Acta Cryst. (1974). A30, 543

An Application of the Unitarity Equation to the Phase Problem of Electron Scattering from Crystals

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(*Received* 14 *December* 1973; *accepted* 20 *January* 1974)

The unitarity equation is used to determine the phases of electron scattering amplitudes from crystals. A sufficient condition is derived for the phases to be determined up to a possible twofold ambiguity. Successful comparison has been made with a theoretical test case.

Introduction

The purpose of this work was to investigate how far the unitarity relation, *viz.* the conservation of electrons, could be used to reduce the phase ambiguity of electron scattering from crystals. The approach was suggested by the successful use of a similar technique in the analysis of high-energy pion–pion scattering (Newton, 1968; Martin, 1969; Tortorella, 1972.) It is based on the fact that the conservation requirement imposes a non-linear constraint upon the scattering amplitude, which, under favourable conditions, may be iterated to yield the phases from a knowledge of the intensities.

In the following section we derive the unitarity relation for elastic electron scattering. In § 2 it is applied to scattering from a crystal with a reflexion-symmetric potential, where it is shown to impose a non-linear constraint upon the scattering amplitude. This is used in § 3 to establish an iterative scheme of phase determination, together with a sufficient condition, equation (3.12), for the existence of a unique solution to which it converges. § 4 contains a successful comparison of the method with test data generated by using the phase-grating approximation for scattering of 500 keV electrons from sodium. The general results are then reviewed in the conclusion.

1. The unitarity equation

If we consider the scattering of electrons from a target, then the asymptotic outgoing scattering states, $|\psi, \text{out}\rangle$, are related to the asymptotic incoming scattering states, $|\psi, \text{in}\rangle$, by a linear operator, S, the scattering matrix (Taylor, 1972)

$$|\psi, \text{out}\rangle = S|\psi, \text{in}\rangle. \tag{1.1}$$

In the absence of bound states, both the sets of asymptotic outgoing and incoming states are complete. It follows that S is a unitary operator:

$$S^+S = 1. \tag{1.2}$$

The above equation is the mathematical expression of the physical requirement that the total number of electrons involved in the scattering process be conserved. It imposes a non-linear constraint upon any description of the process and consequently provides a possible iterative mechanism for augmenting the amount of information available from experimental data.

In order to display it in a usable form we need to introduce several subsiduary concepts, chief of which is the transition matrix, T, defined by

$$S = 1 - iT. \tag{1.3}$$

In terms of the transition matrix the unitarity condition becomes

$$i(T - T^+) = T^+T \tag{1.4}$$

or, considering plane-wave matrix elements,*

$$\langle \mathbf{k}|T|\mathbf{k}_0\rangle - \langle \mathbf{k}|T^+|\mathbf{k}_0\rangle = -i\int \mathrm{đ}^3\mathbf{q}\langle \mathbf{k}|T^+|\mathbf{q}\rangle \langle \mathbf{q}|T|\mathbf{k}_0\rangle. \tag{1.5}$$

Now if T is invariant under time and space reflexions, (the validity of which will be discussed later), then

$$\langle \mathbf{k}|T|\mathbf{k}_0\rangle = \langle \mathbf{k}_0|T|\mathbf{k}\rangle \tag{1.6}$$

and consequently

$$2\,\mathrm{Im}\,\langle \mathbf{k}|T|\mathbf{k}_0\rangle = -\int \mathrm{đ}^3\mathbf{q}\langle \mathbf{q}|T|\mathbf{k}\rangle^*\langle \mathbf{q}|T|\mathbf{k}_0\rangle. \tag{1.7}$$

If the interaction is independent of time and falls off sufficiently rapidly with distance, then energy is conserved by the asymptotic amplitudes. As a result, the transition-matrix elements are proportional to an energy-conserving delta function. This enables the scattering amplitude, $f(\mathbf{k},\mathbf{k})$, to be defined by

$$\langle \mathbf{k}|T|\mathbf{k}_0\rangle = -\frac{2\pi}{m}\bar{\delta}(E_{\mathbf{k}} - E_{\mathbf{k}_0})f(\mathbf{k},\mathbf{k}_0) \tag{1.8}$$

* We employ the notation $\mathrm{đ}^3\mathbf{q} = (2\pi)^{-3}\mathrm{d}^3\mathbf{q}$, $\bar{\delta}^3(\mathbf{q}) = (2\pi)^3\delta^3(\mathbf{q})$.

where $E_{\mathbf{k}}$ is the energy of an electron of mass m corresponding to a momentum $\mathbf{k}$.

