Errors in retrieving the parameters of spectral lines from the absorption spectra. Part 2. The effects of the background and neighboring spectral lines

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The effects of the background component and a wing of a neighboring spectral line on the accuracy of the absorption line parameters retrieval in the presence of random noise have been investigated numerically. The computations have been performed for an absorption spectrum and its frequency derivative. It has been analyzed how the frequency dependence and the parameters of the background affect the error of retrieval of the line position, half-width, and intensity. It was found that adding linear background to the model reduces the errors due to the presence of a neighboring spectral line in determination of the line parameters.

The retrieval of spectral line parameters from an absorption spectrum recorded is a key problem of many applications in spectroscopy and atmospheric optics and is being developed for a long time.[1–6] Nevertheless, the most papers devoted to the determination of line parameters, though describe the methods applied to processing experimental data, pay almost no attention to the methodical issues, such as the effect of neighboring lines[1,2] or the background component.[1,3–5] However, in retrieving the position, half-width, and intensity of a line from an experimentally recorded fragment of a spectrum (or its derivative), the accuracy of determination of line parameters depends on the value of measurement noise, the presence and the nature of the frequency dependence of the background component, the separation from neighboring lines and their intensity, and other features characteristic of the experimental data. Therefore, the results obtained by applying one or another processing technique significantly depend on the features of the spectral fragment processed (number of lines in the spectrum, their possible overlapping, the presence of background, etc.).

In the first part of this paper,[7] the computer experiment was used for analysis of variations in errors of determination of spectral line parameters as functions of measurement noise in the presence of linear or squared background in the spectrum. The aim of this work was to estimate the effect of the background component on the error of determination of the line parameters sought in the presence of random noise. The background component in the simulation of a spectral fragment was described by a linear function of frequency in the form $b(x) = a_0 + a_1x$ or was caused by the presence of a neighboring line with the center lying beyond the spectral fragment processed. The dependence has been investigated of the error of determination of absorption line parameters on the parameters of linear background, intensity, and the distance to the neighboring line (line half-widths were assumed equal).

1. Construction of the model spectral fragment

The calculations were performed for the Voigt profile of a line with the intensity $S = 1$ and the Doppler half-width $\gamma_D = 0.022$ cm^{-1}. The Lorentz half-width γ_L amounted to 0.001 cm^{-1} (Doppler profile) and 0.1 cm^{-1} (Lorentz profile). The central frequency of the line was taken to be 3 conventional units. The frequency scale used was in wave numbers. The width of the model spectral fragment was 0.5 cm^{-1} for the Doppler profile and 4 cm^{-1} for the Lorentz one. The frequency step was, respectively, 0.001 and 0.008 cm^{-1}. The fragment obtained was supplemented with the linear background component or with the wing of the neighboring line and the random noise of 2 or 5% of the absorption coefficient at the center of the studied line k_{max}.

Examples of the model fragments of the spectrum and its frequency derivative for 5% noise are shown in Fig. 1 by the solid line. The dashed lines illustrate the distortions of the model spectral fragment due to the linear background component with the limiting values of the parameters used in the calculations (for illustration, in calculating the model fragment shown in Fig. 1, the Lorentz profile and its derivative were normalized and the random noise was omitted in the dashed curves, although, actually, noise was always present in calculations and the normalization was not carried out).

For the Lorentz line, the model profile was not supplemented with the linear background component,

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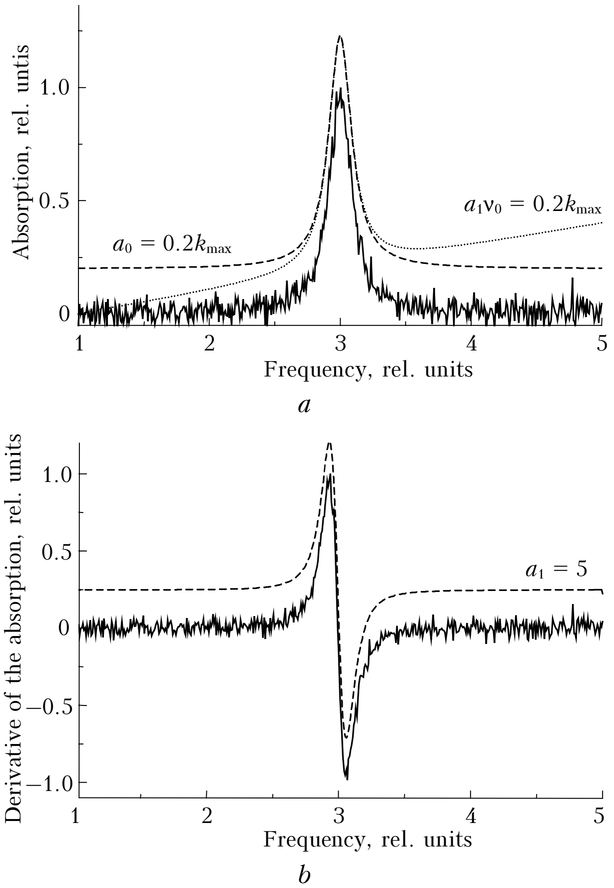


