accepted down to a cut-off value of 4·0, and below this value the $|\varepsilon'|_c$ would be eliminated if $|\varepsilon| < 1{\cdot}0$ and accepted down to $|\varepsilon'|_c > 2{\cdot}8$ if $|\varepsilon| > 3{\cdot}0$. The numbers used for criteria (*a*), (*b*) and (*c*) with myoinositol are larger than those for napthalene because the number of atoms in the asymmetric unit is larger and the $|\varepsilon'|_c$ values are larger for myoinositol. The numbers used here in the application of the criteria are evidently somewhat arbitrary but should serve as a guide. It is not clear at this point how useful the introduction of additional statistical considerations would be for the present, and therefore the investigation of such matters is deferred. It might be pointed out however that further study along such lines would include considerations such as the number of atoms in the asymmetric unit, the relative amount of negative scattering matter, the number of terms contributing to a particular calculation and the variance of the individual terms.

Procedures for phase determination are particularly dependent in their initial stages on relationships among the largest $|\varepsilon'|$ values. Also, it is desirable to have at least ten phases among the larger $|\varepsilon'|$ values per atom in the asymmetric unit for the computation of a Fourier series. Thus the success of a procedure for structure determination, based upon the calculations presented here, depends on how well the computed larger $|\varepsilon'|_c$ are correlated with the larger $|\varepsilon'|_o$.

Aside from phase considerations, it is apparent that useful information should derive from comparing Patterson functions computed from the coefficients $|\varepsilon|^2$ and $|\varepsilon'|^2$ when both positive and negative scattering matter are present.

Mr Stephen Brenner wrote the computing programs and carried out all the calculations. I am indebted to him for his very fine cooperation. The thought to investigate this problem arose from a conversation with Dr Carroll K. Johnson of the Oak Ridge National Laboratory.

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An Alternative Method of Solving the Layer Scaling Equations of Hamilton, Rollett and Sparks

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The relationship between the methods of Dickerson (1959), Rollett & Sparks (1960), and Hamilton, Rollett & Sparks (1965) (HRS) is discussed, together with a short account of why the first two methods are unsatisfactory. An alternative iterative method (the method of 'shortest path') of solving the layer scaling equations of HRS is given which converges faster than the solution given by HRS. An exact solution of the equations of HRS is given which may be applied to situations where a simple weighting scheme may be used. The method of 'shortest path' may be important in protein crystallography where setting up the normal matrix may mean scanning 100000 reflexions and therefore the speed of convergence is of paramount importance.

Introduction

The purpose of this paper is threefold:
(*a*) To give an account of the relationship between the methods of Dickerson (1958), Rollett & Sparks (1960), and Hamilton, Rollett & Sparks (1965).
(*b*) To present an alternative iterative method (the method of 'shortest path') of solving the scaling equations of Hamilton, Rollett & Sparks (1965; we will refer to this paper as HRS), which converges faster than the solution given by these authors. The method of shortest path has the additional advantages that no fudge

factors need to be applied to the shifts, and no *ad hoc* decision need be made as to which film scale factor should be fixed.

(*c*) To give an exact solution to the equations of HRS which may be applied to situations where a simple weighting scheme may be used.

A comparative account of existing methods

Since we follow the methods of HRS closely, the first part of the following will, of necessity, be a restatement of the conclusions of HRS.

The first step in the layer scaling problem is to define the observational equations (*i.e.* that set of equations which we wish to be satisfied as exactly as possible by the right set of scale factors). The scheme proposed by Rollett & Sparks is to write

$$\sqrt{\omega_{hl}}(K_l F_{hl}^2 - F_h^2) = \varphi_{hl} \quad h=1, H, \quad l=1, L \qquad (1)$$

where h is a subscript used to represent the Miller indices for H reflexions on L layers, ω_{hl} is the weight of the reflexion with index h on layer l, K_l is the scale factor of layer l, F_{hl}^2 is the corrected intensity, F_h^2 is the weighted mean of the scaled F^2, and φ_{hl} is the standardized error.