The formal analysis outlined above may be related to concepts which are more familiar in potential scattering by writing the Lippmann–Schwinger equation of scattering (Newton, 1966) in an operator form as

$$T(Z)=V+V(Z-H_0)^{-1}T(Z) \tag{1.9}$$

where H_0 and V are the free and interaction Hamiltonians respectively. It may then be shown (Taylor, 1972) that if the potential falls off sufficiently rapidly, the above transition operator is related to the scattering amplitude by

$$2\pi f(\mathbf{k},\mathbf{k}_0)=-m\lim_{\varepsilon\downarrow 0}\langle\mathbf{k}|T(E_p+i\varepsilon)|\mathbf{k}_0\rangle. \tag{1.10}$$

In a previous publication (Boyce, Burge & McCloughrey, 1972) it was shown that for an infinite crystal with lattice vectors **a**, **b** and **c** respectively, the matrix elements of $T(Z)$ satisfy,

$$\langle\mathbf{k}|T(E+i\varepsilon)|\mathbf{k}_0\rangle=\sum_{\mathbf{L},\mathbf{M}}[1-\tilde{V}G]^{-1}_{0\mathbf{L}}\tilde{V}_{\mathbf{LM}}\times\bar{\delta}^3(\mathbf{k}-\mathbf{k}_0+\mathbf{M}) \tag{1.11}$$

where **L** and **M** denote reciprocal-lattice vectors,

$$\mathbf{L}=l\tilde{\mathbf{a}}+m\tilde{\mathbf{b}}+n\tilde{\mathbf{c}} \tag{1.12}$$

in which $\tilde{\mathbf{a}}$, $\tilde{\mathbf{b}}$ and $\tilde{\mathbf{c}}$ are the unit vectors of the inverse lattice, and are defined in Appendix A. $\tilde{V}_{\mathbf{LM}}$ is the Fourier transform of a single lattice potential, evaluated at $\mathbf{L}-\mathbf{M}$, while $G(\mathbf{k};E)$ is the free-electron propagator corresponding to an energy $E=\hbar^2K^2/2m$

$$G(\mathbf{k};E)=\frac{2m}{\hbar^2}(K^2-k^2+i\varepsilon)^{-1}. \tag{1.13}$$

We now reconsider the assumptions of time and space reflexion invariance employed in the derivation of equation (1.6). As the potential is time-independent, it follows that S, and hence T, is invariant under time reflexion. Under space reflexion, however, the potential transforms as $V(\mathbf{r})\rightarrow V(-\mathbf{r})$. As the summations involved in equation (1.11) are symmetric under reflexion T will be invariant if V is. Therefore we are assuming that

$$V(\mathbf{r})=V(-\mathbf{r}) \tag{1.14}$$

and the class of crystals which can be considered is subject to this restriction. The unitarity relation still has content whenever this condition is relaxed, however its usefulness as an iterative mechanism is greatly reduced.

In the following section we shall consider the case of crystals of finite thickness.

2. The unitarity equation for scattering from a crystal of finite thickness

In the previous section we considered the elastic scattering of electrons from an initial momentum $\mathbf{k}_0$ to a final momentum **k**, by an infinite crystal defined by the lattice vectors **a**, **b** and **c**. In order to describe the experimental situation we must consider crystals of finite width, which will be taken to be along the **c** axis. Bragg's law then applies only to the **a**, **b** plane, and the expression for the transition matrix element takes the form,

$$\langle\mathbf{k}|T|\mathbf{k}_0\rangle=\sum_{\mathbf{M}}F(\mathbf{M},\mathbf{k},\mathbf{k}_0)\bar{\delta}^2[(\mathbf{k}-\mathbf{k}_0)^{\perp\mathbf{c}}+\mathbf{M}] \tag{2.1}$$

