

## The calculator race—1979 is prime

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Physics teachers and students contemplating the purchase of a programmable calculator or a microcomputer are interested in the relative merits of these devices. In this paper we treat some of the relative merits of two such devices, the TI 59 Programmable Calculator<sup>1</sup> with a PC-100A printer and the 8KPET microcomputer.<sup>2</sup>

A straightforward program using the TI 59 Programmable Calculator to generate and print the prime numbers was developed by a freshman student in our calculator physics laboratory. Table I shows an improved form of the program. While it is really not very fast compared with computers and microcomputers, we feel that it is interesting pedagogically. The program omits even numbers by incrementing to the odd number being tested each time by two, and further speeds up the testing by dividing by odd numbers only, starting with three and ending when the square root of the number being tested is reached. The program used no other special properties of prime numbers which might speed it up since speed was of no direct interest to us at first.

It was decided to "race" the TI 59 programmable against the 8KPET microcomputer using somewhat comparable prime number programs. The 8KPET used only a visual display while the TI 59 printed the numbers generated.

The first program tested on the TI 59 included a pause to display the number to be tested next and another pause to display each factor being tried (Table I). These displays added appreciably to the time required and were removed when a little more speed was sought for this "race." Removing these pauses reduced the time between prints by about one third, as is noted in Table II.

Table III shows the Basic program run on the PET microcomputer which follows the same algorithm used in the programmable calculator program. In both cases the two operators agreed to determine how long it takes to go through all the prime numbers to 1979 (2001 is not a prime number!). The prime number generator program is a good benchmark for comparing these two devices since it uses addition, division, and logical comparison repeatedly.

The time for the TI 59 calculator with printer to arrive at the prime number 1979 starting from one, using the program shown in Table I, was 164 min. Removing the two pauses speeded up the calculation appreciably, requiring 110 min to arrive at 1979. The time for the PET to

**TABLE I**  
TI 59 Prime number program

```
LBL; A; 2; NOP; SUM; 00; 3; STO; 01; RCL; 00; PAU;
√X; INT; STO; 02; RCL; 00; ÷; RCL; 01; PAU; =; INV;
INT; EQ; A; RCL; 01; -; RCL; 02; =; GE; 00; 42; 2;
SUM; 01; GTO; 00; 16; RCL; 00; PRT; GTO; A; LBL;
E'; 1; PRT; 2; PRT; 3; PRT; CMS; 1; STO; 00; R/S.
```

**TABLE II**  
Program times

Program and calculator tested	Time to progress from 1 thru all the prime numbers up to 1979
1. TI59; Program shown in Table I	164 min
2. TI59; Program as in Table I but with the two pauses removed	110 min
3. PET Microcomputer Basic program as shown in Table III	3 min

**TABLE III**  
PET Basic prime number program

```
10 N=1
20 PRINT N
30 N=N+2
40 S=N↑.5
50 IF S=INT(S) GOTO 30
60 F=3
70 IF (N/F)=INT(N/F) GOTO 30
80 F=F+2
90 IF F<S GOTO 70
100 PRINT N
110 GOTO 30
```

# Introducing harmonic waves through Fourier synthesis

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## I. INTRODUCTION

Introducing students to the study of harmonics and the nature of composite waves by the method of Fourier synthesis rather than by Fourier analysis seems to have some advantages. Periodic wave synthesis is actually much more easily done than the process of carrying out a Fourier analysis. Furthermore, any system with a graphic display or plotting system is pedagogically useful, as the ability to view the shape of the synthesized curve and to vary the parameters and see the nature of the changes in the wave is interesting and informative.

The microcomputer<sup>1</sup> and the programmable pocket calculator are bringing both Fourier analysis and synthesis<sup>2</sup> into the educational stream for students at several levels. The curves to be synthesized may be ones from the area of applied mathematics, but periodic curves of physical significance and from musical sources are also interesting to study. A Fourier-synthesis algorithm developed while teaching a course in the use of the programmable calculator is presented here, along with three examples of its use.