We define a quantity ψ where

$$\psi = \sum_h \sum_l \varphi_{hl}^2$$

and wish to find that set of K's which make ψ a minimum. The weights are given by

$$\omega_{hl} = 1/K_l^2 \sigma_{hl}^2 \qquad (2)$$

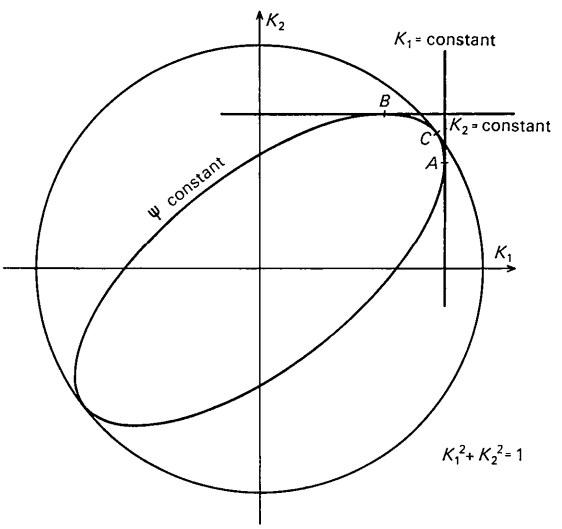

Fig. 1. A geometrical illustration of the scaling of two films: The axes are the scale factors K_1 and K_2. The equations of Rollett & Sparks (1960) for the sum of squares of error (ψ) are homogeneous of degree two. Thus a contour of constant error is an ellipse centred on the origin. The point of minimum (zero) error is the trivial point $K_1 = K_2 = 0$. To find a non-trivial solution Dickerson (1959) puts K_1 = constant or K_2 = constant giving as solutions either *A* or *B*. The Rollett & Sparks constraint ($K_1^2 + K_2^2 = 1$) gives as solution the point *C*.

where σ_{hl} is the standard deviation of F_{hl}^2. The equations (1) have the advantage of being highly symmetrical and simple functions of the weights.

Rollett & Sparks (1960) proceed by assuming that the weights can be put equal to one or, at least, are independent of the scale factors K_l. Therefore they take as the observational equations

$$K_l F_{hl}^2 - F_h^2 = \varphi_{hl} \quad h=1, H, \quad l=1, L. \qquad (3)$$

Since the equations (3) are linear functions of the scale factors, the quantity ψ is a quadratic function (in two dimensions, the contours of constant ψ are concentric ellipses) of the scale factors, and if we are dealing with only two films will have the form shown in Fig. 1. Now the normal equations (the equations obtained by setting $\partial\psi/\partial K_l = 0$ for each K_l in order to find the best set of K's) derived from (1) are homogeneous. The minimum value of ψ is $\psi = 0$ with $K_1 \ldots K_L = 0$. Therefore they will only give a non-trivial solution with the addition of a constraint. The equations of Dickerson (1959) share this property of being homogeneous and are conveniently discussed with those of Rollett & Sparks.

The constraint used by Dickerson is to set one scale factor equal to a constant (*e.g.* K_1 = constant in Fig. 1). If we consider for simplicity a two-film problem then we must find the smallest value of ψ on the line K_1 = constant (Fig. 1), which is the point *A*. Unfortunately, if we choose to make K_2 = constant we arrive at values for the scale factors given by the coordinates of the point *B*, which are different from those of *A*. To avoid this problem Rollett & Sparks chose to make the constraint

$$K_1^2 + K_2^2 = 1 \qquad (4)$$

and therefore arrive at the point *C*. HRS point out that this is just as arbitrary as putting K_1 or K_2 equal to one, and they go on to give a method which avoids these difficulties.