Fig. 1. Example of the model spectrum (*a*) and the spectrum derivative (*b*) with 5% random noise and linear background.

but with the wing of the neighboring line, which was also calculated using Voigt profile with the same values of the half-widths. The intensity of the neighboring line varied from 0.1 to 3 (that is, amounted to from 10 to 300% of the intensity of the line under study), the separation between the line centers was from 2 to 14 half-widths. The boundary of the spectral fragment, included in the processing, from the side of the neighboring line corresponded to the minimum between the studied and neighboring lines, while another boundary remained unchanged, that is, the spectral fragment was asymmetric and included a variable number of points depending on the separation between the lines. As lines approach each other, the minimum between lines disappears, and their profiles merge into a common profile. In this case, the parameters of both lines should be determined simultaneously, and therefore the case that the separation between the lines is shorter than two half-widths was not considered.

2. Results and discussion

When determining the line parameters from the obtained spectral fragment, the nature of the frequency dependence of the background component was assumed unknown, and the calculations were carried out in four ways: 1) by fitting the Voigt profile neglecting the background; 2) with prior removal of the linear background component; 3) with prior removal of the squared background component; 4) with determination of the background parameters from fitting simultaneously with the parameters of the line under study. The prior determination of the parameters of linear background was performed by averaging over several points (about 5% of the total number) in the beginning and in the end of the fragment, while all points of the fragment were used for the prior determination of the parameters of squared background.

The relative errors of retrieval of the line half-width and intensity are measured in percent, while the relative error of the central frequency is measured in percent of the line halfwidth (γ_L for the Lorentz profile and γ_D for the Doppler profile).

2.1. Influence of the parameters of a linear background

In the simulation of the spectral fragment, the parameters of the background component varied in the following ranges: $a_0 = 0–0.2k_{max}$, $a_1\nu_0 = 0–0.2k_{max}$, and only one of the coefficients was varied, while the other one was equal to zero. In the simulation of the derivative of the spectrum, the maximum value of the coefficient a_1 was 20% of the maximum value of the derivative. The relative errors of determination of the central frequency, half-width, and intensity for the Doppler and Lorentz profiles from the spectral fragments with the 5% noise level are shown in Figs. 2 and 3 as functions of the parameters of the background component a_0 and a_1.

The curve numbers correspond to the methods of determination described above. For a comparison, Fig. 3 shows also the line parameters (as functions of the background slope a_1) determined from the fragment of a spectrum of the Lorentz profile with 2% noise. It is seen from Fig. 3 that the noise level most significantly affects the error of retrieval of the central frequency at the slight slope of the background component, while the error of determination of the half-width and intensity is mostly caused by the method chosen for processing.

It can be seen from Figs. 2 and 3 that the maximum errors of determination of the half-width and intensity, naturally, correspond to the fitting with neglected background (curves *1*). The prior removal of the background component decreases the error 1.5 to 3 times, and the use of a linear model of the background (*2*) usually gives better results than the use of squared background (*3*). However, the best results are obtained in the case of fitting the constant and the slope of a linear background simultaneously with the parameters of the line studied (*4*). For the frequency-independent constant of the background, the "Voigt profile + constant" model used in the fitting (that is, $a_1 = 0$, unlike the method *4*) also gives good results (omitted in Figs. 2 and 3), but at $a_1 \neq 0$ the results are much worse.