where **M** is the two-dimensional vector

$$\mathbf{M}=l\tilde{\mathbf{a}}+m\tilde{\mathbf{b}}, \tag{2.2}$$

while we may express vectors in terms of their components in the $\tilde{\mathbf{a}},\tilde{\mathbf{b}}$ plane, and along $\tilde{\mathbf{c}}$, *e.g.*

$$\mathbf{k}=\mathbf{k}^{\perp c}+k^c\tilde{\mathbf{c}}. \tag{2.3}$$

As the total potential falls off sufficiently rapidly in the **c** direction we may extract the delta function which expresses energy conservation and express equation (2.1) in terms of the scattering amplitude as

$$\langle\mathbf{k}|T|\mathbf{k}_0\rangle=\bar{\delta}(k^2-k_0^2)\sum_{\mathbf{M}}f(\mathbf{M},\mathbf{k},\mathbf{k}_0)\bar{\delta}^2[(\mathbf{k}-\mathbf{k}_0)^{\perp\mathbf{c}}+\mathbf{M}]. \tag{2.4}$$

If we reconsider equation (1.11), then it may be observed that, apart from the delta function, the momentum dependence of the amplitude arises from components of the form

$$[\tilde{V}G]_{\mathbf{LM}}=\frac{2m}{\hbar^2}\tilde{V}(\mathbf{L}-\mathbf{M})\{K^2-(\mathbf{k}_0+\mathbf{M})^2+i\varepsilon\}^{-1}. \tag{2.5}$$

For potentials which decrease sufficiently rapidly so that $k_0^2\gg M^2$ for all significant values of **M**, then $(\mathbf{k}_0+\mathbf{M})^2\simeq k_0^2$, and consequently we may regard the scattering amplitude as a function solely of k_0^2 and **M**.

Upon assuming that this approximation holds also for crystals of finite width, the unitarity equation, (1.7), becomes

$$\begin{aligned}\mathrm{Im}\sum_{\mathbf{L}}f(k_0^2,\mathbf{L})\bar{\delta}(k^2-k_0^2)\bar{\delta}^2[(\mathbf{k}-\mathbf{k}_0)^{\perp\mathbf{c}}+\mathbf{L}]&\\=\int\bar{d}^3q\sum_{M,N}f(q^2,\mathbf{M})^*f(k_0^2,\mathbf{N})\bar{\delta}(k^2-q^2)\bar{\delta}(q^2-k_0^2)&\\\times\delta^2[(\mathbf{k}-\mathbf{q})^{\perp\mathbf{c}}+\mathbf{M}]\delta^2[(\mathbf{q}-\mathbf{k}_0)^{\perp\mathbf{c}}+\mathbf{N}]&\end{aligned} \tag{2.6}$$

and consequently

$$\begin{aligned}\mathrm{Im}\,f(k_0^2,\mathbf{L})=\int\bar{d}^3\mathbf{q}\sum_{\mathbf{M}}f(q^2,\mathbf{M})^*f(k_0^2,\mathbf{L}-\mathbf{M})&\\\times\bar{\delta}(q^2-k_0^2)\bar{\delta}^2[(\mathbf{q}-\mathbf{k}_0)^{\perp\mathbf{c}}+\mathbf{L}-\mathbf{M}].&\end{aligned} \tag{2.7}$$

The lemma

$$\int\bar{d}^3\mathbf{q}\bar{\delta}(q^2-k_0^2)\bar{\delta}^2[(\mathbf{q}-\mathbf{k}_0)^{\perp\mathbf{c}}+\mathbf{N}]\simeq(2\pi)^3(2vk_0\tilde{\mathbf{c}})^{-1} \tag{2.8}$$

which is derived in Appendix A, allows the unitarity relation to be reduced to

$$\operatorname{Im} f(k_0^2,\mathbf{L}) = (2\pi)^3(2vk_0\tilde{\mathbf{c}})^{-1} \times \sum_{\mathbf{M}} f(k_0^2,\mathbf{M})^* f(k_0^2,\mathbf{L}-\mathbf{M}). \quad (2.9)$$

The above non-linear equation expresses the conservation of probability during the scattering process. We wish to investigate to what extent it limits the possible scattering amplitudes; specifically how much a knowledge of the modulus of the amplitude, together with the conservation of probability, determines the phase of the amplitude. As the constraining equation involves only a summation the analysis is considerably easier than the corresponding case of central potential scattering.

