. Such distorted $Q_0$ functions, however, can be 'sharpened' by replacing the distance distribution function $H_f(x-l_1)$ by a delta function $\delta(x-l_1)$. After sharpening, the $Q_0$ function is deconvoluted with the FAD method and the $Q_0$ function is obtained as a pure cosine series:

$$q_0(x) = a_0 + \sum_{k=1}^{N_a} a_k \cos \frac{2\pi k}{D_0} x; \quad -\frac{D_0}{2} \leq x \leq \frac{D_0}{2}, \quad (11)$$

where $N_a$ represents the number of coefficients $a_k$, used in the series expansion.

This treatment of distorted $Q_0$ functions has two advantages:

(i) In addition to the Gaussian representation, a development of $q_0$ into a cosine series is gained;
(ii) the process of smearing and sharpening facilitates the answer to the question of uniqueness.

IV. Results
1. Deconvolution of model functions

Model $Q_0$ functions corresponding to arbitrarily chosen model electron density functions $q_0(x)$ are calculated by numerical integration by Simpson’s rule according to $Q_0 = q_0(x) + q_0(-x)$.

These model $Q_0$ functions are deconvoluted using the above presented iterative Gaussian least-squares deconvolution (LSD) method and the resulting electron profile $q_0_{\text{calc}}(x)$ is compared with the initial model electron density function $q_0(x)$.

In the following step the $Q_0$ function of the resulting solution $q_0_{\text{calc}}$, called $Q_0_{\text{recal}}$, is calculated and compared with the input (or function, here the model $Q_0$ function $Q_0_{\text{model}}(x)$.

The first example is seen in Fig. 2. On the left side we see the $Q_0$ function and on the right side the resulting $q_0$ function after five iterations, compared with the model and recalculated functions. The method for estimation of a first set of parameters, referring to the position, width and height of the Gaussians, will be briefly demonstrated in this example.

The first two columns of Table 1 show the positions and heights of the extrema of the $Q_0$ function, where the central maximum is normalized to a value of 100. From the sequence of the maxima and minima and their heights and positions, one can estimate in a simple manner a first parameter set $x_0, x_1, c_1, l_1$, using equations (2), (7), (9).

For convenience, we choose the position of the first Gaussian of $q_0(x)$ as origin, i.e. $x_1 = 0$, fixed. This is allowable because Patterson functions are independent of the choice of the origin. The following search can be considered as an estimation of initial values of a Gaussian analysis with constraints:

From the number of the extrema a solution based on a 4-Gaussian model is attempted ($N_0 = 4$).

At first the parameter $c$ is estimated to be $c = 0.008$. This follows from the half-width of the last maximum in $Q_0(x)$ of 13 Å.

The factor $w_e$ is then $(\pi/2c)^{0.5} = 14$. From the position and the height of the last maximum of $Q_0$ we find: $l_1 = 198$ Å; $A_1 = 2.2/14$ or $A_1 = 0.4$.

The next inner maximum of $Q_0$ enables us to estimate two further parameters: $2A_1 A_2 = 6/5/14$; thus $A_2 = 0.58$ and $x_2 = 25$ Å.

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Fig. 2. Iterative Gaussian LSD method applied to a model function. Model profile $q_0$ (curve I) on the right side, corresponding convolution square $[Q_0(x)_{\text{model}}]$ on the left side; result of the deconvolution procedure (curve II) on the right side and its corresponding convolution square $[Q_0(x)_{\text{recalced}}]$ on the left side; $H_f(x)$ is considered as a delta function.
Table 1. Estimation of the parameters of the first approximation of $q_0$ (example 1) and comparison with the 'best' values found after five iterations; the $R_Q$ values after each iteration are also given.