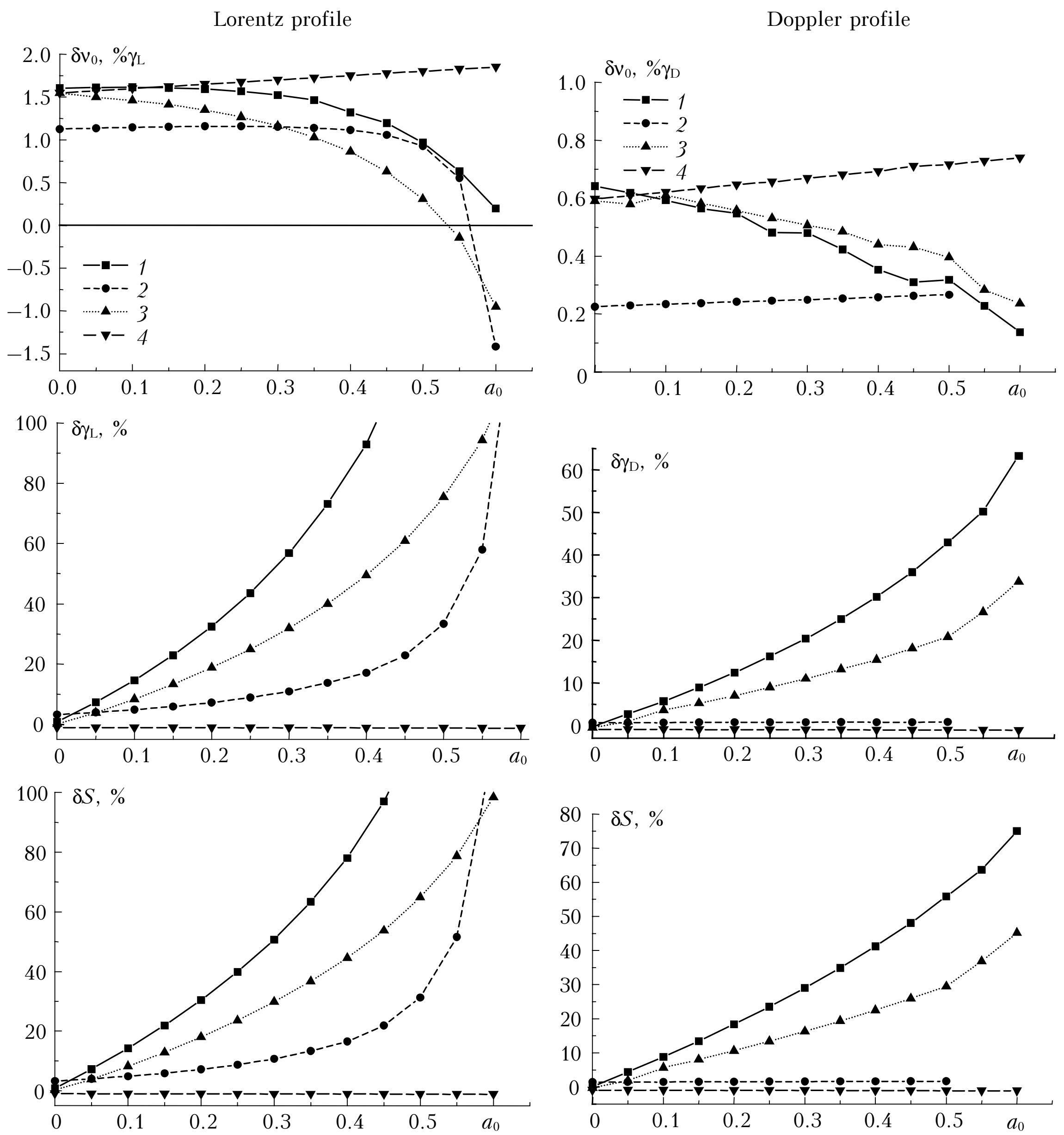


Fig. 2. Relative errors of line parameters retrieved from the spectral fragment vs. the background constant a_0.

The error of determination of the central frequency for the chosen variability range of the parameters of the background component appeared to be the smallest with the prior removal of the linear background and amounted to ≈1.2% γ_L (0.001 cm^{-1}) for the Lorentz profile and smaller than 0.0001 cm^{-1} for the Doppler one with the contribution of the background component within 15% k_{max} and the 5% noise level. The relative errors of determination of the half-width and intensity from the Lorentz spectral fragment by methods *1–3* appeared to be somewhat higher than those for the Doppler profile and close for both types of the profiles with the simultaneous fitting of line parameters and the background (method *4*).

The relative errors of determination of line parameters from the fragment of the frequency derivative of the spectrum with the 5% noise level were determined only as functions of the slope angle of the spectral background (Fig. 4), since the contribution of the constant disappears upon differentiation.

The errors of retrieval of the half-width and intensity from the fragment of the derivative turned out to be within 2% for any method of determination of line parameters and weakly dependent on a_1 (in the case of retrieval of the parameters from the spectrum close values of the errors, weakly dependent of the background parameters were obtained only with the line and background parameters fitted simultaneously, whereas for other methods the errors strongly depended on the background).

However, the error of retrieval of the central frequency from the derivative proved to be higher than in the case of the spectrum itself for all the methods.

