Acta Cryst. (1976). A**32**, 920

A note on the conversion of the tangent formula to an optimization problem. By ARTHUR M. LESK, *Fairleigh Dickinson University, Teaneck, New Jersey* 07666, *U.S.A.*

(*Received* 10 *February* 1976; *accepted* 22 *March* 1976)

It is shown that the sets of phase angles of a structure which satisfy the tangent formula correspond also to extremal values of a function $G=-\frac{1}{6}\sum_{\mathbf{h}}\sum_{\mathbf{k}}|E_{\mathbf{h}}E_{\mathbf{k}}E_{\mathbf{h}-\mathbf{k}}|\cos(\varphi_{\mathbf{k}}+\varphi_{\mathbf{h}-\mathbf{k}}-\varphi_{\mathbf{h}})$. This fact may simplify the computational implementation of the tangent formula and those of its extensions that can also be formulated as optimization problems.

The tangent formula (Karle & Hauptman, 1956) was originally stated as a set of simultaneous (approximate) equations:

$$\tan\varphi_{\mathbf{h}}=\frac{\sum_{\mathbf{k}\neq\mathbf{h}}|E_{\mathbf{k}}E_{\mathbf{h}-\mathbf{k}}|\sin(\varphi_{\mathbf{k}}+\varphi_{\mathbf{h}-\mathbf{k}})}{\sum_{\mathbf{k}\neq\mathbf{h}}|E_{\mathbf{k}}E_{\mathbf{h}-\mathbf{k}}|\cos(\varphi_{\mathbf{k}}+\varphi_{\mathbf{h}-\mathbf{k}})} \qquad (1)$$

in which $\varphi_{\mathbf{h}}$ is the phase corresponding to the normalized structure factor $E_{\mathbf{h}}$. Multiplication of each equation by the corresponding quantity:

$$\cos\varphi_{\mathbf{h}}\,.\,[\sum_{\mathbf{k}\neq\mathbf{h}}|E_{\mathbf{k}}E_{\mathbf{h}-\mathbf{k}}|\cos(\varphi_{\mathbf{k}}+\varphi_{\mathbf{h}-\mathbf{k}})]\,,$$

transposing, and applying standard trigonometric identities, produces the system of equations:

$$\begin{aligned}\sum_{\mathbf{k}\neq\mathbf{h}}|E_{\mathbf{k}}E_{\mathbf{h}-\mathbf{k}}|\,[\cos\varphi_{\mathbf{h}}\sin(\varphi_{\mathbf{k}}+\varphi_{\mathbf{h}-\mathbf{k}})\\ -\sin\varphi_{\mathbf{h}}\cos(\varphi_{\mathbf{k}}+\varphi_{\mathbf{h}-\mathbf{k}})]\\ =\sum_{\mathbf{k}\neq\mathbf{h}}|E_{\mathbf{k}}E_{\mathbf{h}-\mathbf{k}}|\sin(\varphi_{\mathbf{k}}+\varphi_{\mathbf{h}-\mathbf{k}}-\varphi_{\mathbf{h}})=0\,.\end{aligned} \qquad (2)$$

Hauptman has derived, and examined the practical utility of, a number of modifications of this system of equations, which he called *modified* tangent procedures (Hauptman, 1971; Hauptman & Weeks, 1972). The modified tangent procedures contain additional terms that make stronger use of the probability distribution of the phases. Both the system of equations (2) and the modified tangent procedures could be solved by the principle of least squares.