3. Existence and uniqueness of solutions

In order to analyse equation (2.8) it is convenient to define

$$F(\mathbf{L}) = \frac{(2\pi)^3}{2vk_0\tilde{\mathbf{c}}} f(k_0^2,\mathbf{L}) \quad (3.1)$$

as the equation becomes

$$\operatorname{Im} F(\mathbf{L}) = \sum_{\mathbf{M}} F(\mathbf{M})^* F(\mathbf{L}-\mathbf{M}) \quad (3.2)$$

where **L** and **M** are two-dimensional vectors in the **ab** plane of reciprocal space, as given by equation (2.2). We wish to determine sufficient conditions for a knowledge of the modulus of $F(\mathbf{L})$ to determine its phase uniquely and to enable it to be calculated by iterating equation (3.2). This problem has already been solved for an isolated spherically symmetric potential. (Newton, 1968; Martin, 1969; Tortorella, 1972.) The analysis which follows is a direct application of the earlier results to the case of a crystal.

Let the amplitude $F(\mathbf{L})$ have modulus $G(\mathbf{L})$ and phase $\varphi(\mathbf{L})$. The unitarity equation becomes

$$G(\mathbf{L}) \sin \varphi(\mathbf{L}) = \sum_{\mathbf{M}} G(\mathbf{M})G(\mathbf{L}-\mathbf{M}) \times \cos\{\varphi(\mathbf{M})-\varphi(\mathbf{L}-\mathbf{M})\}. \quad (3.3)$$

For $\mathbf{L}=\mathbf{0}$ the equation is

$$G(\mathbf{0}) \sin \varphi(\mathbf{0}) = \sum_{\mathbf{M}} G(\mathbf{M})G(-\mathbf{M}). \quad (3.4)$$

Therefore the principal value of the phase of the centre spot is uniquely determined. We may utilise this by rewriting equation (3.3) for $\mathbf{L}\neq\mathbf{0}$ as

$$RG(\mathbf{L}) \sin\{\varphi(\mathbf{L})-\zeta\} = \sum_{\mathbf{M}}{}' G(\mathbf{M})G(\mathbf{L}-\mathbf{M}) \times \cos\{\varphi(\mathbf{M})-\varphi(\mathbf{L}-\mathbf{M})\}, \quad (3.5)$$

where the prime indicates that the terms $\mathbf{M}=\mathbf{0}$ and $\mathbf{M}=\mathbf{L}$ are to be omitted from the sum, while

$$R^2 = 1-4G(\mathbf{0}) \sin \varphi(\mathbf{0}) + 4G^2(\mathbf{0}) \quad (3.6)$$

and

$$\{1-2G(\mathbf{0}) \sin \varphi(\mathbf{0})\} \tan \zeta = 2G(\mathbf{0}) \cos \varphi(\mathbf{0}). \quad (3.7)$$

The above equation suggests that we consider the mapping

$$\varphi \rightarrow \mathscr{M}(\varphi) \quad (3.8)$$

where

$$\mathscr{M}(\varphi) = \zeta + \sin^{-1}[R^{-1} \sum_{\mathbf{M}}{}' H(\mathbf{L},\mathbf{M}) \times \cos\{\varphi(\mathbf{M})-\varphi(\mathbf{L}-\mathbf{M})\}] \quad (3.9)$$

with

$$H(\mathbf{L},\mathbf{M}) = \frac{G(\mathbf{M})G(\mathbf{L}-\mathbf{M})}{G(\mathbf{L})} \quad \text{if} \quad G(\mathbf{L})\neq 0$$
$$= 0 \quad \text{if} \quad G(\mathbf{L}) = 0. \quad (3.10)$$

Upon defining

$$Q = \sup_{\mathbf{L}} \{\sum_{\mathbf{M}}{}' H(\mathbf{L},\mathbf{M})\} \quad (3.11)$$

we may state the following theorem:

If

$$Q < \alpha\{4\alpha^2G^2(\mathbf{0})+1\}^{1/2} - 2\alpha^2G(\mathbf{0}) \quad (3.12)$$

where

$$\alpha = \left(\frac{\sqrt{17}-1}{8}\right)^{1/2} \quad (3.13)$$

then

$$\varphi = \mathscr{M}(\varphi) \quad (3.14)$$

has a unique solution which may be obtained by iterating the equation.