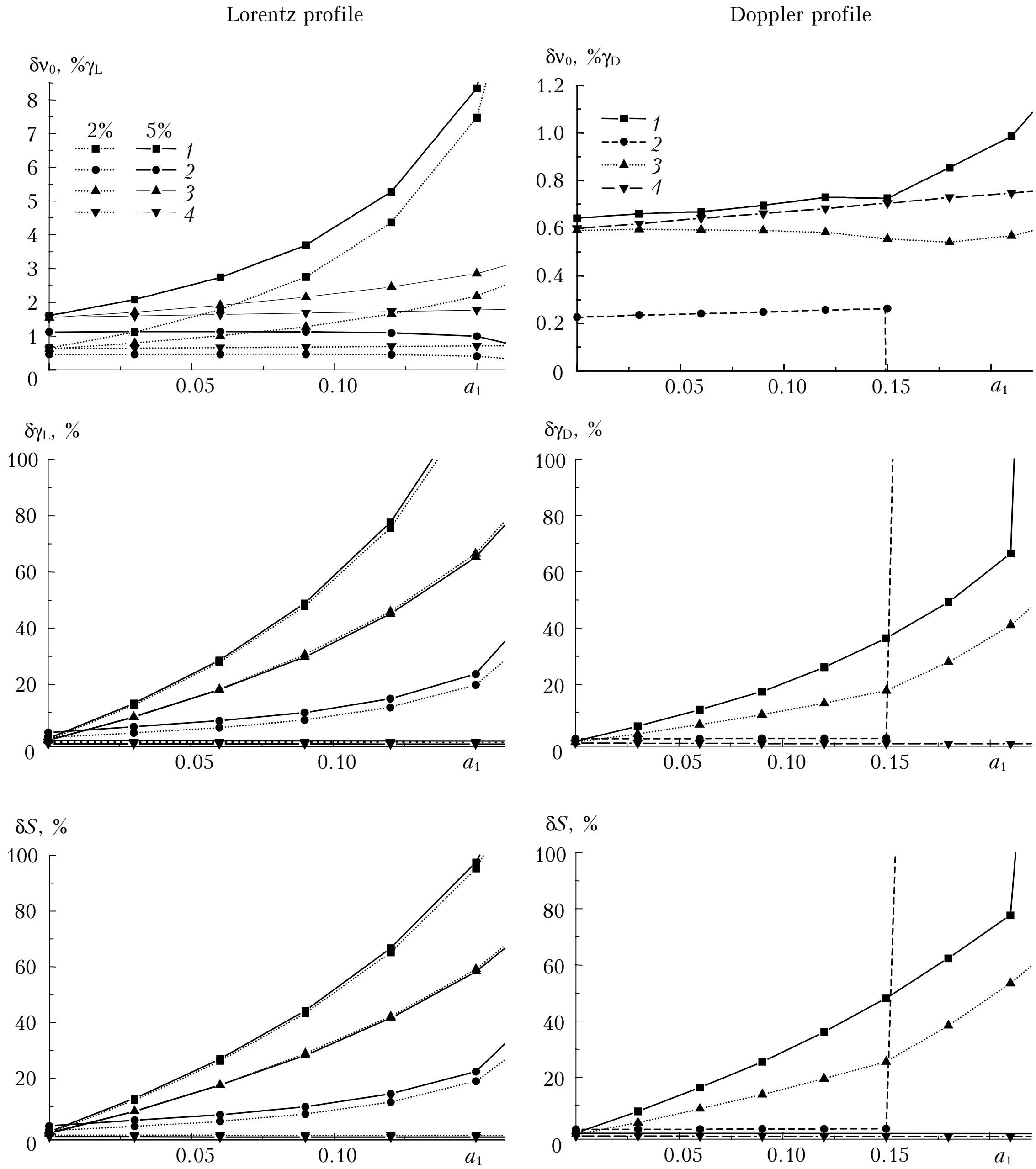


Fig. 3. Relative errors of line parameters retrieved from the spectral fragment vs. the background slope a_1.

The irregular shape of the curves in Fig. 4 indicates that, when the line parameters are determined from a fragment of the derivative, random noise affects the obtained parameters more strongly than in the case of using the spectrum itself.

2.2. Influence of the width of the spectral fragment

To study the influence of the width of the spectral fragment on the errors of determination of spectral line parameters from the model fragment of the Lorentz profile with the 5% noise level without the background component, the fragments with the width of 2, 4, 6, ..., 20 half-widths, symmetric about the central frequency of the studied line, were analyzed sequentially. The relative errors in the retrieved parameters of a line studied from the spectrum and its derivative are shown in Fig. 5 as functions of the width of the spectral fragment.

The line parameters were determined without removal of the background (curves *1* in Fig. 5), with prior removal of the squared background (*2*), and with determination of the background parameters using simultaneous fitting of the line parameters (*3*). The close results obtained with the prior removal of the squared background and without the removal of background for the spectral fragment indicate that the prior removal of the background in the cases, when it is actually absent in the spectrum, has no marked