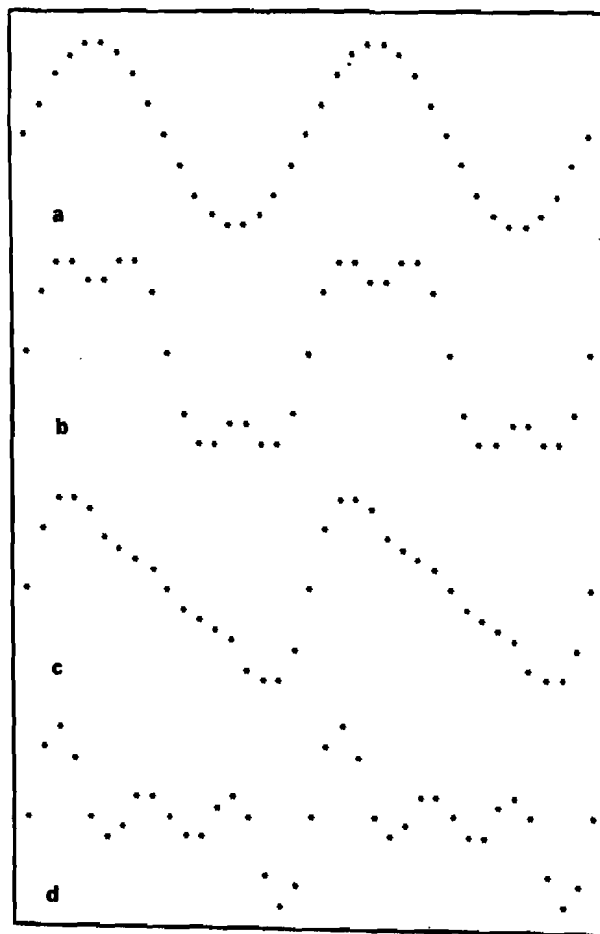


Fig. 1. (a) First harmonic reference; (b) square wave; (c) string plucked  $1/5$  from one end; (d) transmitted wave from a string.

## II. FOURIER SYNTHESIS

The mathematical form which we use for introducing Fourier harmonic synthesis is

$$y(x) = \sum_M (A_M \sin Mx + B_M \cos Mx), \quad (1)$$

where  $M$  is the harmonic number, usually starting with one, and  $A_M$  and  $B_M$  are the amplitudes of the sine and cosine terms, respectively, for the  $M$ th harmonic. This series is easy to program unambiguously, and many interesting examples of Fourier series contain either sine terms or cosine terms only. Thus the harmonic number  $M$  and the two amplitudes are all that are needed for each harmonic to be included and one of the amplitudes frequently is zero. Occasionally the relative amplitudes and the phase angle of each harmonic component are specifically given, but a straightforward trigonometric expansion will result in a form compatible with Eq. (1).

The Fourier series shown in Eq. (1) was used to produce the synthesized curves displayed in Figs. 1(a), 1(b), 1(c), and 1(d). The short program with user notes shown in the Appendix can be used with either the TI 58 or TI 59 with the printer.<sup>3</sup>

Each harmonic curve was calculated at 19 values of  $x$  equally spaced between  $0^\circ$  and  $360^\circ$  and summed into 19 data registers to produce the synthesis. The calculation for each harmonic is completed in a little over 45 seconds. The numbers resulting after each successive synthesis are automatically listed and the results can be plotted after the listing is complete. Additional cycles can be plotted when desired, and this feature is especially useful when the final harmonic to be considered has been included in the synthesis.

## III. EXAMPLES

The first curve shown in Fig. 1(a) is a sine curve, the first harmonic, displayed primarily as a frame of reference for the three synthesized curves that follow. All three of the synthesized curves include only up to the third harmonic shown in Table I. All four curves were obtained using  $N = 18$ .