<table>
<thead>
<tr>
<th>Extrema of $Q_0$</th>
<th>Parameters</th>
<th>'Best' set after five iterations</th>
<th>Numbers of iterations</th>
<th>$R_Q$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x$ (Å)</td>
<td>$Q_0(x)$</td>
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<td></td>
<td></td>
</tr>
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<td>100.0</td>
<td>$A_1$</td>
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<td>1</td>
</tr>
<tr>
<td>24</td>
<td>-56.0</td>
<td>$A_2$</td>
<td>0.58</td>
<td>2</td>
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<td>13.0</td>
<td>$A_3$</td>
<td>-1.40</td>
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</tr>
<tr>
<td>70</td>
<td>-30.0</td>
<td>$A_4$</td>
<td>1.06</td>
<td>4</td>
</tr>
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<td>48.0</td>
<td>$c$</td>
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<td>5</td>
</tr>
<tr>
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<td>$x_3$</td>
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<td>80.0</td>
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<tr>
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<td>$c_1$</td>
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</tr>
<tr>
<td>250</td>
<td>0.0</td>
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</table>

Fig. 3. Deconvolution of a $Q_0$ function including a statistical distance distribution function $H_i(x)$ with a standard deviation of 10%. Same model function $q_0$ as in Fig. 2.

Fig. 4. Application of the deconvolution method to the $Q_0$ function of a model like that in Fig. 2, but inverted with respect to the ordinate axis [changing of inside to outside and vice versa (no statistical distortions)].
The minimum at \( x = 150 \text{ Å} \) renders \( 2A_1A_3 + A_2^2 = 11.0/14. \)
Therefore \( A_3 = 1.4 \) and \( x_3 = 48 \text{ Å}. \)
From the next minimum we get \( x_4 = 80 \text{ Å} \) and from the
central maximum of \( Q_0 \) (= sum \( A_f^2 \)) we obtain an initial
value of 1.06 for \( A_4. \)

The following computer run based on the least-squares
program of Marquardt (1963) is relatively insensitive to the
estimated heights of the Gaussians \( |A_f| \) but it has been found
very essential that the estimated signs and the spacings be-
tween the Gaussians of the first set roughly correspond to
the signs and positions of the extrema of the \( Q_0 \) function.

The estimated parameters of the first set and the 'best'
values of the parameters, found by the Gaussian LSD pro-
cedure after five iterations, are represented in Table 1. The
lowering of the corresponding \( R_Q \) values after each iteration
is also seen in this table.

The next example (Fig. 3) shows the deconvolution of a
distorted \( Q_0 \) function. It corresponds to the same \( q_0 \) func-
tion, but includes a statistical distance distribution function \( H_1(x - l_1) \) with a standard deviation of 10%. Comparing the
\( Q_0 \) functions of Figs. 2 and 3, we see that the outer extrema
of \( Q_0(x) \) are smeared in Fig. 3 according to the term \( Q_{m2} \times H_1.\)

The result of the Gaussian LSD procedure, obtained
after five iterations, is presented on the right side of Fig. 3
(curve II) and agrees very well with the input \( q_0 \) function.
In Figs. 4 and 5 the deconvolution of two further \( Q_0 \) func-
tions is represented. They are generated by the same \( \mu_m \) func-
tions as in the first example, but the inside and the outside
of the model are inverted.

The above-mentioned proof of the iterative Gaussian de-
convolution method as applied to the distorted \( Q_0 \) func-
tions of Figs. 3 and 5 is seen in Figs. 6 and 7. After the dis-
tance distribution functions \( H_1 \) have been replaced by delta
functions, the 'sharpened' \( Q_0 \) functions are immediately de-
convoluted, yielding electron density functions \( q_0 \) in the
form of cosine series, which agree very well with the model
electron density functions of Figs. 3 and 5.

All the previous model \( q_0 \) functions are generated as a sum
of four Gaussian functions. Fig. 8 shows the deconvolution
of a \( Q_0 \) function belonging to a completely arbitrarily, nu-
merically given model \( q_0 \) function (right side). In this case
differences remain between the resulting electron density \( q_0 \)
and the initial model electron density \( q_0 \), indicating an error
caused by the type of representation of \( q_0 \), here the develop-
ment of \( q_0 \) into a sum of six Gaussians. The differences, how-
ever, are small and suitable to give a realistic estimation of error brackets of electron densities \( q_0 \), determined by this Gaussian LSD method.