The reason why the method of Rollett & Sparks breaks down may be understood as follows. If we use the observational equations (3), the effect of halving K_1 and K_2 (keeping their ratio constant) is to quarter the value of ψ. Therefore it is always possible to obtain smaller values of ψ by reducing the scale factors while keeping their ratio constant. Hence the need for a constraint. Let us consider a third film which is represented only by a few weak spots. The constraint is now

$$K_1^2 + K_2^2 + K_3^2 = 1. \qquad (5)$$

Since (3) is weak its contribution to the sum of squares of the errors ψ is numerically small. The absolute magnitude of ψ can be decreased by making K_1 and K_2 as small as possible. On account of the constraint this can only be done by making K_3 relatively large, but this is allowed because its magnitude has only a small effect on the error ψ. Thus we see that weak films in a batch scaled by Rollett & Sparks's method will have scale factors which are systematically too large.

The solution to this predicament lies in the form of the equations (1). If we halve the values of all the K's

in equation (1) we do not affect the value of the error ψ, since the weights also depend upon the scale factors. Therefore, if we plot the error as a function of the scale factors it must consist of a set of radial lines (Fig. 2). ψ is a homogeneous function of the K's but of degree zero rather than degree two as it is in the equation (3) (the form used by Rollett & Sparks). Therefore no arbitrary constraint is necessary in solving for the minimum value of ψ, as long as we allow the weights to be explicit functions of the scale factors.

To solve the problem we must find an algorithm to locate that radial line on which ψ is a minimum. A method of doing this has been given by HRS. We give an alternative method below.

An alternative iterative method for solving the scaling equations of Hamilton, Rollett & Sparks

In the following we find it algebraically more convenient to work with the inverse scale factor G_l $(=1/K_l)$. This notation was introduced by HRS. In the following we use subscript h to denote Miller indices, l to denote film number, and m to denote film number in a second summation. Rewriting equations (1) with G for K, we have

$$\frac{1}{\sigma_{hl}}(F_{hl}^2 - G_l F_h^2) = \varphi_{hl} \quad h=1, H, \quad l=1, L. \tag{6}$$

We wish to minimize ψ with respect to the inverse scale factors, where

$$\psi = \sum_h \sum_l \frac{1}{\sigma_{hl}^2}(F_{hl}^2 - G_l F_h^2)^2. \tag{7}$$

Now

$$F_h^2 = \frac{\sum_m \frac{G_m}{\sigma_{hm}^2} F_{hm}^2}{\sum_m \frac{G_m^2}{\sigma_{hm}^2}} \tag{8}$$

and putting $\beta_{hl} = \dfrac{F_{hl}^2}{\sigma_{hl}}$ and $\alpha_{hl} = \dfrac{G_l}{\sigma_{hl}}$

we have

$$\psi = \sum_h \sum_l \left[\beta_{hl} - \frac{\alpha_{hl} \sum_m \alpha_{hm}\beta_{hm}}{\sum_m \alpha_{hm}^2} \right]^2. \tag{9}$$

Symbolically, let us write equation (9) as

$$\psi = \sum_\alpha E_\alpha^2 \tag{10}$$

to express the fact that it is a sum of squares (α stands for a summation over h and l). To find the minimum value of ψ we set each derivation with respect to the variable G equal to zero, *i.e.*

$$\frac{\partial \psi}{\partial G_l} = 0 \quad l=1, L \tag{11}$$

in turn.

If we have starting values for the set G_l then we may use the Taylor expansion for ψ (where ΔG is the shift in G).

$$\psi = \psi_0 + \sum_l \left(\frac{\partial \psi}{\partial G_l}\right)_0 \Delta G_l + \sum_l \sum_m \tfrac{1}{2} \left(\frac{\partial^2 \psi}{\partial G_l \partial G_m}\right)_0 \Delta G_l \Delta G_m + etc. \tag{12}$$

We may minimize $\psi - \psi_0$ (let us call this ψ') in the normal way using conditions (11) and find that the condition is given by

$$\mathbf{A}\Delta\mathbf{G} = \mathbf{r} \tag{13}$$

where the $L \times L$ matrix $\mathbf{A}$ has elements

$$A_{lm} = \frac{1}{2}\left(\frac{\partial^2 \psi}{\partial G_l \partial G_m}\right)_0 \tag{14}$$

and the column vector $\mathbf{r}$ has elements

$$r_l = -\frac{1}{2}\left(\frac{\partial \psi}{\partial G_l}\right)_0. \tag{14a}$$

Now consider the case $\psi = \sum_\alpha E_\alpha^2$.