The first synthesis example shown in Fig. 1(b) is the interesting approximation to the square wave<sup>4</sup> obtained using the first two terms only of the Fourier series for the square wave

$$Y(x) = \sin x + (1/3)\sin 3x + (1/5)\sin 5x, \quad (2)$$

etc. The synthesis of the curve characteristic of the violin string<sup>5</sup> plucked  $1/5$  from the end is shown in Fig. 1(c). The triangular shape of the curve is beginning to develop. The third synthesized curve, Fig. 1(d), is an approximation to the curve expected for the transmitted wave from a vibrating string.<sup>5</sup>

Other curves can be synthesized and compared with ex-

fractive index at room temperature, *ca* 2.3.<sup>13</sup> This is consistent with other evidence for relaxation processes below room temperature.<sup>2,9,14,15</sup> The molecular motion involved is very likely torsion about the chain axes as suggested by Bunn and Garner.<sup>13</sup> The fact that the relaxation is evident in both dielectric loss and proton

resonance data implies that both the dipolar and paraffinic parts of the molecules are moving, even at low temperatures.

#### ACKNOWLEDGMENT

We take this opportunity to express our thanks to Dr. W. P. Slichter who, in addition to supplying the specimens, contributed many enlightening discussions. We are also indebted to Dr. R. H. Boyd, E. I. du Pont de Nemours Company, for making his manuscript available to us prior to publication.

<sup>13</sup> C. W. Bunn and E. V. Garner, *Proc. Roy. Soc. (London)* **189**, 39 (1947).

<sup>14</sup> A. J. Curtis, National Bureau of Standards, dielectrics results (unpublished).

<sup>15</sup> K. Schmieder and K. Wolf, *Kolloid-Z.* **134**, 149 (1953).

## Determination of Atomic Distributions in Liquid Lead-Bismuth Alloys by Neutron and X-Ray Diffraction\*

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AND

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The intensity of scattered neutrons and x-rays has been measured for molten alloys and pure components in the system lead-bismuth. A specially designed diffraction spectrometer has been constructed for the x-ray determinations. The diffraction data have been treated to give atom distributions, and the first main peak in the distribution curves for solutions up to about 60 wt % bismuth corresponds to 12 nearest neighbors, with the value falling to about 7.7 for pure bismuth. No unusual features have been found in the eutectic region, but the density decrease on melting of lead-rich solids is puzzling in view of the retention of 12 nearest neighbors at a mean distance shorter than in the crystal. A model of average pentagonal dodecahedral coordination is suggested to account for this and for the spacing of first maxima in the distribution curves.

### INTRODUCTION

ALTHOUGH diffraction yields much more detailed knowledge of the structure of crystals than it does for liquids, this technique has nevertheless provided valuable information as to the arrangement of atoms in liquids. It has been used extensively for the examination of the elements, as well as a number of compounds, but relatively little work has been done on binary metallic systems.<sup>1</sup> Since it is frequently possible

to interpret physical properties in terms of structure it seemed desirable to investigate a series of liquid alloys through the whole range of composition, especially with the hope that various conjectures regarding alloys might be examined and that a correlation might be made between structural trends and trends found in the physical behavior of the system with changing composition.

For example, the existence of inhomogeneities together with superposition of independent atomic distributions near the eutectic composition has been suggested,<sup>2</sup> as well as the possibility of compound formation,<sup>3</sup> and of the persistence of competing residual

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† Neutron work carried out at Oak Ridge National Laboratory.

‡ Taken in part from thesis submitted for degree of Master of Science, 1959.