2. Deconvolution of the \( q_0 \) function of wet erythrocyte ghost membranes

Erythrocyte ghost membranes (or hemoglobin-free erythrocytes) can be prepared so that they form a one-dimensional system of stacked and flattened vesicles as is schematically shown in Fig. 1. The same deconvolution procedures can then be applied to the experimental \( q_0 \) function, derived from the small angle scattering data of such stacks of wet erythrocyte ghost membranes.

On the one hand, the scattered intensity function exhibits three orders of a periodicity of 600 Å, and two broad maxima at Bragg spacings of 110 and 66 Å; therefore we have \( L = 600 \) Å. On the other hand, from the modulations of the \( q \) function we find a unit-cell extension (corresponding to the sum of double membrane extension and intra-unit cell interspace between single membranes) of ca 300 Å. That means, that the \( q_0 \) function is already isolated without an additional separation procedure.

The result of the iterative Gaussian LSD procedure, using a four-Gaussian model of \( q_0(x) \), is seen in Fig. 9. The corresponding set of 'best' parameters, found by the iterative deconvolution procedure with a four-Gaussian model, is listed in Table 2. Additionally, the 'best' parameters found with a three-Gaussian model are given. The reduction of the \( R_0 \) value from 0.0049 (three-Gaussian model) to 0.0033 (four-Gaussian model) indicates that the fourth Gaussian is an essential part of the electron density profile.

It is important to note that in every example \(-q_0(x)\) represents an equivalent solution. In the case of erythrocytes additional information, e.g. from biochemistry and other

![Fig. 7. Fourier-analytical deconvolution of the sharpened \( q_0 \) function of model II (see Fig. 5).](image)

![Fig. 8. Deconvolution of a \( q_0 \) function referring to a numerically chosen model \( q_0 \) function (curve I, right side). The resulting \( q_0 \) function, after application of the iterative Gaussian LSD method is also seen on the right side (curve II) and its \( q_0 \) function is given by \( q_0 \), recalc (left side). A statistical distance distribution function \( H_1(x) \) with a standard deviation of 6% has been included.](image)
V. Discussion

Generally, the field of application of the iterative Gaussian LSD method is restricted to structure determinations within a range between low resolution and medium resolution (Δx_{min} ~ 15 Å). It cannot be expected to determine positions of individual atoms, and only the position, thickness and relative electron density of characteristic layer-like regions (e.g. protein layers or polar head groups of lipid layers) will be resolved. In this special case, however, a stepwise enhancement of details of the electron density function \( Q_0(x) \) by a successive increase of the number of Gaussians used in the model function, appears advantageous.

Regarding the fact that the \( Q_0 \) function corresponds only to distances between nearest neighbors, a distinction between lattice distortions of the first kind, that retain long-range order, and lattice distortions of the second kind (loss of long-range order) is unnecessary. For more details concerning the influence of lattice distortions on the complete \( Q \) function see the related chapter of the book by Vainshtein (1966) or the paper by Kreutz & Pape (1975).

Influence of experimental errors, correction factors and 'cut-off' effect

A decisive criterion of any method is its sensitivity to errors. Let us shortly examine the propagation of different errors that can affect the process of Fourier transformation of the scattering intensity yielding the complete autocorrelation function \( Q(x) \).

The statistical error of the data points, obtained by proportional-counter measurements or as sampled densitometer tracings of films, will produce a hump in the \( Q \) function lying outside the region of the \( Q_0 \) function. Therefore the \( Q_0 \) function method is only slightly affected by the statistical error of the data.

Correction factors like the Lorentz factor are sources of systematic errors that affect the complete Fourier transform. Their influence cannot be characterized in a general form; however, the advantage of the method, of describing the solution \( Q_0 \) by a minimal number of parameters, facilitates the investigation of the effect of different Lorentz factors on the resulting parameters of the solution \( Q_0 \).