The proof of the theorem proceeds by showing that subject to the condition expressed by equation (3.12) $\varphi \rightarrow \mathscr{M}(\varphi)$ is a contraction mapping in a suitable metric space. We define the norm $\|\cdot\|_\infty$ by

$$\|\varphi\|_\infty = \sup_{\mathbf{M}\neq\mathbf{0}} |\varphi(\mathbf{M})-\zeta| \quad (3.15)$$

and consider the set

$$\varepsilon = \{\varphi \mid \|\varphi\|_\infty < \infty\}. \quad (3.16)$$

As the space $\langle \varepsilon, \|\cdot\|_\infty \rangle$ is isomorphic to l_∞, the space of bounded sequences, it is a Banach space. It is shown in Appendix B that $\varphi \rightarrow \mathscr{M}(\varphi)$ is a strict contraction mapping if $\varphi \in \mathscr{F}$ where

$$\mathscr{F} = \{\varphi \mid \|\varphi\|_\infty \leq \sin^{-1}(R^{-1}Q)\} \quad (3.17)$$

and the conditions of equation (3.12) apply. But $\mathscr{F}$ is a closed subset of ε and is thus complete, therefore, by the contraction-mapping principle, $\varphi \rightarrow \mathscr{M}(\varphi)$ has a unique fixed point which may be obtained by iteration.

Physically this means that if equation (3.12) is satisfied then the phase of the scattered amplitude is uniquely determined by its modulus. It is possible that the phase may still be determined even if equation (3.12) is not satisfied, since when and how it becomes ambiguous are at present unanswered questions.

In considering equation (3.9) rather than equation

(3.5) a principal value restriction was imposed. Thus, given a solution of equation (3.9), $\varphi(\mathbf{L})$, either $\varphi(\mathbf{L})$ or $\pi-\varphi(\mathbf{L})$ is a solution of equation (3.5), leading to a twofold ambiguity for each spot. In any physical case, however, the phases are likely to vary little between adjacent spots, so that this ambiguity is unlikely to provoke significant difficulty.

4. A test example

In order to make use of the analysis presented above it is necessary to obtain absolute measurements of experimental intensities. As these measurements were not available the method was tested by comparison with theoretical data which was generated by using the phase-grating approximation.

In terms of the scattering matrix, the phase-grating approximation corresponds to the assumption

$$S=\exp(-iV) \tag{4.1}$$

where V is the reduced potential of the scattering material. Upon comparison with equation (1.2) it may be seen that if the potential is Hermitian, then the approximation satisfies the unitarity equation and hence provides a valid example against which the iterative scheme may be tested. From equation (1.3) it follows that the phase-grating approximation for the transition matrix is

$$T=i\{\exp(-iV)-1\} \tag{4.2}$$

and that it satisfies the Lippmann–Schwinger equation to first order in V.

If the specimen is a crystal of finite width along the **c** axis, then the phase-grating approximation to the scattering amplitude, defined by equation (1.8) is,

$$f(\mathbf{k},\mathbf{k}_0)=i\sum_{\mathbf{L}}[\exp(-i\tilde{V})-1]_{0\mathbf{L}}\bar{\delta}^2(\mathbf{k}-\mathbf{k}_0-\mathbf{L}) \tag{4.3}$$

where

$$\tilde{V}_{\mathbf{LM}}=\int \mathrm{d}^3r\,\exp\{i\mathbf{r}\,.\,(\mathbf{L}-\mathbf{M})\}V(\mathbf{r}) \tag{4.4}$$

and

$$\mathbf{L}=l\tilde{\mathbf{a}}+m\tilde{\mathbf{b}}, \tag{4.5}$$

the integration in the **c** direction being over the thickness of the crystal.

The amplitudes corresponding to the scattering of 500 keV electrons by a layer of crystalline sodium three unit cells thick were calculated using equation (4.3) for diffraction spots within the circle $(l^2+m^2)^{1/2}=10$, the lattice potential being obtained by Fourier transforming the appropriate structure factors (*International Tables for X-ray Crystallography*, 1962). The moduli and phases so obtained are shown in Tables 1 and 2 respectively.

