Final state

APPLICATION OF PUNCHED CARD EQUIPMENT TO THE ANALYSIS OF COMPLEX SPECTRA

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The punched card tabulating and sorting equipment generally used in statistical and accounting work has been applied to the analysis of complex spectra into term values. The wave numbers of the lines are punched on the special cards provided for use with the machines. The method enables one either to determine wave number differences which frequently occur or to isolate those line pairs showing a given frequency difference. The advantages of the method include high speed, accuracy as high as desired without checking with an adding machine, and the fact that only one simple modification is needed of standard equipment that is available almost everywhere.

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1. Introduction.

The analysis of complex spectra into term values constitutes an important part of empirical spectroscopy. This analysis is conducted by means of various theoretical or empirical principles of which the most important is the Ritz Combination Principle: Each spectral line has a wave number which is the difference of a pair of terms taken from a sequence called a term series. The analysis of a complicated spectrum is very tedious; many trials are needed to discover the numerous terms from which the still more numberous frequencies are formed.

As a result mechanical aids to the process have been developed. Laporte introduced the method of plotting the wave numbers of the lines of the spectrum to scale on a strip of paper and using a pair of dividers to locate line pairs having a common difference. When two pairs of lines show the same difference this fact may be fortuitous or it may indicate, according to the Ritz principle, that the two pairs of lines have a pair of terms in common. When this happens we know the interrelation of four term values.

The interval sorter described by G. R. Harrison[3] is based on an elabora-

[3] G. R. Harrison, Rev. Sci. Ins. 3, 753 (1932); 4, 581 (1933).

tion of the Laporte method. The wave numbers of the lines are punched to scale on a paper strip. This strip is doubled back on itself, the length of the loop being determined by the wave number difference for which one is searching. The fact that two lines show a certain difference is recorded photographically when the punchings on the two ends of the loop coincide, allowing a light beam to pass.

The method about to be described is numerical rather than graphical in

character. It depends upon the use of the rather elaborate punched card equipment of the International Business Machines Corporation[4]. To adapt

[4]It may be that the punched card equipment of other manufacturers could be used in the same way.

this equipment to the present problem we have had to make some alterations in the method of using the machines and to add one simple piece of auxiliary apparatus. It should perhaps be emphasized that no changes in the standard machines themselves are necessary.

2. Punched Card Equipment.

Numerical data are punched on cards (Fig. 1) and the present design allows eighty digits to be carried by a single card. In actual use the card is divided into fields each with as many digits as are necessary to carry the numerical information. In the machines we have used the tabulators will accept only numbers up to eight digits but we are informed that the newer tabulators will accept numbers up to fifty digits. The numbers are punched on the cards by either hand punches or by electric punches. The electric punches are self fed and possess means for copying any portion of a given card on another card.

The principal machines are a sorter and a tabulator. When the sorter is set to sort on any column it divides the cards according to the numbers punched in that column. This machine is used to arrange the cards in numerical order in any field.

In the tabulator the cards pass two sets of brushes, the upper and the lower. Each set has eighty brushes, one for each column on the cards. The brushes make contact thru the holes which are punched in the cards, the phase

of the electrical impulse produced in any brush being governed by the position of the number punched in the corresponding column of the card. Thus the impulse for a nine comes earliest in the cycle while that for a zero comes last. The upper set of brushes is used largely for controlling the processes carried out by the machine in a way that will be touched on later. The lower brushes may be connected to counting banks of dials called counters by flexible leads equipped with jack connections. When this is done the contents of the cards add into the counters to which the corresponding brushes are wired. By the use of certain "controls" the machine can be made to stop, print the total from the counters, clear itself, and resume operation. Instead of printing the totals they may be punched on a new set of cards by a "summary punch" electrically connected with the tabulator. Some tabulators in use are designed to allow the direct subtraction of the value of any card desired. The installations which we have used do not possess this feature and we have always accomplished subtraction by adding the complement, a method of procedure which is perfectly satisfactory for the present purpose.

