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Some remarks on the relation between the Harker–Kasper inequality and the Okaya–Nitta linear inequalities.

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Okaya & Nitta (1952) have derived structure-factor inequalities for a centrosymmetrical structure in which unitary structure factors appear only in linear form. The most useful among these so-called linear inequalities are

$$\left.\begin{aligned} |U_H \pm U_{H'}| &\le \{(1\pm U_{H+H'}) + m^2(1\pm U_{H-H'})\}/2m \\ |U_H \pm U_{H'}| &\le \{m^2(1\pm U_{H+H'}) + (1\pm U_{H-H'})\}/2m\,, \end{aligned}\right\} \quad (1)$$

where U_H is the unitary structure factor for the reflexion $H = hkl$, and m is any positive number. These inequalities correspond to the following Harker–Kasper inequality (Harker & Kasper, 1948):

$$|U_H \pm U_{H'}| \le \sqrt{\{(1\pm U_{H+H'})(1\pm U_{H-H'})\}}\,, \quad (2)$$

which has been shown to be the most powerful among analogous inequalities (Grison, 1951). As already remarked in the paper of Okaya & Nitta, (1) is less powerful than (2) in limiting phase relations of structure factors. This can easily be shown as follows.

In general for any real or complex numbers a_i's and b_i's

$$|\sum_i a_i b_i| \le \sqrt{\{\sum_i |a_i|^2 \sum_i |b_i|^2\}} \le \tfrac{1}{2}(\sum_i |a_i|^2 + \sum_i |b_i|^2)\,, \quad (3)$$

the first half of this relation being the Cauchy inequality. If we put

$$a_i = \begin{Bmatrix} 1 \\ m \end{Bmatrix} \sqrt{n_i}\,.\begin{Bmatrix} \cos \\ \sin \end{Bmatrix} \{2\pi(px_i + qy_i + rz_i)\}$$

$$b_i = \begin{Bmatrix} m \\ 1 \end{Bmatrix} \sqrt{n_i}\,.\begin{Bmatrix} \cos \\ \sin \end{Bmatrix} \{2\pi(p'x_i + q'y_i + r'z_i)\}$$

in one of the inequality relations of (3),

$$|\sum_i a_i b_i| \le \tfrac{1}{2}(\sum_i |a_i|^2 + \sum_i |b_i|^2)\,,$$

we obtain (1). On the other hand, the same substitution in the Cauchy inequality leads to (2). Hence, from (3), (2) is more powerful than (1) as a phase-limiting inequality.

The relation between (1) and (2) can be seen more clearly by graphical representation. Choosing the double sign in (1) and (2) so that the left-hand side may be equal to, say, $|U_H| + |U_{H'}|$, and putting

$$|U_H| + |U_{H'}| = k,\ 1\pm|U_{H+H'}| = X,\ 1\pm|U_{H-H'}| = Y,$$

then (1) becomes

$$\left.\begin{aligned} k &\le X/2m + mY/2 \\ k &\le mX/2 + Y/2m \end{aligned}\right\} \quad (4)$$

and (2) becomes

$$k \le \sqrt{(XY)}\,. \quad (5)$$

Inequality (5) requires that the allowed values of X and Y must lie on the positive side of a rectangular hyperbola $xy - k^2 = 0$, while (4) requires that they must lie on the positive side of two straight lines, $x/2m + my/2 - k = 0$ and $mx/2 + y/2m - k = 0$. Now these two straight lines prove to be tangents to the above hyperbola with direction coefficients $-1/m^2$ and $-m^2$ respectively, and are situated symmetrically with respect

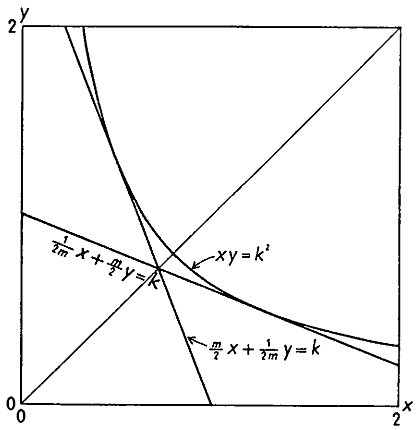

Fig. 1. Graphical representation of the relation between the two inequalities (1) and (2).

to the straight line $x = y$ (Fig. 1). Thus it can be seen that (2) restricts an allowed region for X and Y by a rectangular hyperbola, whereas in (1) the same role is played by two tangents to this hyperbola with direction coefficients varying with m; the limit imposed by (1) is therefore less severe than that set by (2).

From the practical point of view, there is little difference in usefulness between these two inequalities. Indeed, for $F(hk0)$'s and $F(0kl)$'s of tetragonal ethylenediamine sulphate, both inequalities gave the same number of structure factors of which the signs could be determined (Okaya & Nitta, 1952; Sakurai, 1952). It may thus be safely asserted that the linear inequalities are much more convenient to use in analytical application, while the Harker–Kasper inequality (2) can be used very easily by means of a graphical method (Sakurai, 1952).

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