Then

$$\frac{\partial^2 E_\alpha^2}{\partial G_l \partial G_m} = 2\frac{\partial E_\alpha}{\partial G_l}\frac{\partial E_\alpha}{\partial G_m} + 2E_\alpha \frac{\partial^2 E_\alpha}{\partial G_l \partial G_m}. \tag{15}$$

If the quantities E_α are linear functions of the G_l (as they will be near a minimum of ψ) we may put the second term in equation (12) equal to zero, whereupon (13) become the familiar normal equations with

$$A_{lm} = \sum_\alpha \left(\frac{\partial E_\alpha}{\partial G_l}\right)_0 \left(\frac{\partial E_\alpha}{\partial G_m}\right)_0$$
$$r_l = -\sum_\alpha E_\alpha \left(\frac{\partial E_\alpha}{\partial G_l}\right)_0. \tag{16}$$

Putting these equations in the form of (9) instead of the symbolic form (10), we may evaluate the derivatives in (16) and find that

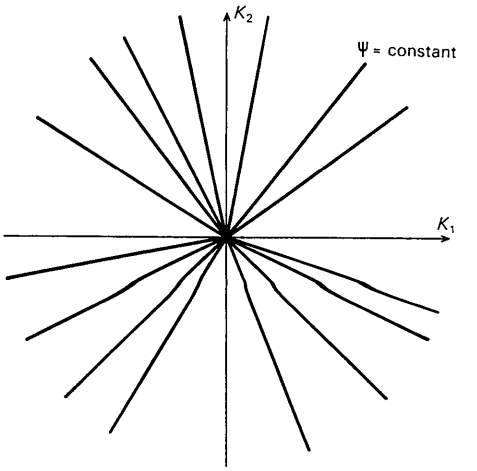

Fig. 2. The equations of HRS for the sum of squares of error (ψ) are homogeneous of degree zero, thus contours of constant ψ have the form of radial lines. If all the values of the K's are proportionately increased or decreased, any value of ψ remains unaltered. Therefore to solve these equations no extra constraints are required.

$$A_{lm}=\sum_h\left\{\frac{\delta_{lm}}{\sigma_{hl}^2}\frac{\left[\sum_k \frac{G_kF_{hk}^2}{\sigma_{hk}^2}\right]^2}{\left[\sum_k \frac{G_k^2}{\sigma_{hk}^2}\right]^2}+\frac{F_{hl}^2F_{hm}^2}{\sigma_{hl}^2\sigma_{hm}^2\left[\sum_k \frac{G_k^2}{\sigma_{hk}^2}\right]}-\frac{\left[\sum_k \frac{G_kF_{hk}^2}{\sigma_{hk}^2}\right][F_{hm}^2G_l+F_{hl}^2G_m]}{\sigma_{hl}^2\sigma_{hm}^2\left[\sum_k \frac{G_k^2}{\sigma_{hk}^2}\right]^2}\right\} \quad (17)$$

and

$$r_l=\sum_h\left\{\frac{F_{hl}^2}{\sigma_{hl}^2}\frac{\left[\sum_k \frac{G_kF_{hk}^2}{\sigma_{hk}^2}\right]}{\left[\sum_k \frac{G_k^2}{\sigma_{hk}^2}\right]}-\frac{G_l}{\sigma_{hl}^2}\frac{\left[\sum_k \frac{G_kF_{hk}^2}{\sigma_{hk}^2}\right]^2}{\left[\sum_k \frac{G_k^2}{\sigma_{hk}^2}\right]}\right\}. \quad (18)$$

Now the E_α's are homogeneous functions of G_l of degree zero. If the value about which the Taylor expansion is made is given by the vector $\mathbf{G}^\circ$ ($\mathbf{G}^\circ$ are the starting values) we have

$$\sum_l G_l^0\left[\frac{\partial E_\alpha}{\partial G_l}\right]_0=0 \quad \text{(Euler's theorem)}. \quad (19)$$