<sup>1</sup> Diffraction studies of liquid alloys previously reported include: (a) Al-Sn, Al-In, Bi-Sn: A. I. Bublik and A. G. Buntar, *Kristallografiya* **3**, 32-42 (1958). Data for several compositions. (b) Hg-Zn: D. M. Karlikov, *Ukrain. Fiz. Zhur.* **3**, 370-4 (1958). Density functions given for three alloys. (c) Bi-Pb, Bi-Sn, Sn-Zn, Al-Hg: O. S. Lashko and O. V. Romanova, *Ukrain. Fiz. Zhur.* **3**, 375-84 (1958). Density functions given for eutectics. (d) In-Sb, Sn-Sb: Krebs, Hauke, and Weygand, *Angew. Chem.* **70**, 468-9 and 474 (1958). Density functions given for InSb and SnSb. (e) In-Sb: R. C. Buschert, Thesis, Purdue University, 1957. Density function given for InSb. (f) Tl-Hg: R. E. Smallman and B. R. T. Frost, *Acta Met.* **4**, 611-18 (1956). Intensity data for four alloys. (g) Na-K: N. S. Gingrich and R. E. Henderson, *J.*

*Chem. Phys.* **20**, 117-20 (1952). Density functions given for five alloys and pure components. (h) Au-Sn: H. Hendus, *Z. Naturforsch.* **2**, 505-21 (1947). Intensity given for liquid AuSn. (i) Sn-Bi, Sn-Pb, Pb-Bi: H. Richter, *Physik. Z.* **44**, 406 (1943). Intensities by electron diffraction for selected compositions. (j) K-Hg, Tl-Hg: F. Sauerwald and W. Teske, *Z. anorg. u. allgem. Chem.* **210**, 247 (1933). Intensity data for several alloys. (k) Na-K: K. Banerjee, *Indian J. Phys.* **3**, 399 (1929). Intensity data for several alloys.

<sup>2</sup> Reference 1(h).

<sup>3</sup> A discussion of various possibilities as to degree of binding is given by F. Sauerwald, *Z. Metallk.* **41**, 97-104 (1950).

the Franck-Condon principle the differences between the energies of these absorption bands may be much smaller than the differences in the corresponding activation energies so that it might, therefore, be very difficult to resolve the various bands.

In order to check this idea, S. Barile and the authors, undertook measurements of the absorption coefficient at the temperature of dry ice and were able to resolve

the absorption band at 2280Å into two bands. These two bands had also been found by S. Smakula.<sup>10</sup>

#### ACKNOWLEDGMENT

The authors are indebted to Dr. Gerhart Groetzinger and Dr. Philip Schwed for valuable discussions.

<sup>10</sup> S. Smakula (private communication).

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## Neutron Diffraction and Atomic Distribution in Liquid Lead and Liquid Bismuth at Two Temperatures

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Neutron diffraction patterns have been obtained on liquid lead and liquid bismuth at two temperatures. The patterns differ only slightly at the different temperatures, the main peak being slightly shorter and broader and shifted slightly to smaller angles at the higher temperatures. The diffraction patterns have been analyzed to obtain information on the atomic distribution. The first main peak in the distribution curve for liquid lead is at 3.40Å and represents about 9.4 atoms. The first main peak in the curve for liquid bismuth is at 3.35Å and represents about 7.7 atoms. The second most prominent concentration of atoms occurs at 6.6Å for both lead and bismuth.

#### INTRODUCTION

THIS work was undertaken with the purpose of obtaining neutron diffraction patterns on liquid lead and liquid bismuth at two temperatures and of analyzing these patterns in order to obtain information on the atomic distribution in the liquid. These two elements have conveniently large neutron scattering cross sections. Bismuth and lead are the only liquid metals which have been studied by neutron diffraction<sup>1</sup> and, in the case of lead, the results differ somewhat from those obtained by x-ray diffraction methods.<sup>2</sup> The previous neutron diffraction work with these liquids made use of an instrument with a spread in angle and wavelength. While this arrangement did help to overcome the disadvantage of a low neutron beam intensity, it introduced complications in the interpretation of the data. It was hoped that the neutron spectrometer<sup>3</sup> available would be capable of giving good patterns because of its relatively intense well-defined monochromatic beam and the relative simplicity of obtaining experimental results.

#### EXPERIMENTAL

The equipment used consisted of a neutron spectrometer and recording system<sup>3</sup> and a special furnace to hold the metal in the liquid state at a controlled temperature.