Using the moduli of the amplitudes, equation (3.12) was verified to hold. A unitary set of phases was then generated by iterating equation (3.9), starting from a random set of phases. The resulting set is shown in Table 3. The phases were found to be independent of the initial values employed in the iteration, and may be observed to be within 2% of the expected phases of the phase-grating approximation. Therefore the test case confirms the efficacy and uniqueness of the iterative procedure.

Table 1. *Amplitudes* ($\times 10^3$) *obtained using the phase-grating approximation*

h \ k	0	1	2	3	4	5	6	7	8	9	10
0	33·5		9·32		4·74		2·74		1·73		1·08
1		13·0		6·13		3·52		2·16		1·33	
2	9·32		6·79		4·14		2·53		1·63		1·05
3		6·13		4·41		2·87		1·89		1·19	
4	4·74		4·14		3·01		2·09		1·37		
5		3·52		2·87		2·16		1·49		1·05	
6	2·74		2·53		2·09		1·53		1·08		
7		2·16		1·89		1·49		1·10			
8	1·73		1·63		1·37		1·08				
9		1·33		1·19		1·05					
10	1·08		1·05								

Table 2. *Phases* ($\times 10$) *obtained using the phase-grating approximation*

h \ k	0	1	2	3	4	5	6	7	8	9	10
0	1·04		2·89		4·31		5·45		5·99		5·73
1		2·25		3·75		4·91		5·75		6·12	
2	2·89		3·55		4·60		5·58		6·03		5·52
3		3·75		4·46		5·36		5·90		6·04	
4	4·31		4·60		5·26		5·79		6·13		
5		4·91		5·36		5·75		6·11		5·44	
6	5·45		5·58		5·79		6·09		5·81		
7		5·75		5·90		6·11		5·90			
8	5·99		6·03		6·13		5·81				
9		6·12		6·04		5·44					
10	5·73		5·52								

Table 3. *Phases* ($\times 10$) *obtained by iterating the unitarity equation*

h \ k	0	1	2	3	4	5	6	7	8	9	10
0	1·04		2·88		4·29		5·42		5·97		5·83
1		2·24		3·73		4·88		5·72		6·14	
2	2·88		3·53		4·57		5·56		6·02		5·64
3		3·73		4·44		5·33		5·88		6·09	
4	4·29		4·57		5·23		5·76		6·14		
5		4·88		5·33		5·72		6·11		5·55	
6	5·42		5·56		5·76		6·09		5·89		
7		5·72		5·88		6·11		5·97			
8	5·97		6·02		6·14		5·89				
9		6·14		6·09		5·55					
10	5·83		5·64								

5. Conclusions

By considering the elastic scattering of electrons from thin crystals having reflexion-symmetric potentials, a method has been developed for determining the phases from the absolute intensities of the diffraction spots. A condition, equation (3.12), has been derived which guarantees that the phases so obtained are subject to at most a twofold ambiguity of the form α or $\pi-\alpha$. In any experimental case it is expected that the quasi-smooth variation of phase between adjacent diffraction spots will further reduce the ambiguity.

The method has been sucessfully tested against data generated by using the phase-grating approximation for 500 keV electrons scattering from a thin crystal of sodium. Possible further developments of the method include an investigation of when and how ambiguity may arise if equation (3.12) is violated, the introduction of inelastic scattering, and the relaxation of the condition of reflexion symmetry of the potential.

The authors wish to thank Professor R. E. Burge for much advice and constant encouragement during the work.

APPENDIX A

In order to establish the relation

$$\int \mathrm{d}^3\mathbf{q}\,\bar{\delta}(q^2-k_0^2)\bar{\delta}[(\mathbf{q}-\mathbf{k}_0)^{\perp\mathbf{c}}+\mathbf{N}] = (2\pi)^3(2v)^{-1}\{(\mathbf{N}.\tilde{\mathbf{c}})^2+\tilde{\mathbf{c}}^2(k_0^2-N^2)\}^{-1/2} \quad (A.1)$$

we expand in terms of the reciprocal-lattice vectors $\tilde{\mathbf{a}}$, $\tilde{\mathbf{b}}$ and $\tilde{\mathbf{c}}$, which are defined by

$$\tilde{\mathbf{a}}=2\pi v^{-1}\mathbf{b}\times\mathbf{c} \quad (A.2)$$

and its cyclic permutations, with

$$v=\mathbf{a}\,.\,(\mathbf{b}\times\mathbf{c}) \quad (A.3)$$

being the cell volume.