Hence

$$\sum_l\sum_\alpha\left(\frac{\partial E_\alpha}{\partial G_m}\right)_0\left(\frac{\partial E_\alpha}{\partial G_l}\right)_0 G_l^0=\sum_l A_{lm}G_l^0=0 \qquad m=1, L.$$

Therefore the vector $\mathbf{G}^\circ$ is an eigenvector of $\mathbf{A}$ of eigenvalue zero. Therefore $\mathbf{A}$ has zero determinant, and equations (13) are either inconsistent or admit many solutions differing by a multiple of $\mathbf{G}^\circ$. The latter is the case because (19) can be written

$$\sum_l G_l^0 r_l=0 \quad (19a)$$

showing that $\mathbf{r}$ is orthogonal to $\mathbf{G}_0$.

Returning to Fig. 2, we may now see the geometrical meaning of the approximation of using the truncated Taylor expansion for ψ in place of the full expansion (equation 12), or in other words, of using the quadratic form

$$\psi'=\Delta\mathbf{G}^T\mathbf{A}\Delta\mathbf{G} \quad (20)$$

in place of the true form (9). We have shown above that $\mathbf{A}$ has one zero eigenvalue corresponding to $\mathbf{G}^\circ$, therefore (20) represents an open ended cylinder and lines of constant ψ are parallel to the vector $\mathbf{G}^\circ$. The effect of the approximate expression (12) therefore has been to move the origin of Fig. 2 to infinity so that sets of radial lines become parallel. To solve the problem we wish to find the axis of this cylinder.

The most efficient way to find the axis of the cylinder from a starting point (*e.g.* point G_0 in Fig. 3) is to intersect the cylinder axis by the shortest path from $\mathbf{G}_0$ (*i.e.* at right angles to $\mathbf{G}_0$). In comparison, the method of HRS (whose setting up of the problem is formally identical with that given above) is to proceed along any path G_l=constant until it intersects the axis of the cylinder (see Fig. 3). As long as the linear Taylor expansion is a good approximation for the observational equations, the difference is of little importance, but if the starting value is well away from the axis of the cylinder then the approximation (12) will be better for small shifts, and therefore it is better to use the shortest path. The method of HRS may produce inordinately large shifts if G_l=constant is nearly parallel to the axis of the cylinder, which will happen if film l is weak. To avoid problems of this kind (especially attempts of $\mathbf{G}$ to move out of the positive quadrant) HRS find it necessary to place limits on the values of the shifts during refinement. Notice that the constraint used by HRS to solve the equations is the same as Dickerson's, but does not now lead to different solutions for different constraints as applied to different equations.

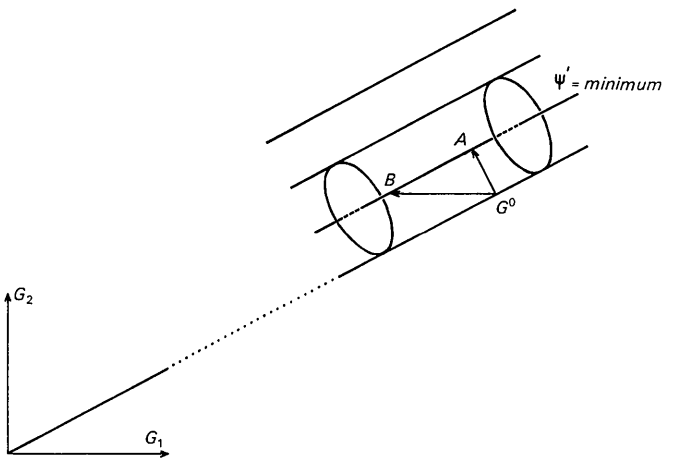

Fig. 3. A linear approximation to the equations of HRS may be obtained by a Taylor expansion. The effect of this approximation is to make contours of constant error into parallel lines rather than radial lines. Starting from a trial solution $G^0(G_l=1/K_l)$ we may reach the line of minimum error by an infinite number of paths. HRS use the path G_l=constant and arrive at a solution B. We give a method for finding the shortest path to the point A. The points A and B are equivalent except for an arbitrary scalar multiplier.