5. Application to Analysis of Spectra.

As has been pointed out by Harrison[5] there are two rather distinct functions which mechanical aids may perform in the analysis of spectra. First there is the problem of finding the wave number differences which frequently occur between lines of the spectrum; the other function is to discover as many as possible of the line pairs which show a given difference. To obtain differences which frequently occur in the spectrum an ordered, selected, and not too long list of wave numbers is made and a code identification

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[5] G. R. Harrison, Rev. Sci. Ins. 4, 584 (1933).

number attached to each. These wave numbers as well as their identifications are punched on cards. If now a duplicate set were made up and interleaved with the original and if the "controls" were properly arranged to add one card into the counting bank, subtract the next and summary punch the difference we would have difference cards showing the difference in the wave numbers of the two original cards. To get all of the differences we would have to shift the relation between the two sets of cards one place at a time. If the differences were all obtained in this way we could arrange them in order ~~to~~ of magnitude with the sorter and then all equal differences would fall together. The cards could then be listed by the tabulator and frequently occurring differences would be very evident. These ideas represent our first thoughts on the subject but they are given here because they furnish a basis for explanation of the modifications necessary to make the method practical.

To avoid the need of subtraction we may punch complements on the second set of cards. For brevity we shall often refer to the two sets of cards as the A cards and the B cards. To avoid mixing the code identification numbers which serve to indicate the lines from which the given difference arises the code punching may be shifted on the B cards so that the code number on any B card will enter the counter to one side of that from the corresponding A card. These numbers will both be summary punched and will appear side by side on the difference cards clearly indicating the origin of the given difference.

The standard controlling device on the machines employs two sets of brushes, the upper and the lower. When the punching on the card at a selected group of upper brushes is the same as that at the corresponding group

of lower brushes the machine "passes control" and does not stop. However if the cards differ the machine will "control", stop, summary punch or print the total, clear the counters and resume operation. The machine may be made to pass one A and one B card and then stop by the following device. A one digit control is used, which means that one digit in the card at the upper brushes and at the lower brushes must agree to have the machines pass control. The A cards are punched 1, 1 in two blank columns, say in columns 37 and 38. The B cards are punched blank, 1 in the same two columns. (See Fig. I). The wires from the controlling device go to upper brush 38 and lower brush 37. The A cards are presented first and arrive at the lower brushes just as a B card arrives at the upper brushes. A little reflection will make it clear that the machine will pass control in this case but control and stop the machines when a B card is at the lower brushes and an A card is at the upper brushes.

In order to use the capacity of the machines to the best advantage and to make the work as rapid as possible it is desirable to work in several fields at once. The machines which we have used have had five counters each with nine counting wheels one of which is used for a carry over, thus giving a capacity of eight digits. The code numbers for identification require space in the counters but one code number for a card will suffice, the position of the difference in the list or on the summary card being sufficient to decide its origin. So one counter is sufficient for identification and we may work differences in the other four counters. It seems best in the present problem to punch the first four wave numbers on the first card, the next four on the next card, etc. An A card so punched is illustrated in Fig.

1, which shows the identification and control punchings. The B card has been modified in a way next to be described.

The greatest difficulty yet remaining with the basic scheme is the need of shifting the A and B cards relative to each other in order to obtain all differences. The failure of several attempts to do this conveniently resulted in the following modification of the method which removes the necessity of shifting the cards. The B cards are left blank in the fields in which wave numbers are punched on A cards. They contain the control punching which has been described, a diagonal punching in some field not otherwise used say 0 in column 70, 1 in 71, etc. up to 9 in 79 and an X punching in column 80 (Fig. 1). When card A passes the lower brushes it adds the contents of its various fields into the counters being used. Card B is however blank in the fields which are punched in the A card and which are wired to the counters. The brushes covering the diagonal punching, 70 to 79 if we use the B punching illustrated in Fig. 1, are wired to the one piece of auxiliary apparatus. This piece of apparatus is shown schematically in Fig. 2.

As will be seen by referring to this drawing the numerical impulse from the diagonal punching is led into a set of horizontal bars which form a "set up board". Just above this set up board is a multiple contact relay. Numerical impulses for any number desired can be selected by clipping flexible leads on the bars and this number is distributed into wires leading to the counters by the relay. The relay is needed to prevent mixing of the original A impulses which are also connected to the same counters. The same number, which in the present application is the complement of a frequency number is added

into all counters simultaneously but of course the A cards add different numbers into the various counters. It happens that the tabulator possesses a class selector circuit that may be used to control the relay. The X punched in column 80 of the B cards sets up the circuit as this card passes the upper brushes. The code indication for the number set up on the board can be supplied by a card on the copy rack of the summary punch or it can be more conveniently supplied by wires clipped to the set up board. This auxiliary apparatus is conveniently mounted in a box and may be connected to the tabulator by inserting about fifty jacks, the exact number depending on the number of places to which one is working. The complete set up (Fig. 3) ready to analyse spectra can be made in about fifteen minutes.