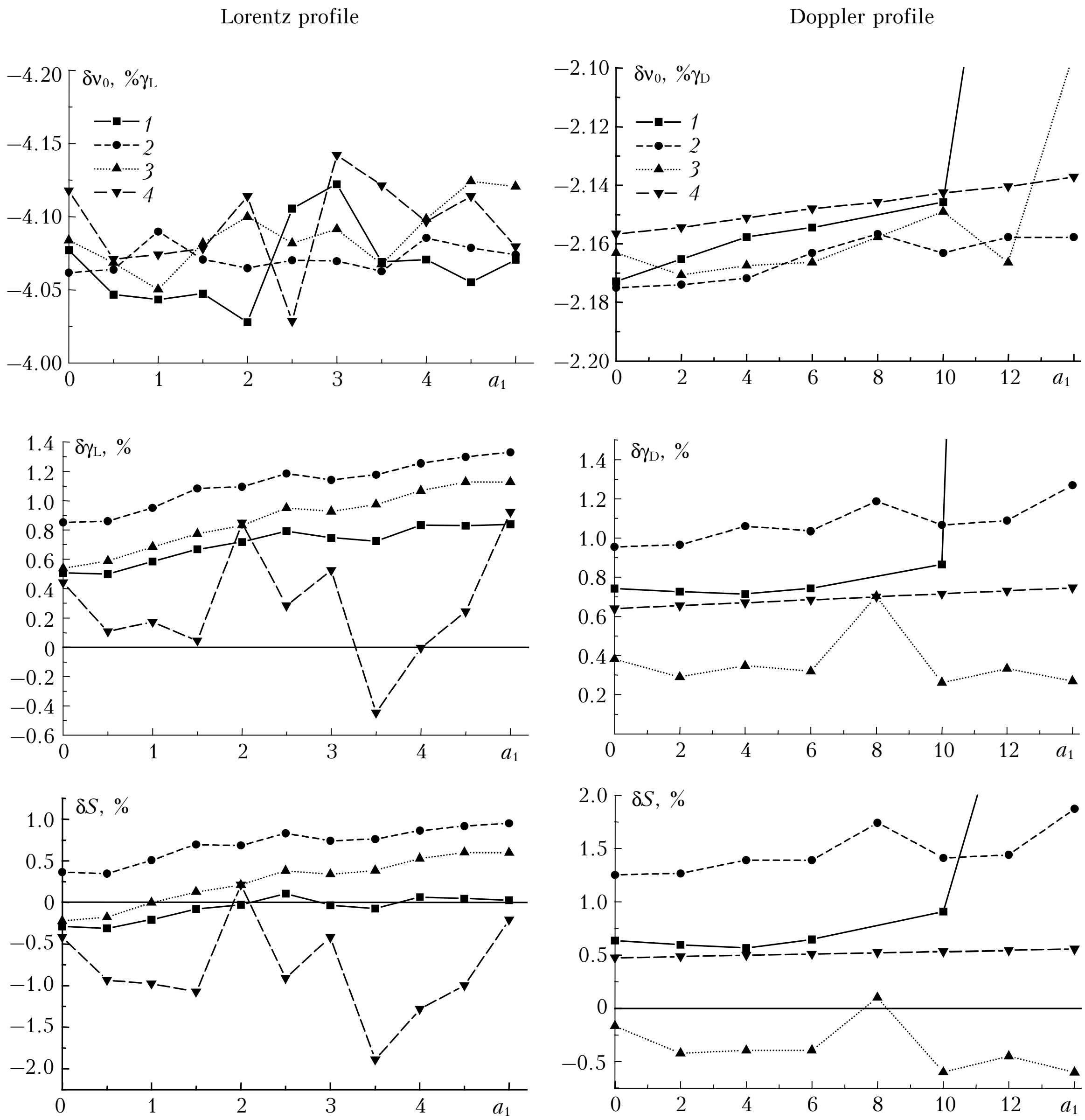


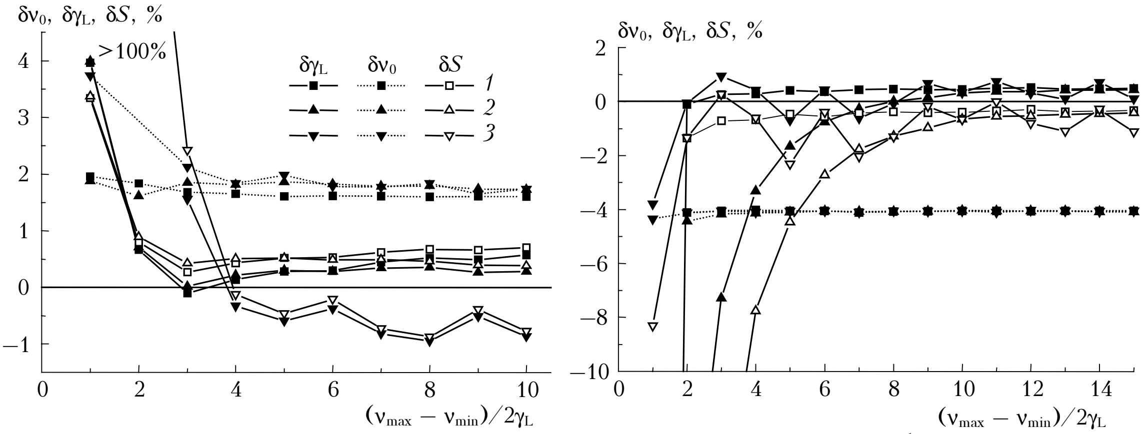
Fig. 4. Relative errors of line parameters retrieved from the fragment of the spectrum derivative vs. the background constant a_1.

influence on the errors of retrieval of the parameters, whereas determination of the background parameters from fitting in this case can lead to somewhat greater errors in determination of the line half-width and intensity for the case of a narrow fragment.

When line parameters are retrieved from the derivative of the spectrum, the prior removal of the background does not affect the error of determination of the central frequency, but can lead to large errors in retrieval of half-widths and intensities.