The neutron diffraction spectrometer consisted of a monochromatizing crystal with collimating slits, a monitoring system for maintaining a neutron beam of nearly constant intensity, a BF<sub>3</sub> slow neutron proportional detector arranged to scan the diffracted beam out to about 110 degrees, and the associated electronic circuits and recording system. A copper crystal reflecting a relatively strong neutron beam of 1.16Å from the (111) planes was employed to give the patterns used in the analysis. The wavelength spread was about 2 percent at the center of the beam, and the sensitive angle of the detector was about 2 degrees. The BF<sub>3</sub> neutron detector scanned through the diffraction angles at a rate of 8 degrees per hour for most of this work, and the pulses from it operated the rate meter and recording potentiometer. The data were obtained in the form of a chart showing counts per minute against scattering angle.

Two preliminary low temperature runs on liquid bismuth were made using a heating system which applied heat to one end of the sample. The remainder of the low and all the higher temperature runs were

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<sup>1</sup> O. Chamberlain, *Phys. Rev.* **77**, 305 (1950).

<sup>2</sup> H. Hendus, *Z. Naturforsch.* **2A**, 505 (1947).

<sup>3</sup> Made available by H. Levy and S. W. Peterson, similar to that described by E. O. Wollan and C. G. Shull, *Phys. Rev.* **73**, 830 (1948).

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## Atomic and Electronic Distributions in Liquid Nitrogen, Nitric Oxide, and Nitrous Oxide

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(Received May 17, 1943)

The monochromatic x-ray diffraction patterns for liquid nitrogen, nitric oxide and nitrous oxide have been obtained and analyzed by the Fourier integral method to obtain the atomic or electronic distributions. The diffraction patterns show one main peak and only faint peaks or plateaus at larger angles. The distribution curves show diatomic aggregates in liquid nitrogen and nitric oxide comparable to those found in the gaseous states. A linear molecule for nitrous oxide is consistent with the present data while a triangular molecule is not.

### INTRODUCTION

THE diffraction patterns produced by x-rays when scattered by liquids are of interest both in a qualitative way and as regards the information they can give concerning the "structure" of the liquid. The x-ray diffraction patterns produced by monatomic liquids may be analyzed in a systematic way to give the radial distribution of atoms about a given atom, using the theory of Zernicke and Prins,<sup>1</sup> and Debye and Menke.<sup>2</sup> The diffraction pattern produced by a polyatomic liquid is not so directly interpreted in terms of the distribution of atoms, but does give, by a direct analysis, the distribution of electrons in the liquid. A successful analysis by either of these theories depends first on a careful determination of the diffraction pattern out to large angles for that liquid, the relative intensity of the scattered x-rays, as well as the position of the diffraction peaks, being of importance.

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<sup>1</sup> F. Zernicke and J. Prins, *Zeits. f. Physik* **41**, 184 (1927); *Zeits. f. Physik* **56**, 617 (1929).

<sup>2</sup> P. Debye and H. Menke, *Physik. Zeits.* **31**, 797 (1930); *Ergeb. d. Tech. Rontgenk.* (1931), Vol. 2.

The present work was undertaken both to seek to improve on earlier work on the diffraction pattern produced by liquid nitrogen and for the first time actually to carry out analyses of this pattern and those of liquid nitric oxide and nitrous oxide so as to obtain direct information concerning the atomic and electronic distributions in these liquids.

The diffraction pattern produced by liquid nitrogen was one of the first to be obtained, pictures having been taken by Keesom and de Smedt<sup>3</sup> about 1923. Using molybdenum radiation filtered through zirconium and an evacuated camera of 2.75-cm radius, they found two peaks in the pattern for liquid nitrogen, the main peak at  $\sin \theta/\lambda = 0.139$  and a second peak at about 0.208.

