A New Method of Analysis of the Structure of H_α and D_α

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(Received December 28, 1936)

The interferometer pattern due to a group of spectral lines can be expressed as a Fourier series, and the coefficients of this series can be regarded as the quantities to be measured. These coefficients can also be computed in terms of the positions, intensities, and the parameters describing the shapes of the lines. Although the equations cannot be explicitly solved for the latter quantities in terms of the Fourier coefficients, numerical means can be used to find the parameters which best reproduce the observed values. This method has been applied to two plates of H_α and D_α. The results indicate that to fit the observations with the four strongest lines given by the theory it is necessary to make the separations of the two most intense components some 2 percent less than the theoretical value.

ONE of the principal difficulties in the analysis of fine structure patterns, especially in the light elements, lies in the fact that the widths of the component lines are of the same order of magnitude as their separations. This makes the object under consideration really a continuous spectrum whose intensity distribution must be analyzed, rather than a spectrum of discrete lines. Such a spectrum requires a quite different method of description and must be characterized by a different set of numbers than a true line spectrum. When an interferometer is used to study the spectrum the periodicity of the pattern suggests the use of a Fourier series for describing it, and the method of analysis to be described is one in which the coefficients of this Fourier series are regarded as the characteristics of the spectrum. To compare the observations with spectroscopic theory, however, these characteristic coefficients must be interpreted in terms of intensities and positions of elementary component lines.

Method of Analysis

Consider first the Fabry-Perot interferometer pattern to be expected from a single elementary line. After it has been expressed in terms of intensity as a function of the distance from the center of the pattern, the scale can be made linear by squaring the abscissae. The intensity will then be a periodic function whose period can be determined with considerable accuracy. The range of wave-length represented by the separation of successive orders is called the spectral range and may be designated by s. This quantity is strictly a function of the order of interference, but it varies so slowly that over the three or four orders in which one is usually interested it may be treated as constant. Then let $\theta=2\pi\lambda/s$ be the variable in terms of which the pattern is to be described. θ may be called the angular order of interference.

If the line under consideration were strictly monochromatic, and if the resolving power of the interferometer were infinitely high, the intensity of the pattern would be zero except for a series of points separated by the distance 2π. However, neither of these conditions is satisfied and one needs to consider three principal causes of line breadth.

(*a*) The natural width, due to the finite lifetimes of the states involved, or classically due to the damping of the oscillations, gives a line whose shape is

$$I_n(\theta-\theta_0)=\beta/\{(\theta-\theta_0)^2+\beta\}^2. \tag{1}$$

θ_0 is the position of the maximum, and β is a constant which depends upon the lifetimes of the initial and final states. The broadening due to collisions gives a line of the same shape so that these two effects can be treated together by giving to β a suitable value.

(*b*) In hydrogen the most important source of broadening is the Doppler effect caused by the motion of the emitting atoms. This gives a line whose form is

$$I_D(\theta-\theta_0)=e^{-\alpha(\theta-\theta_0)} . \tag{2}$$

The quantity α depends upon the mass of the emitting molecule and the temperature. $\alpha = Ms^2\nu^2/8\pi RT$, where M is the molecular weight, ν is the frequency of the center of the line, R is the gas constant and T is the absolute temperature.

(c) The third source of broadening is the finite resolving power of the interferometer. This causes an apparent line form given by

$$I_i(\theta-\theta_0) = 1 + 2\sum_{n=1}^{\infty} r^n \cos n(\theta-\theta_0), \quad (3)$$

where r is the reflecting power of the interferometer plates.

These three functions can be combined to give the resultant form of the interference fringes due to a single line.

$$J(\theta, \theta_0) = \int_{-\infty}^{\infty} d\theta_2 \int_{-\infty}^{\infty} d\theta_1 I_i(\theta-\theta_2) I_D(\theta_2-\theta_1) \times I_n(\theta_1-\theta_0) \quad (4)$$

$$= B_0' + \sum_{n=1}^{\infty} (B_n' \cos n\theta + A_n' \sin n\theta),$$

where $B_0' = \pi^{\frac{1}{2}}$, $B_n' = 2\pi^{\frac{1}{2}} r^n e^{-n^2/4\alpha - n\beta} \cos n\theta_0$,

$$A_n' = 2\pi^{\frac{1}{2}} r^n e^{-n^2/4\alpha - n\beta} \sin n\theta_0.$$

These expressions for the coefficients assume a line of unit intensity, and they are of course all proportional to the intensity.

If the pattern is due to a superposition of different elementary lines, the coefficients of the Fourier series (4) are superpositions of contributions from the different lines. Hence

$$B_0 = \pi^{\frac{1}{2}} \sum_{j=1}^{N} I_j,$$

$$B_n = 2\pi^{\frac{1}{2}} r^n e^{-n^2/4\alpha} \sum_{j=1}^{N} e^{-\beta_j n} I_j \cos n\theta_j, \quad (5)$$

$$A_n = 2\pi^{\frac{1}{2}} r^n e^{-n^2/4\alpha} \sum_{j=1}^{N} e^{-\beta_j n} I_j \sin n\theta_j.$$

In these expressions the subscript j denotes a quantity belonging to the jth elementary line. The quantities I_j are the various intensities.