The computational procedure equivalent to the geometrical method described above (the 'shortest path' method) is as follows:

(1) Compute **A** (of order L) (equation 17).

(2) Compute **r** (equation 18).

(3) Diagonalize **A** and find the matrix of the eigenvectors $\boldsymbol{\beta}$. Put the eigenvector of smallest eigenvalue at the L'th (last) position.

We have $$\mathbf{A}\Delta\mathbf{G}=\mathbf{r}; \tag{21}$$

therefore $$\boldsymbol{\beta}\boldsymbol{\beta}^T\mathbf{A}\boldsymbol{\beta}\boldsymbol{\beta}^T\Delta\mathbf{G}=\mathbf{r}\,. \tag{22}$$

Let us call the diagonalized matrix $\mathbf{D}(=\boldsymbol{\beta}^T\mathbf{A}\boldsymbol{\beta})$, put $\boldsymbol{\beta}^T\Delta\mathbf{G}=\Delta\mathbf{G}'$ and $\boldsymbol{\beta}^T\mathbf{r}=\mathbf{r}'$

therefore $$\mathbf{D}\Delta\mathbf{G}'=\mathbf{r}'\,. \tag{23}$$

The smallest element of **D** is theoretically zero and in practice will be very near zero.

(4) Solve for $\Delta G'_1 \ldots G'_{L-1}$ and put $\Delta G_L=0$ [this is essentially the method of Diamond (1958)].

(5) Rotate back to find $\Delta\mathbf{G}(=\boldsymbol{\beta}\Delta\mathbf{G}')$.

(6) Put new $\mathbf{G}^\circ=\mathbf{G}^\circ+\Delta\mathbf{G}$.

We show the results of our method [Table 1(*a*)] compared with the method of HRS on a 14-parameter problem (HRS) [Table 1(*b*)]. In each case the starting values were unity. Table 1(*b*) shows the result of using HRS method and fixing film 5, and Table 1(*c*) shows the effect of fixing film 14 (in order to facilitate comparison the scale factors are rescaled after each cycle to make $G_1=1$). After cycle (3), root mean square error of 1(*a*) is 0·004345, whereas for 1(*b*) we have 0·04172 and for 1(*c*) 0·02677. The largest error of 1(*a*) is 0·00921 whereas the largest error of 1(*b*) is 0·09782 and of 1(*c*) is 0·06639 all in film 6.

The convergence of 1(*a*) is appreciably faster than 1(*b*) or 1(*c*) and this may be important in protein crystallography, where setting up the normal matrix may mean scanning 100000 reflexions and therefore speed of convergence is of paramount importance.

In the method of HRS fixing a film is equivalent to crossing out the appropriate row and column in the normal matrix and right hand side and solving the rest. By doing this we should produce a normal matrix which has a non-zero determinant and can therefore be solved. However, if the film chosen is poorly linked or is very weak the resulting determinant is still very near zero, and thus the solution is subject to problems of rounding error and overflow. An example is shown in Table 1(*c*). By fixing film 14 in the HRS test problem a slightly wrong scale factor for film 14 has been produced. Film 14 has only 3 reflexions. Therefore it would seem to be best to fix a strong film when using the method of HRS. Note that no restrictions of any kind have been found necessary in using the method of shortest path.