Now if we expand

$$\mathbf{q}=\tilde{\mathbf{q}}_a\mathbf{a}+\tilde{\mathbf{q}}_b\mathbf{b}+\tilde{\mathbf{q}}_c\mathbf{c}, \quad (A.4)$$

then by choosing a particular coordinate frame we may easily show that

$$\int \mathrm{d}^3\mathbf{q}=\frac{(2\pi)^3}{v}\int \mathrm{d}^3\tilde{\mathbf{q}} \quad (A.5)$$

while at $\mathbf{q}^{\perp\mathbf{c}}=-\mathbf{N}$

$$\delta(q^2-k_0^2)=\tfrac{1}{2}\Delta^{-1/2}\{\delta(\tilde{\mathbf{q}}_c-q_+)+\delta(\tilde{\mathbf{q}}_c-q_-)\} \quad (A.6)$$

where

$$\tilde{\mathbf{c}}^2q_\pm=\mathbf{N}\,.\,\tilde{\mathbf{c}}\pm\Delta^{1/2} \quad (A.7)$$

with

$$\Delta=(\mathbf{N}\,.\,\tilde{\mathbf{c}})^2+(k_0^2-N^2)\tilde{\mathbf{c}}^2. \quad (A.8)$$

But q_- corresponds to the backward-scattering amplitude, which is negligible, therefore, upon combining equations (A.5) and (A.6),

$$\int \mathrm{d}^3\mathbf{q}\,\bar{\delta}(q^2-k_0^2)\bar{\delta}^2[(\mathbf{q}-\mathbf{k}_0)^{\perp\mathbf{c}}+\mathbf{N}] = (2\pi)^3(2v)^{-1}\Delta^{-1/2} \quad (A.9)$$

which is the required equality.

If $k_0^2\gg N^2$, then $\Delta\simeq k_0^2\tilde{\mathbf{c}}^2$, and hence

$$\int \mathrm{d}^3\mathbf{q}\,\bar{\delta}(q^2-k_0^2)\bar{\delta}^2[(\mathbf{q}-\mathbf{k}_0)^{\perp\mathbf{c}}+\mathbf{N}]\simeq(2\pi)^3(2vk_0\tilde{c})^{-1} \quad (A.10)$$

which is the form used in equation (2.8).

APPENDIX B

From equation (3.9)

$$\|\mathscr{M}(\varphi)\|_\infty\le\sup_{\mathbf{L}\neq0}\sin^{-1}[R^{-1}\sum_{\mathbf{M}}{}'H(\mathbf{L},\mathbf{M})]\le\sin^{-1}(R^{-1}Q) \quad (B.1)$$

where Q is defined by equation (3.11). Hence

$$\mathscr{F}=\{\varphi|\,\|\varphi\|_\infty\le\sin^{-1}(R^{-1}Q)\} \quad (B.2)$$

is mapped into itself by $\varphi\to\mathscr{M}(\varphi)$.

In order to derive sufficient conditions for the mapping to be strictly contractive we consider

$$\|\mathscr{M}(\psi)-\mathscr{M}(\varphi)\|_\infty = \sup_{\mathbf{L}\neq0}|\sin^{-1}A(\psi)-\sin^{-1}A(\varphi)| \quad (B.3)$$

where

$$A(\varphi)=R^{-1}\sum_{\mathbf{M}}{}'H(\mathbf{L},\mathbf{M})\cos\{\varphi(\mathbf{M})-\varphi(\mathbf{L}-\mathbf{M})\} \quad (B.4)$$

and hence

$$|A(\psi)-A(\varphi)|\le2R^{-2}Q\sum_{\mathbf{M}}{}'H(\mathbf{L},\mathbf{M})\times\sin\tfrac{1}{2}\{\psi(\mathbf{M})-\varphi(\mathbf{M})-\psi(\mathbf{L}-\mathbf{M})+\varphi(\mathbf{L}-\mathbf{M})\}\le2R^{-2}Q^2\|\psi-\varphi\|_\infty. \quad (B.5)$$