Eq. (5) is the desired connection between the quantities predicted by the usual spectroscopic theory, and the Fourier coefficients characteristic of the pattern. If all of the theoretical quantities were known it would only be necessary to calculate the Fourier coefficients and compare them with the observed ones. However, the theoretical quantities are not always satisfactorily known. The temperature in a discharge tube is only roughly known; the relative intensities of the lines in a pattern are often dependent upon the conditions of excitation; and the width parameter β is not usually known with any accuracy. Furthermore, although relative positions are usually given by the theory, the origin of θ is not easily determined experimentally. The practical problem is thus to invert the equations (5) and to determine from the observed Fourier coefficients the parameters of the component lines. Of course, this cannot be uniquely done since there is an infinity of coefficients from which to determine a finite number of parameters, and due to experimental errors the coefficients will not be strictly consistent. It is thus necessary to adopt a criterion for what constitutes the best set of parameters and then to find them, essentially by trial.

Let $J(\theta)$ be the interferometer pattern which would be obtained from the assumed parameters, and let $K(\theta)$ be the observed pattern. Let the patterns be expressed as Fourier series in which the coefficients of the observed pattern are designated by asterisks. Then the quantity

$$\Delta = \frac{1}{\pi} \int_0^{2\pi} \{J(\theta) - K(\theta)\}^2 d\theta \quad (6)$$

may be taken as a measure of the difference between the two curves. By this criterion all parts of the curve of equal extent in θ are given equal weights. The quantity Δ can then be expressed in terms of the Fourier coefficients.

$$\Delta = 2(B_0 - B_0^*)^2 + \sum_{n=1}^{\infty} \{(B_n - B_n^*)^2 + (A_n - A_n^*)^2\}. \quad (7)$$

The derivative of Δ with respect to any parameter can be determined from this equation, so that after a set of parameters has been tried they can be changed in the proper direction to produce a reduction in Δ. When the derivatives

TABLE I.

PLATE	86				78			
	H_α		D_α		H_α		D_α	
LINE	OBS.	CALC.	OBS.	CALC.	OBS.	CALC.	OBS.	CALC.
B_0	93.28		75.12		103.76		70.10	
B_1	6.07	5.95	1.47	1.28	1.78	2.12	2.28	2.87
B_2	42.81	43.54	56.55	55.42	42.05	41.65	41.04	41.43
B_3	4.86	3.48	7.12	6.47	2.33	1.63	4.55	3.37
B_4	1.49	2.03	6.38	8.77	0.63	1.85	5.00	4.82
B_5	0.14	0.06	−0.08	0.45	−0.65	−0.01	−0.09	0.32
B_6	0.16	0.02	0.77	0.73	−0.30	0.02	−1.12	0.27
A_1	0.63	0.78	1.08	0.57	4.63	4.39	1.84	2.40
A_2	3.19	4.10	2.08	1.53	−0.70	−1.16	4.76	4.91
A_3	−2.24	−3.12	−8.73	−7.15	−1.87	−1.51	1.40	−0.59
A_4	1.22	1.11	4.89	4.28	−0.64	0.52	3.27	2.72
A_5	−0.42	−0.14	0.66	−1.74	−0.18	−0.06	0.67	−0.42
A_6	−0.55	0.01	−0.15	0.43	0.44	0.00	0.13	0.30
Δ	4.78		17.26		4.72		11.38	
r	0.82		0.84		0.70		0.71	
α	1.20		2.30		1.25		2.50	
I_1	100		100		100		100	
I_2	89		96		98		91	
I_3	21		22		21		19	
I_4	12		10		13		11	
θ_1	2°		1°		2°		6°	
θ_2	191°		190°		184.7°		189°	
θ_3	120°		121°		120°		135°	
θ_4	340°		335°		335°		340°	
d	.817872 cm		.817872		.801310		.801310	
$\Delta\nu_0$	.61117 cm^{-1}		.61117		.62380		.62380	
$\Delta\nu_{12}$	.320 cm^{-1}		.320		.317		.317	
$\Delta\nu_{23}$	.120 cm^{-1}		.117		.112		.094	
$\Delta\nu_{14}$	.037 cm^{-1}		.044		.047		.045	
Δp	6.7804				6.6366			
$\Delta\nu$	4.1440 cm^{-1}				4.1399			
e/m	1.7592×10^7				1.7610×10^7			

with respect to all of the parameters are small and change sign with a small change in the parameters, the set of parameters is called the best.

APPLICATION TO H_α AND D_α.