An exact solution for a simple weighting scheme

Returning to equation (9), this may be simplified by taking together all terms corresponding to a given reflexion h. This is most simply accomplished by considering the variables α_{hl} and β_{hl}, for each h, as points in space having L dimensions (L is number of layers). By applying the theorem of Pythagoras we find

$$\psi=\sum_h\left\{\sum_l \beta_{hl}^2-\frac{(\sum_l \alpha_{hl}\beta_{hl})^2}{(\sum_l \alpha_{hl}^2)}\right\}. \tag{24}$$

The first term on the right hand side of (24) is independent of the G_l's; therefore to minimize ψ we must maximize U where

$$U=\sum_h\frac{(\sum_l \alpha_{hl}\beta_{hl})^2}{\sum_l \alpha_{hl}^2} \tag{25}$$

$$=\sum_h\frac{(\sum_l G_l F_{hl}^2/\sigma_{hl}^2)^2}{\sum_l G_l^2/\sigma_{hl}^2}\,. \tag{26}$$

We may find the maximum of U by setting each of the derivatives of U with respect to G_l equal to zero. If we attempt to do this with equation (26) we are led to an intractable set of equations.

However, if the weights are all equal or can be written in the form $x_h y_l$ (*i.e.* the product of a term dependent solely upon the reflexion index with one dependent solely upon the film number) we must maximize

$$\frac{\sum_h(\sum_l G_l F_{hl}^2)^2}{\sum_l G_l^2}\,. \tag{27}$$

This is equivalent to maximizing

$$\sum_h(\sum_l G_l F_{hl}^2)^2 \tag{28}$$

subject to the restriction

$$\sum_l G_l^2=1 \tag{29}$$

and is, therefore, an eigenvalue problem. The solution is given by finding the eigenvector with the largest eigenvalue of the normal matrix with elements

$$A_{lm}=\sum_h F_{hl}^2 F_{hm}^2\,. \tag{30}$$

The similarity of this solution to that given by Rollett & Sparks (1960) is apparent although we are attempting to find the maximum eigenvalue rather than the minimum, and the diagonal terms are different.

The initial attractiveness of the above solution, which has the advantages of the method of Rollett & Sparks, must be tempered by the realization that it cannot deal with the situation of many layers each of which intersects another layer only along a common row. In this common situation each film or set of data contains only a fraction of the total reflexions and

frequently has no data in common with some other layer. We normally deal with this by putting the weights equal to zero for reflexions not represented on this layer. However, we have made the restriction that all weights must be unity and cannot, therefore, use this trick. Unfortunately this makes the above method unusable in most circumstances.

The utility of the method we have just given lies in scaling films together with many common data, and therefore it is particularly useful for two films. Whether the loss of the weighting scheme is important must be decided by experience. At least the method is free from systematic errors.

We are pleased to acknowledge a number of helpful discussions of the scaling problem with Dr J. S. Rollett. We are grateful to Dr Rollett for providing the test data for the 14-parameter problem. We are grateful for the advice of our colleagues, in particular that of Dr R. Diamond.

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Table (1*a*). *Method of shortest path*

Film number	Cycle numbers 1	2	3	4	5	6	7	8	9
1	1·00000	1·00000	1·00000	1·00000	1·00000	1·00000	1·00000	1·00000	1·00000
2	1·02642	1·11545	1·15616	1·16046	1·16179	1·16185	1·16186	1·16186	1·16186
3	1·00909	1·07462	1·12380	1·12821	1·12830	1·12829	1·12829	1·12829	1·12829
4	0·83554	0·72818	0·73241	0·73512	0·73531	0·73531	0·73531	0·73531	0·73531
5	0·99103	1·11814	1·17168	1·17368	1·17401	1·17400	1·17400	1·17400	1·17400
6	1·03762	1·17104	1·25723	1·26709	1·26840	1·26843	1·26844	1·26844	1·26844
7	0·39557	0·23758	0·22879	0·22997	0·23002	0·23002	0·23002	0·23002	0·23002
8	0·39728	0·22931	0·21186	0·21288	0·21301	0·21302	0·21302	0·21302	0·21302
9	0·38432	0·21685	0·19853	0·19930	0·19936	0·19936	0·19936	0·19936	0·19936
10	0·38749	0·20516	0·16919	0·16504	0·16498	0·16498	0·16498	0·16498	0·16498
11	0·47485	0·40127	0·41541	0·41567	0·41577	0·41577	0·41577	0·41577	0·41577
12	0·48843	0·45682	0·47808	0·47793	0·47804	0·47804	0·47804	0·47804	0·47804
13	0·88923	0·83178	0·84201	0·84443	0·84465	0·84465	0·84465	0·84465	0·84465
14	0·74247	0·76882	0·76767	0·77219	0·77264	0·77267	0·77266	0·77267	0·77267