Further, the above-presented method is not specifically influenced by the well-known 'cut-off' effect of the intensity
function. After background subtraction an intensity function is always obtained which continuously decreases to zero at a defined value \( b_{\text{max}} \) and finer details of \( \varrho_0(x) \) than \( \Delta x = 1/2b_{\text{max}} \) cannot be resolved. A desired effect, however, is the rearrangement of the information content of an intensity curve during the process of Fourier transformation. The part of the information regarding the unit-cell structure is concentrated from the whole intensity interval to the inner region of the \( Q \) function, i.e. the region of the \( Q_0 \) function. Thus, if the \( Q_0 \) function is separable, the \( Q_0 \) deconvolution method is preferable to a Fourier analysis of the scattered intensity.

The question of uniqueness

The deconvolution of an undistorted \( Q_0 \) function of a structure with centrosymmetry has an unambiguous solution \( \varrho_0(x) \) except for the reflection about the abscissa, \( -\varrho_0(x) \) (Hosemann & Bagchi, 1962, p. 121). The uncertainty which remains for distorted \( Q_0 \) functions is caused by the smearing of the convolution product \( Q_m2 \) with the distance statistics \( H_l(x) \). Hence we may require that the details of \( Q_m2 \) should not be completely smeared out and we restrict ourselves to distance statistics with a standard deviation equal to or lower than about 15%.

A possibility of surveying the number of solutions \( \varrho_0 \) is then given by the following procedure: Let the single-layer thickness be given by \( w \) and the double layer extension by \( D_0 \geq 2w \). Then the first term of equation (3), \( 2Q_m \), is defined only within the interval \((0, w)\), where it clearly predominates with respect to the second term. The remaining interval \((w, D_0)\) contains only values of the second term \( Q_m2 \times H_1 \). But this region is not sufficiently well defined to serve as a domain for determining a solution \( \varrho_m \) by an iterative method. However, it is possible to extrapolate the outer part \( Q_m2 \times H_1 \) towards the inner interval \((0, w)\) with a sufficient accuracy and subtract it from the complete \( Q_0 \) function.

Thus, the two terms of equation (3) are separated from each other and we proceed according to a method similar to that of Weick (1974) in his analysis of the X-ray diffraction of hollow spherical vesicles, where also the autocorrelation function and the smeared convolution product from an electron density distribution were given separated from each other.

The total number of solutions \( \varrho_m \) of the first part \( 2Q_m \) can be found systematically under the assumption that the number, the width, the sign, and the positions of the peaks of the electron density function \( \varrho_m \) can be deduced from the corresponding number, width, signs, and positions of the peaks of the generalized Patterson function \( Q_0(x) \).

From the resulting set of solutions only such solutions \( \varrho_m \) remain which simultaneously satisfy the second part of equation (3), i.e. \( Q_m2 \times H_1 \). The question of the finally remaining number of solutions \( \varrho_m \) must be investigated separately for each particular case.

In the case of erythrocyte ghosts the remaining solutions have been the Gaussian sequences \((+ + + , \text{ from outside to inside})\) and the inverted solution \(-\varrho_m(- + - )\), whose parameters are listed in the lower part of Table 2. As has been mentioned above, the second solution \(-\varrho_m \) was discriminated against by taking additional information from other biophysical and biochemical investigations into account.

**Conclusion**

By contrast with other known deconvolution methods (e.g. Hosemann & Bagchi, 1962, p. 121; Kreutz, 1968, p. 20; Worthington et al., 1974) the presented deconvolution procedure demonstrates the following advantages:

(i) The parameters describing the structure \( \varrho_m \) can be directly determined from the \( Q_0 \) function (Patterson analysis) and the number of these parameters can be held to a minimum;
(ii) a statistical distance distribution between the two parts of the unit cell can be taken into account quantitatively and, thereafter, can be eliminated very easily;
(iii) the complete computing time is very short.

The authors wish to thank Mrs Walburga Herbst and Mr Robert Mull for helping prepare the manuscript, Mrs Gerlinde Heppeler and Mrs Sophia El-Deeb for drafting the
figures. The computer calculations were performed at the Rechenzentrum of the University of Freiburg. Program descriptions are available from the authors.

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