It can be seen from Fig. 5 that the width of the spectral fragment does not affect the errors of determination of line parameters regardless of the processing method used, if the spectral fragment has the width of no less than 8–10 line half-widths (4–5 half-widths on each side of the center). If smaller spectral fragment is used, the errors in retrieval of the half-width and intensity increase markedly. It should be noted that, in processing narrower spectral fragments, the errors of determination of the half-width and intensity from fitting simultaneously with the background parameters are larger than in the case of the prior removal of the background, whereas the prior removal of the background is least correct when processing narrower fragments of the derivative of the spectrum.

When the background parameters are determined from the fitting, the errors of retrieval of the half-width and intensity increase for spectral fragments narrower than 8 half-widths. However, if the background parameters are not fitted, the fragment narrowing to 5–6 half-widths does not lead to an increase in the error of retrieval of spectral line parameters. In the case of the derivative of the



a *b*

Fig. 5. Relative errors in parameters of the studied line retrieved from the fragment of the spectrum (*a*) and its derivative (*b*) vs. the width of the spectral fragment.

spectrum, no marked increase in the errors of retrieval of the half-width and intensity is observed even when the fragment is narrowed to four half-widths both with the neglect of the background and with fitting of its parameters, but the prior removal of the background worsens the results for the fragments narrower than 14–15 half-widths. This suggests that, in processing of a spectrum, the preferable way is to remove the background component, while for the derivative of the spectrum it is better to simultaneously fit the line and background parameters.

The errors in determination of the central frequency are much more resistant to both the width of the fragment and to the method the background is taken into account. Only the fitting of background parameters during the processing of the spectral fragment with the width smaller than 6 line half-widths causes an increase in the error as compared to the other methods.

The errors of retrieval of spectral line parameters as functions of the width of the spectral fragment calculated in such a way can be found in Ref. 8. The calculations were performed for the Lorentz spectral fragment without the background component and a 2% level of random noise. The fitting involved the "Voigt profile + constant" model with simultaneous determination of the frequency independent background and the line parameters. In this case, the width of the spectral fragment influenced the errors of retrieval of the parameters when spectral fragments narrower than 14–15 half-widths were processed (cf. ≈ 8 half-widths in this paper). The different minimum widths of the fragment, starting from which the error does not decrease with the increasing fragment width, is likely caused by the fact that in Ref. 8 the spectrum included much smaller number of points (5 points at the line halfwidths), whereas in this work we use 12 points per half-width for the Lorentz spectrum. In addition, there is a difference in the background model used: in this work, the slope of the background was a fitted parameter, along with the background constant.

2.3. Influence of neighboring line

The errors in retrieval of the parameters of the line under study (intensity S, central frequency ν_0) from the spectral fragment as functions of the intensity and the separation of the neighboring line (intensity S_n, central frequency ν_1) for the Lorentz profile with a 5% random noise without an addition of the background component are shown in Fig. 6. The parameters of the line studied were determined by all the four methods described above.

It can be seen from Fig. 6 that the errors in determination of the parameters of the line studied are proportional to the intensity of the neighboring line. The dependence of these errors on the separation between the lines is nonlinear. The effect of the neighboring line cannot be compensated for by prior removal of even the squared background, and the results obtained with and without the removal of the background are close. However, introducing additionally the linear background into the model and determining its parameters from the fitting along with the parameters of the line under study, it is possible to almost half the error in determination of the half-width and intensity as compared with that of other methods for the interline separation of 5 half-widths. However, for a denser set of lines this difference decreases. Thus, the addition of linear background during the fitting partly compensates for the effect of the neighboring line, if it is sufficiently separated from the line under study. However, as the lines approach each other, the joint fitting of the parameters of both lines is needed.

The presence of the neighboring line with the half intensity at the separation about four half-widths introduces the error up to 5% of the half-width in the determination of the central frequency and about 7–10% in the determination of the intensity and half-width.

Analogous calculations were also performed for the fragment of the derivative of the spectrum, and their results are shown in Fig. 7. It can be seen from Figs. 6 and 7 that, with the use of the derivative, the absolute values of the errors in parameters are smaller than in the case of the spectrum itself.