Table 1(*b*). *Method of Hamilton, Rollett & Sparks*
Fixing film 5

Film number	Cycle numbers 1	2	3	4	5	6	7	8	9
1	1·00000	1·00000	1·00000	1·00000	1·00000	1·00000	1·00000	1·00000	1·00000
2	1·01602	1·05890	1·11200	1·14936	1·15996	1·16168	1·16185	1·16186	1·16186
3	1·00555	1·03296	1·07733	1·11535	1·12730	1·12828	1·12829	1·12829	1·12829
4	0·89243	0·79813	0·74575	0·73334	0·73463	0·73528	0·73531	0·73531	0·73531
5	0·99449	1·04236	1·11333	1·16129	1·17285	1·17397	1·17401	1·17402	1·17401
6	1·02271	1·08288	1·17062	1·24265	1·26553	1·26827	1·26843	1·26844	1·26844
7	0·51659	0·32619	0·25222	0·23170	0·22988	0·23001	0·23002	0·23002	0·23002
8	0·51838	0·32164	0·24100	0·21581	0·21284	0·21299	0·21301	0·21302	0·21302
9	0·50478	0·30742	0·22733	0·20226	0·19925	0·19935	0·19936	0·19936	0·19936
10	0·50813	0·30052	0·20935	0·17377	0·16547	0·16498	0·16498	0·16498	0·16498
11	0·59621	0·45986	0·41981	0·41432	0·41543	0·41576	0·41577	0·41577	0·41577
12	0·60924	0·49224	0·47177	0·47533	0·47772	0·47804	0·47804	0·47804	0·47804
13	0·92912	0·87232	0·84431	0·84134	0·84394	0·84462	0·84465	0·84465	0·84465
14	0·82488	0·77431	0·76206	0·76736	0·77166	0·77257	0·77264	0·77265	0·77265

Table 1(*c*). *Method of Hamilton, Rollett & Sparks*
Fixing film 14

Film number	Cycle numbers 1	2	3	4	5	6	7	8	9
1	1·00000	1·00000	1·00000	1·00000	1·00000	1·00000	1·00000	1·00000	1·00000
2	1·02026	1·07249	1·12939	1·15602	1·16098	1·16181	1·16186	1·16186	1·16186
3	1·00700	1·04264	1·09354	1·12319	1·12809	1·12830	1·12829	1·12829	1·12829
4	0·86817	0·77571	0·73602	0·73337	0·73508	0·73531	0·73531	0·73531	0·73531
5	0·99307	1·05831	1·13671	1·16928	1·17367	1·17400	1·17400	1·17400	1·17400
6	1·02878	1·10385	1·20205	1·25719	1·26740	1·26840	1·26844	1·26844	1·26844
7	0·45896	0·29447	0·23898	0·22990	0·22996	0·23002	0·23002	0·23002	0·23002
8	0·46074	0·28870	0·22596	0·21316	0·21291	0·21301	0·21302	0·21302	0·21302
9	0·44724	0·27502	0·21256	0·19963	0·19930	0·19936	0·19936	0·19936	0·19936
10	0·45056	0·26646	0·19153	0·16832	0·16505	0·16498	0·16498	0·16498	0·16498
11	0·53960	0·43578	0·41412	0·41467	0·41566	0·41577	0·41577	0·41577	0·41577
12	0·55309	0·47345	0·47131	0·47675	0·47795	0·47804	0·47804	0·47804	0·47804
13	0·91232	0·85873	0·84009	0·84245	0·84441	0·84465	0·84465	0·84465	0·84465
14	0·78942	0·76883	0·76490	0·77157	0·77529	0·77420	0·77465	0·77457	0·77456