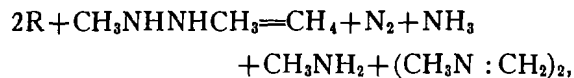
### THEORY AND METHOD OF EVALUATING THE FOURIER INTEGRAL

The equation used for liquid nitrogen has been developed previously<sup>4</sup> in the literature and may

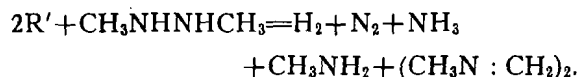
<sup>3</sup> W. H. Keesom and J. de Smedt, *Proc. Amst. Akad. Sci.* **26**, 112 (1923).

<sup>4</sup> B. E. Warren, *J. App. Phys.* **8**, 645 (1937).

reactions (1) and (2) require a third molecule of the hydrazine for ultimate decomposition giving over-all

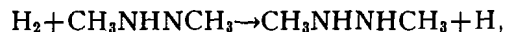


or



The observed quantum yield of 0.3 as opposed to the analytical yield of 3 is probably due to a reversal of (1a) or its equivalent. Henkin and Taylor<sup>2</sup> in the study of the addition of hydrogen atoms to azomethane found complete conversion of the azomethane to dimethylhydrazine even when the ratio of atomic hydrogen to azomethane was much less than 0.5 whereas, had the addition occurred entirely by steps involving atomic hydrogen, the ratio would have to have been at least two. It was obvious that some of the hydrogenation was occurring through hydrogen molecules and the reaction of the radical formed by

addition of one hydrogen atom to azomethane, with hydrogen :



appeared very plausible as a Walden inversion type reaction. This reaction is equivalent to a reversal of (1a) and, since the maximum energy of activation of addition of hydrogen to azomethane was found to be 3-4 kcal., will occur quite readily reducing the quantum yield as found.

The recent observation of Birse and Melville<sup>15</sup> that the efficiency of the primary process in ammonia photolysis is 0.58 rather than one indicates, since no fluorescence has been detected in ammonia and the pressure dependence of the quantum yield is less than would be expected for any collisional process, that there is some mechanism for internal degradation of the energy. This might also be present in the hydrazine molecule.

<sup>15</sup> E. A. B. Birse and H. W. Melville, Proc. Roy. Soc. A175, 164 (1940).

## The Diffraction of X-Rays by Liquid Oxygen\*

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(Received May 17, 1942)

The x-ray diffraction pattern of liquid oxygen at 89°K shows an intense peak at  $\sin \theta/\lambda = 0.157$ , and very weak peaks at 0.35 and at 0.5; that at 62°K shows an intense peak at 0.159, and weak peaks at 0.35 and at 0.5. The atomic distribution curves have peaks at 1.3A, 2.2A, 3.4A, and 4.2A for 89°K, and at 1.25A, 2.15A, 3.2A, and 4.1A for 62°K. The first peaks are due to the interatomic distance in the diatomic molecule, the second may be due to triatomic oxygen, and the others may be due to higher molecular aggregates.

### INTRODUCTION

A STUDY of the diffraction of x-rays by liquid oxygen is of interest not only for its contribution to the field of x-ray diffraction, but also for the information it may supply to our knowledge of molecular aggregates in liquid oxygen. The present work was undertaken to obtain as complete a diffraction pattern of liquid oxygen as possible and to analyze this pattern for the

\* A preliminary report of this work was presented at the December, 1940 meeting of the American Physical Society.

atomic distribution curve. This has been done for liquid oxygen at 89°K and at 62°K.

One of the earliest studies in the field of x-ray diffraction by liquids was done with liquid oxygen by Keesom and de Smedt. In their first work,<sup>1</sup> copper radiation filtered through nickel was used in an evacuated camera of 2.75-cm radius. Two peaks in the intensity curve were reported, the main peak at  $\sin \theta/\lambda = 0.151$  and a weak second-

<sup>1</sup> W. H. Keesom and J. de Smedt, Proc. Amst. Akad. Sci. 25, 118 (1922).