Table I shows the results of the application of this method of analysis to two plates of H_α and D_α. These plates were taken with a grating spectrograph of two meters focal length equipped with a grating of 48,000 lines per inch. This provided enough dispersion to separate the two lines. Intensity marks were photographed on each plate. A microphotometer curve was made of each pattern and this was transformed into a curve of intensity as a function of the distance from the center of the pattern. The abscissae were then squared and two or three orders were averaged together to give the pattern to be analyzed. To permit this averaging it was necessary to apply a correction which took account of the lack of uniformity of illumination of the slit. This correction was determined from the relative intensities of the maxima and minima in successive orders.

To determine the Fourier coefficients, ordinates were taken from the curves at intervals corresponding to 3°. These were multiplied by the corresponding values of the trigonometric functions and the products added. Since the analysis is based on the true Fourier coefficients, and not on a set which will give an exact fit for a certain finite number of ordinates, it is necessary to determine them by a process of integration such as this, rather than by fitting the curve at some selected points. It was concluded from the behavior of the coefficients, that the functions of 6θ could be used, but for higher multiples of θ the coefficients were deemed not to have much significance because of experimental uncertainties.

After the Fourier coefficients had been measured a set of trial parameters was selected. These represented estimates of the breadth parameters and of the positions and intensities of four component lines. The possible fifth line was neglected because of its low intensity. Since the coefficient B_0 is the sum of the intensities, it was used to eliminate the intensity of the first component. From the assumed parameters the corresponding Fourier coefficients were computed, and then either by inspection of the result, or by working out the derivatives of Δ with respect to the various parameters, changes were made and the calculation repeated. By continuing this process the parameters listed in the table were obtained. These are not necessarily the final results which would be obtained if the process were carried out indefinitely, but they make the value of Δ relatively small, and the derivatives of Δ also small. Their accuracy is probably about all that is justified by the accuracy of the photometry.

In this analysis the parameter β was neglected. The natural width of most of the component lines is dominated by the width of the $2p$ level. This is such as to give to β a value of 0.1. However, if all of the component lines have the same value of β the effect on the Fourier coefficients can be produced by a reduction in the reflection coefficient r. Portions of the components designated as 2 and 3 are due, however, to transitions to the $2s$ level. If this level were isolated it would be metastable and very narrow. Since it coincides with the $2p_{\frac{1}{2}}$ level it is subject to a good deal of perturbation, and hence is probably much broadened. For this reason, as well as to avoid the introduction of more parameters than would be justified by the number of usable Fourier coefficients, all of the lines were treated as having the same natural breadth, and this was included in the parameter r.

In the table are listed the observed and computed values of the Fourier coefficients, and the values of the parameters which were used in the computations. For ease in comparison I_1 was set at 100 in each case. d is the separation of the interferometer plates in cm, $\Delta\nu_0$ is the wave number difference corresponding to unit difference in order of interference. This has been corrected for the index of refraction of air. The succeeding $\Delta\nu$'s represent the wave number differences between the components designated by the subscripts. Δp is the difference in order of interference between the two strong components of H_α and D_α and $\Delta\nu$ is the corresponding wave number difference.

The two plates analyzed were taken under slightly different conditions. The interferometer separations were different as indicated. For plate 86 the current density was about 25 ma per sq. cm while for plate 78 it was about 45 ma per sq. cm. The pressure of helium in both cases was about 0.5 mm. The hydrogen pressure was small but unknown since it was due to the dissociation of the water frozen to the walls of the discharge tube. The effect of the difference in current shows up in the different values of r. This indicates a rather considerable broadening due to the increase in current. The values of α correspond to temperatures in the neighborhood of 100°K. The values of $\Delta\nu_{12}$ differ by about 1 percent between the two plates although they are both definitely less than the value 0.328 cm^{-1} given by the theory. To make sure of this difference an attempt was made to use parameters corresponding to this separation in the analysis of D_α on plate 86. The minimum value of Δ which could be obtained in this way was nearly twice the value given in the table.

One might suspect that the difference between the two plates indicates a trend toward the theoretical value as the current is decreased. A study of several more plates will be necessary to establish the presence or absence of such a trend, but the fact that for plate 86 the value of r is as high as can be expected after allowing for the 0.1 taken off by the natural width suggests that in this case the external disturbances have been reduced to a very small value, but that the assumed four-line structure is inadequate to explain the observations if the theoretical separations are to be used. This is in agreement with the previous conclusions of Dr. Hsieh and myself,[1] and of Gibbs and Williams,[2] although Shane and Spedding[3] concluded that they had no evidence of deviations from the theory.

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[1] Houston and Hsieh, Phys. Rev. **45**, 263 (1934).
[2] Williams and Gibbs, Phys. Rev. **49**, 416 (1936).
[3] Shane and Spedding, Phys. Rev. **47**, 33 (1935).