But $\sin^{-1}x$ is a convex function of x, therefore

$$|\sin^{-1}A(\psi)-\sin^{-1}A(\varphi)|\le(1-R^{-2}Q^2)^{-1/2}|A(\psi)-A(\varphi)| \quad (B.6)$$

and, upon combining equations (B.5) and (B.6), the condition for a strict contractive mapping

$$\|\mathscr{M}(\psi)-\mathscr{M}(\varphi)\|_\infty<\|\psi-\varphi\|_\infty \quad (B.7)$$

becomes

$$2R^{-2}Q^2(1-R^{-2}Q^2)^{-1/2}<1, \quad (B.8)$$

viz.

$$Q<\alpha R$$

where

$$\alpha=\left(\frac{\sqrt{17}-1}{8}\right)^{1/2}. \quad (B.9)$$

Now

$$\sin\varphi(\mathbf{0}) = \sum_{\mathbf{M}} H(\mathbf{0},\mathbf{M}) = \sum_{\mathbf{M}}{}' H(\mathbf{0},\mathbf{M}) + G(\mathbf{0}) \leq Q + G(\mathbf{0}). \quad \text{(B.10)}$$

Hence a sufficient condition to satisfy equation (B.8) is

$$Q < \alpha[1 - 4G(\mathbf{0})Q]^{1/2} \quad \text{(B.11)}$$

i.e.

$$Q < \alpha[4\alpha^2 G^2(\mathbf{0}) + 1]^{1/2} - 2\alpha^2 G(\mathbf{0}). \quad \text{(B.12)}$$

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Acta Cryst. (1974). A**30**, 548

Facetting the Dodecahedron

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(*Received* 15 *September* 1973; *accepted* 14 *February* 1974)

Rules are given for the construction of facetted polyhedra which ensure that the reciprocal figures are also polyhedra. The complete set of 22 facetted dodecahedra is enumerated, depicted and correlated with the stellations of the icosahedron.

Introduction and definitions

The name *polyhedron* implies a definition in terms of the flat polygonal faces of the figure. This viewpoint leads naturally to the idea of stellating a polyhedron by extending the planes of the faces to meet again at new edges and vertices. Less obvious is the dual process, *facetting*, in which the vertices are linked together to give new edges and new faces (or *facets*). Coxeter (1963) has given an authoritative account of both constructions but treats only those cases where the derived polyhedra have regular polygonal faces or vertices. This is a severe restriction, satisfied by only five of the 59 stellated icosahedra enumerated by Coxeter, Du Val, Flather & Petrie (1938). It does, however, have the effect of ensuring that the derived polyhedra have well-defined reciprocals, a condition not met by many of the 59 icosahedra.

The operation of reciprocating a polyhedron (P) consists in constructing a set of points reciprocal to the planes of the faces of P; the centre of P is taken as the centre of inversion. The new points are identified with the vertices of the reciprocal (R); they are linked by edges whenever the corresponding faces of P have an edge in common. It follows that the vertices of P are reciprocal to the faces of R and that P and R are topologically dual. Clearly it is possible to define the facetions of P and the stellations of R in such a way as to maintain duality. However, one cannot construct 59 facetted dodecahedra by reciprocating the stellated icosahedra of Coxeter *et al.* (1938), since these were described as *solids* built up from fundamental cells defined by the extended faces of the icosahedron. The reciprocal cells overlap one another and so cannot be used in an analogous way. If, however, one treats a polyhedron as a *surface*, defining precisely how the faces are to be joined together, the construction of the reciprocal follows automatically. This procedure leads to a convenient description of facetting, through the definitions which follow:

1. An *edge* is a straight line connecting two *vertices*.

2. A *polygon* is an endless chain of coplanar edges in which every vertex lies at the end of two and only two edges. The edges may intersect to give star or skew polygons but the intersections are not counted as vertices.

3. A *face* (or *facet*) is a plane surface with a polygonal boundary. If the chain of edges winds round the centre n times the face will have n layers, which may be connected by a winding point.

4. A *polyhedron* is an unbounded surface composed of faces joined together along their edges in such a way that every edge of the polyhedron is the edge of two and only two faces. The faces may intersect but the intersections are not counted as edges.

So far, this follows Coxeter (1963), but does not