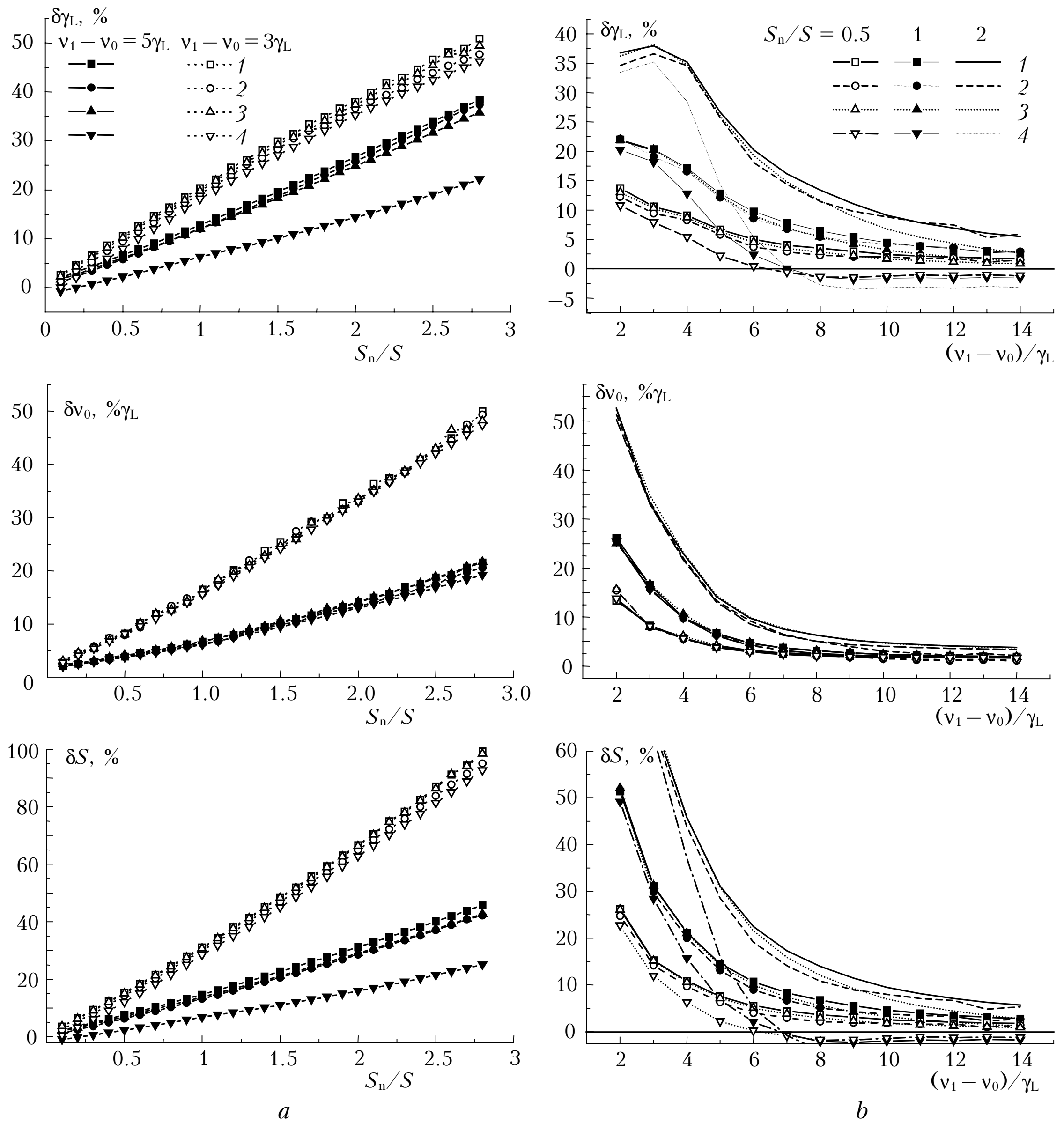


Fig. 6. Relative errors in parameters of the studied line retrieved from the fragment of the spectrum vs. the intensity (*a*) and the separation (*b*) of the neighboring line.

The dependence of the errors on the intensity of the neighboring line is also close to linear, and the errors increase sharply as the separation between the lines becomes smaller than 5–6 half-widths. As in the previous cases, the processing of the derivative indicates that 1) random noise markedly affects the obtained values of line parameters and 2) determination of the background parameters from the fitting gives the best results, while the prior removal of the background component is much less efficient.

Conclusions

1. The neglect of the background component in determining the line parameters from the absorption spectrum can lead to the error in determination of the intensity and half-width up to 100% for the Lorentz profile and up to 80% for the Doppler profile at the background level near the line center up to 20% of the absorption at the line center in the case of 5% random noise in the spectrum.

2. With the unknown nature of the background component, the prior removal of the linear background or, especially, addition of a linear function into the model during the fitting decreases the errors in determination of spectral line parameters down to 1–2% even with a 5% noise and 20% background levels.

3. The errors in determination of the line parameters from the derivative of the spectrum depend only slightly on the method the background component is taken into account and do not exceed 1.5–2% for the intensity and half-width under conditions described above. However, systematic errors can arise in determination of the line center.