The complement of a frequency number is placed on the set up board, and the cards are passed thru the machine, thus giving the differences of the given frequency number with all the rest. By repeating, all differences are obtained. Meanwhile the summary punch has copied all differences and the composite code showing the numbers from which they arose on a new set of cards. These cards are then sorted and listed as above described. It will be necessary to sort and list on each difference field separately but the listing may be so carried out that equal differences come near each other in the list. Each list will of course include the code.

The method described above is slightly altered when applied to the problem of finding line pairs showing a given difference. Now the ordered wave number list is much larger, perhaps including all known lines. The order of punching the wave numbers on the cards may advantageously be different; for instance, if there were four hundred lines the first card would contain the

1st, the 101st, the 201st and the 301st lines. The given difference is placed on the set up board and is added to each wave number. No summary punch is used but the sums are listed directly. Comparison of the resulting list with the original wave number list indicates by an agreement a pair of lines showing the given difference.

4. Experimental Application.

At the suggestion of Dr. W. F. Meggers we have used the spectrum of Fe I to develop the method. No completely systematic analysis of this spectrum was attempted but numerous machine runs were made leading to the selection of the procedure which has been described. Some idea will now be given of the speed and results of the method.

A skilled operator will punch three hundred A cards an hour each carrying four wave numbers. An equal length of time will be needed for verifying the punching on the cards. The B cards are all identical and may be punched very quickly by using the copying feature of the electric punch. When summary cards are being punched for use in finding frequently occurring differences, about fifteen difference cards are produced per minute. The time required for subsequent sorting and listing is about two hours per thousand differences cards (four thousand differences). All equal differences fall together or nearly so in four ordered printed columns and are easily marked allowing any tolerance desired. The code numbers indicating the lines from which any differences arise are carried in parallel columns. In such an actual list comprising the results of 1800 difference cards which were however selected so that the differences would fall in the range between 6900 cm^{-1} and 8300 cm^{-1} the differences of several frequently recurring differences in

iron were clearly indicated.

In the determination of line pairs which show a given difference the speed of the method is of course much greater. The cards punched for this purpose are placed in the tabulator which is set to print from the counters upon control. The given difference is placed on the set up board and the tabulator started. Thirty pairs of cards pass thru the tabulator in one minute which means that the machine is doing two sums every second. No attention on the part of the operator is necessary except to refill the card hopper if the run is a long one. While the machine is making one list one may check a previously obtained list for lines showing the given difference. In the experimental application of the method, known wave number differences were used and the line pairs showing the given difference were very quickly and easily found. After a little practice the machine made lists may be checked with the original wave number list at a rate of at least three thousand entries (in each list) per hour.

The method here described has exhibited the following characteristics:

1. Only the one simple device needs to be added to standard equipment which is of very general availability. This equipment is not altered in any way.
2. The accuracy is high. In the machines we have used one may work to eight significant figures which is of course sufficiently accurate for most spectroscopic work. The new machines will allow this accuracy to be extended as much as desired. Since this method gives direct numerical results no adding machine is needed to check the results obtained.

3. The method is rapid. The speed is not as great as that reported by Harrison for his interval sorter. However it seems likely that if the two method were compared in application to the more complex spectra and working at the accuracy necessary to resolve these spectra the present method would compare favorably with the use of the interval sorter.
4. The method will give trouble free operation over long periods of time. The reputation of the punched card equipment is well known and the additional relay used has given no trouble at all.
5. All of the operations described can be delegated to the ordinary clerical help accustomed to the use of the machines.

The authors wish to acknowledge the kind assistance of the Tabulating Division of the International Business Machines Corporation in providing machines and apparatus.

The British Tabulating Machine Company of London has developed a "rolling total" machine which will make it unnecessary to use any auxiliary apparatus, and entirely eliminates the use of B cards. Either of the problems of spectrum analysis discussed above may be handled on this foreign equipment.