# *Personal Reminiscences*

H. Lipson

## *Fourier Strips*

In 1932, C. A. Beevers and H. Lipson at Liverpool were attempting to work out the structure of $CuSO_4 \cdot 5H_2O$—a triclinic crystal with two formula units in the unit cell. They had established that the copper atoms were in special positions, but the problem seemed to be much too difficult for the trial-and-error methods that were then currently in use. Beevers then suggested trying the Fourier methods that W. L. Bragg (1929) was advocating for the determination of structures; they had been tried out on diopside but they had not yet been used for an unknown structure.

The problem however was how to carry out the summations. There were 95 intensities and it was decided that, in the light of the limit of resolution, over five hundred points would have to be considered in the asymmetric part of the unit cell. This was considered to be a formidable task.

Beevers made the first exploration. Taking one point only, he worked out the contribution of *all* the F's; it took him 40 minutes. On the basis of this, assuming a 20-hour week (they had other duties as well!) they reckoned that it would take about eight months to make the complete survey. This would not do! They therefore tried to think of improved methods, involving long strips of paper with sine-curve ordinates written on them; one read off numbers in prearranged sequences and the other multiplied them by the observed F's on a slide rule basis. With these artifices the first Fourier synthesis was completed in a month (with, it may be remarked, most pleasing success).

During the process new ideas were forthcoming and by means of these the synthesis was checked by performing it again in rows along the other axis, and the mission was accomplished in two weeks. The results showed suprising agreement.

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The methods still seemed unsystematic and clumsy, mostly because each curve of cos $2\pi(hx + ky)$ parallel to the x axis had to start at a separate value of ky. Lipson then had the idea of expanding the function into cos $2\pi hx$ cos $2\pi ky$—sin $2\pi hx$ sin $2\pi ky$, so that the ky terms could be considered as amplitudes rather than phases. This simple idea—which at first sight seemed retrograde—made the whole computation much easier since all the amplitudes for one k could be added together once and for all; it could be carried out quite efficiently by one person who had the necessary arithmetical ability.

The procedure involved working out the various sine curves, entering them in a book, and adding the columns of figures (Beevers and Lipson, 1934). Lipson thought it rather wasteful to lose the figures each time; obviously a curve with a particular amplitude was likely to recur, and so was worth-while preserving for further use. Therefore he entered the numbers on strips, and filed them for future use. After a few summations he had an imposing collection, which he added to systematically in any spare moments.

Thus the Fourier strips originated. Beevers, who had then moved to Manchester, made a copy and then suggested that further printed copies be made. Professor W. L. Bragg and Mr. R. W. James were very sympathetic and after much consideration of the enormous cost involved (about £100!) seventy sets were produced and given or sold to other laboratories (Lipson and Beevers, 1936). As usual in research, the production of the strips involved much more work than was expected, but the final results seem to have well justified the trouble and cost of their preparation. Beevers has continued to produce sets of strips and by now (1961) three hundred sets have been supplied to laboratories all over the world.

### *Intensity Statistics*

The idea of making use of a statistical survey of the intensities diffracted by a crystal arose in 1942. *Nature* received two letters from S. H. Yü (1942a, b) in China claiming that absolute intensities could be derived from relative ones. The letters were sent to be refereed at Cambridge, but they did not give enough detail for the methods to be properly assessed. A. J. C. Wilson thought that the claim was unreasonable, but H. Lipson pointed out that if one assumed any arbitrary positions for the atoms in a unit cell the general level of the F's should be the same as for the correct structure. He suggested the

rather clumsy procedure of working out such a set of F's and scaling the observed ones to give the same total; Wilson however looked into the theory and found a simpler procedure based upon Patterson's ideas of interatomic vectors.

Wilson (1942) tried out this procedure on data for copper sulphate and the alums, and found that, although it gave correct orders of magnitude, it was not very accurate. The methods were worth using, but they had to be modified as more accurate atomic positions were obtained. The work was then dropped in favour of more immediate practical problems.

After the war, Wilson returned to the problem that had been worrying him: why did not the alums and copper sulphate give better results? He traced the discrepancy to the fact that some heavy atoms lay on special positions and this discovery induced him and Rogers to explore the influence of symmetry or intensity distributions. From this exploration arose the extensive list of papers published by them and their co-workers at Cardiff.

*References*

1. Lipson & Beevers, *Proc. Roy. Soc.* A 1934, *146*, 570.
2. Lipson & Beevers, *Proc. Phys. Soc.* [London] 1936, *48*, 772.
3. Wilson, A. J. C. (1942). *Nature*, 150, 152.
4. Yü, S. H. (1942a). *Nature*, 149, 638.
5. Yü, S. H. (1942b). *Nature*, 150, 151.

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