Because the analysis of Hauptman & Weeks shows that both the original tangent formula and the modified tangent formula can be formulated as optimization problems, it is interesting to note that solution of the system of equations (2) is equivalent to determining an extremal point of a function. For if

$$G=-\tfrac{1}{6}\sum_{\mathbf{h}}\sum_{\mathbf{k}}[|E_{\mathbf{h}}E_{\mathbf{k}}E_{\mathbf{h}-\mathbf{k}}|\cos(\varphi_{\mathbf{k}}+\varphi_{\mathbf{h}-\mathbf{k}}-\varphi_{\mathbf{h}})]\,,$$

then

$$\frac{\partial G}{\partial\varphi_{\mathbf{l}}}=|E_{\mathbf{l}}|\sum_{\mathbf{k}}[|E_{\mathbf{k}}E_{\mathbf{l}-\mathbf{k}}|\sin(\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}-\mathbf{k}}-\varphi_{\mathbf{l}})]\,. \qquad (3)$$

Although the definition of G contains a double summation, compared to the two single summations of the equations (1), an equation of type (1) must be evaluated for every value of **h** whereas one evaluation of G contains information about the entire set of phases.

This formula (3) for the derivatives of G depends on the assumption that the summations are effectively infinite, and that Friedel's law holds. It can be derived by noting that:

$$\begin{aligned}&\frac{\partial}{\partial\varphi_{\mathbf{l}}}\cos(\varphi_{\mathbf{k}}+\varphi_{\mathbf{h}-\mathbf{k}}-\varphi_{\mathbf{h}})\\ &=-\sin(\varphi_{\mathbf{k}}+\varphi_{\mathbf{h}-\mathbf{k}}-\varphi_{\mathbf{h}})\frac{\partial}{\partial\varphi_{\mathbf{l}}}(\varphi_{\mathbf{k}}+\varphi_{\mathbf{h}-\mathbf{k}}-\varphi_{\mathbf{h}})\\ &=-\sin(\varphi_{\mathbf{k}}+\varphi_{\mathbf{h}-\mathbf{k}}-\varphi_{\mathbf{h}})\times(\delta_{\mathbf{kl}}-\delta_{\mathbf{k},-\mathbf{l}}+\delta_{\mathbf{h}-\mathbf{k},\mathbf{l}}\\ &\quad-\delta_{\mathbf{h}-\mathbf{k},-\mathbf{l}}-\delta_{\mathbf{hl}}+\delta_{\mathbf{h},-\mathbf{l}})\,.\end{aligned}$$

Writing

$$\begin{aligned}\frac{\partial G}{\partial\varphi_{\mathbf{l}}}&=\tfrac{1}{6}\sum_{\mathbf{h}}\sum_{\mathbf{k}}|E_{\mathbf{h}}E_{\mathbf{k}}E_{\mathbf{h}-\mathbf{k}}|\sin(\varphi_{\mathbf{k}}+\varphi_{\mathbf{h}-\mathbf{k}}-\varphi_{\mathbf{h}})\\ &\quad\times(\delta_{\mathbf{kl}}-\delta_{\mathbf{k},-\mathbf{l}}+\delta_{\mathbf{h}-\mathbf{k},\mathbf{l}}-\delta_{\mathbf{h}-\mathbf{k},-\mathbf{l}}-\delta_{\mathbf{hl}}+\delta_{\mathbf{h},-\mathbf{l}})\,,\end{aligned}$$

$\partial G/\partial\varphi_{\mathbf{l}}$ is expressed, after evaluating the delta functions, in terms of six single summations. Applications of Friedel's law shows that each of these is equal to

$$\tfrac{1}{6}\sum_{\mathbf{k}}|E_{\mathbf{l}}E_{\mathbf{k}}E_{\mathbf{l}-\mathbf{k}}|\sin(\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}-\mathbf{k}}-\varphi_{\mathbf{l}})\,.$$

Thus, any set of phases for which the tangent formula is satisfied, or which satisfies the system of equations (2), corresponds also to the vanishing of the partial derivatives of G; *i.e.* to a set of phases for which G has an extremum.

This relation may simplify the computational implementation of the tangent formula and those of its extensions that can also be formulated as optimization problems.

Work supported by U.S. National Science Foundation research grants GJ-35327 and DCR74-24390.

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