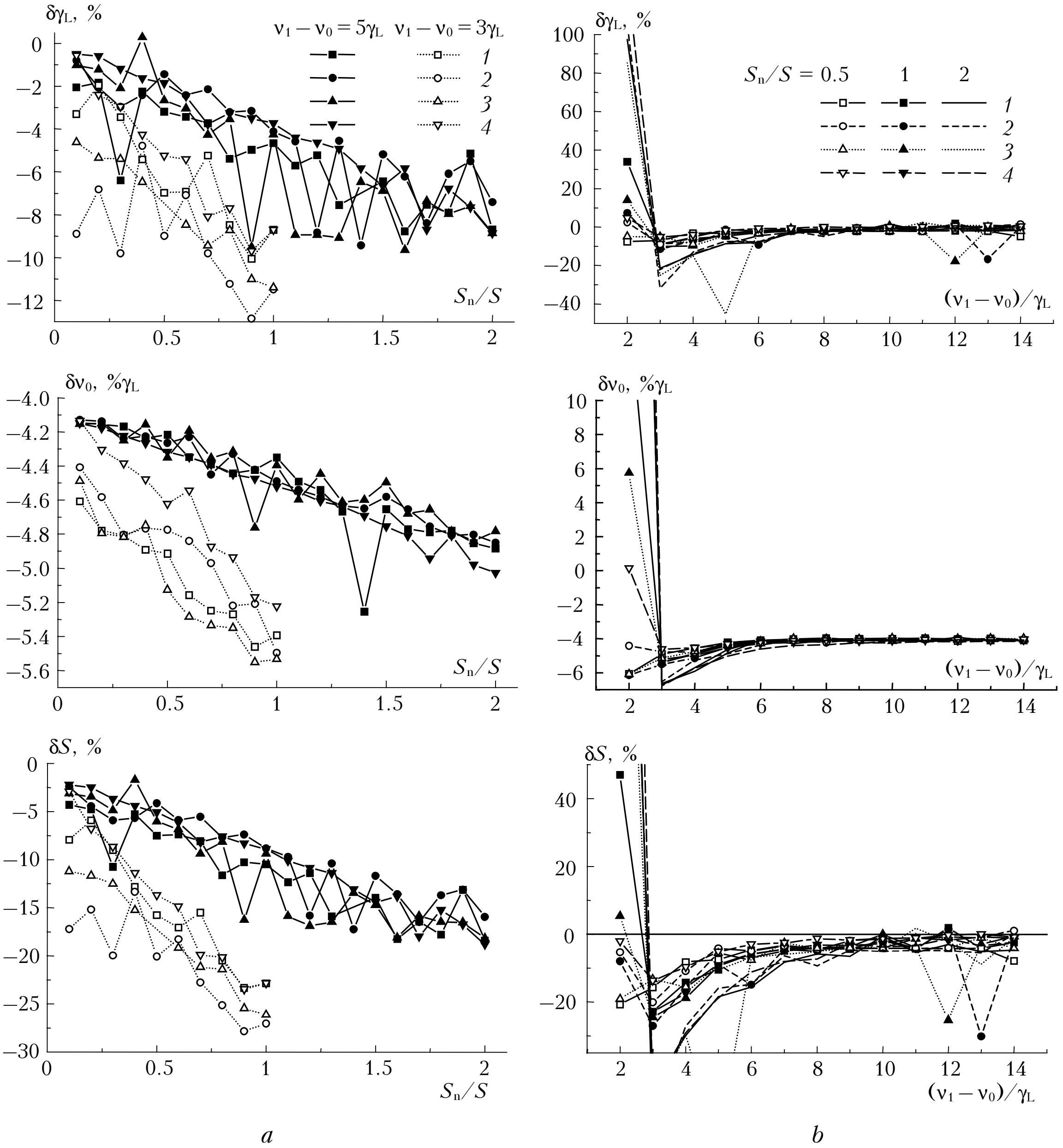


Fig. 7. Relative errors in parameters of the studied line retrieved from the fragment of the derivative of the spectrum vs. the intensity (*a*) and the separation (*b*) of the neighboring line.

4. The decrease of the width of the spectral fragment to less than 8 half-widths for the spectrum itself leads to an increase of the error of retrieval of the half-width and intensity made with simultaneous fitting of the background parameters. However, with the prior removal of the background component, the spectral fragment can be narrowed to 6 half-widths without any marked increase in the errors of determination of the half-width and intensity.

5. For the derivative of the spectrum, the error in determination of the intensity without background correction increases as the spectral fragment becomes narrower to less than 10 line half-widths. However, the introduction of a linear background in the model used for the fitting allows the intensity and half-width to be determined accurate to 3% for the spectral fragment about four half-widths wide.

6. The accuracy of determination of the central frequency of the line under study only slightly depends on the width of the spectral fragment used.

7. The presence of the wing of a weak (more than halved intensity) line in the recorded spectrum leads to the error in determination of the parameters of the line under study no higher than 2–3% with the separation between the lines larger than five half-widths and up to 5% with the separation of three half-widths.

8. The error in determination of the parameters of the line studied from the spectral fragment is proportional to the intensity of the interfering line and achieves 50% for the half-width, 50% of half-

width for the central frequency, and 100% for the intensity if the intensities of the interfering and studied lines relate to each other as 3:1 and the interfering line is separated by 3γ.

9. In the presence of the interfering line in the spectrum, the prior removal of the background components is inefficient. However, the addition of a linear background to the model of the line profile during the fitting 1.5 to 2 times decreases the errors in determination of the half-width and intensity at least for the lines separated by no less than 4 to 5 half-widths.

10. The use of the fragment of the frequency derivative of the spectrum for determination of spectral line parameters yields the parameters with smaller (by 2 to 2.5 times) error, but the artificial addition of the background component does not compensate for the effect of the interfering line.

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