Errors in retrieving the parameters of spectral lines from the absorption spectra. Part 1. Effect of background and measurement noise

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The parameters of a spectral line profile are calculated from the fragment of a model absorption spectrum and its frequency derivative using different methods for fitting and removal of the background component. The effect of measurement noise and background on the accuracy of retrievals of the absorption line parameters is analyzed.

Introduction

The data on absorption line parameters are widely used in solving various problems in atmospheric optics. Along with theoretical calculations,[1] experimental data are the main source of information on the line parameters. Usually, such data are represented by a Fourier transform, transmission and absorption spectra.[2] Determination of the line parameters from spectra of different types has some peculiarities. Using numerical simulation, we have analyzed the effect of the background component and measurement noise on the accuracy of retrieval of a line position, its halfwidth, and intensity from a fragment of the corresponding absorption spectrum.

Simulation of a spectral fragment

In the general case, the absorption spectrum recorded can be presented as

$$\tilde{f}(x_i) = f(x_i) + \xi(x_i)\,, \qquad (1)$$

$$f(x_i) = b(x_i) + \sum_{j=1}^{N_L} k_{\max j}\, F(x_i, \nu_{0j}, \gamma_j),$$

$$i = 1, \ldots, N;\ j = 1, \ldots, N_L,$$

where $b(x)$ is the background component; $k_{\max}$ is the absorption coefficient at the center of a line; F is the type of the absorption line profile; ν_0 and γ are the line position and the profile halfwidth; N is the number of points in the spectrum recorded; N_L is the number of spectral lines, whose absorption is significant within the portion of the spectrum under consideration; ξ is the measurement noise.

The background component may have different origin and is mostly determined by the characteristics of the receiving system (ADC, optics transmittance, spectral sensitivity of the detector, and others). In practice, three types of the background component are usually considered[3]:

$$b(x) = a_0 + a_1 x\,, \qquad (2)$$

$$b(x) = a_0 + a_1 x + a_2 x^2\,, \qquad (3)$$

$$b(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3.$$

Here a_0, a_1, a_2, a_3 are the unknown parameters of the background model.

In our calculations, we used the Doppler profile of a spectral line for simulation of the fragment of the spectrum or its derivative. The width of the model fragment was equal to 30 halfwidths, γ, of an absorption line, the line position ν_0 was placed at the center of the fragment. To simulate the experiment, the background component and noise have been added to the calculated absorption coefficient. The noise was simulated with a generator of normally distributed random numbers; the noise value in the calculations varied from 0 to 20% at normalization to the absorption coefficient at the line center $k_{\max}$.

The type of the background is usually unknown in processing the experiment. To study the effect of the background model on the accuracy of retrieval of the spectral line parameters, we have carried out three series of model calculations: without the background component, with the linear component given by Eq. (2), and with the squared background component given by Eq. (3). The coefficients a_0, a_1, and a_2 were taken so, that the value of the background component at the line center was no larger than 8% of $k_{\max}$ and the slope of the background component provided the difference in the values at the line width no more than 0.2% of $k_{\max}$. The presence of neighboring lines was ignored in the calculations.

Figure 1 depicts some examples of the model absorption spectrum with the background component and without it. The absorption spectrum includes 1-% noise, and the spectrum derivative is shown noise-free, because the background is hidden in the presence of even 1-% noise.

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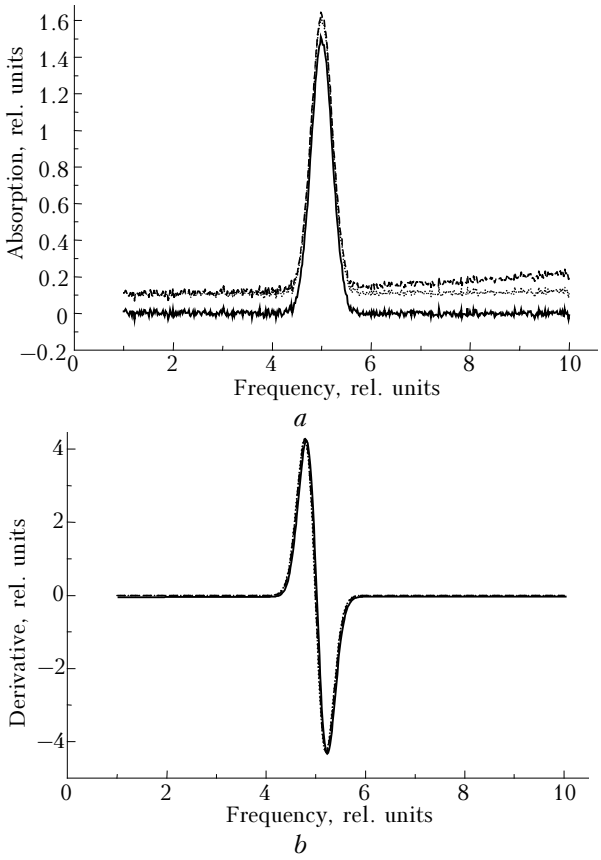

Fig. 1. Model fragments of absorption spectrum (*a*) and its derivative (*b*).

Methods for determination of spectral line parameters

Mostly, the methods for processing the experimental data involve minimization, in some way, of the discrepancy between the calculated model of the spectrum and measurements:

$$\Delta = \sqrt{\frac{1}{N-M}\sum_{i=1}^{N}\left(\tilde{y}(x_i) - f(x_i,p)\right)^2};$$

$$\{p_j\} = p_1,\ldots,p_M, \quad N > M,$$

where $\tilde{y}$, f are the measured and model spectra; $\{p_j\}$, $j = 1, \ldots, M$, are the spectral line parameters sought, M is the number of sought parameters ($M = 3$ for the Doppler profile).

Estimation of the vector p reduces to solution of the system of equations:

$$\partial\Delta^2 \big/ \partial p_j = 0, \qquad j = 1,\ldots,M .$$

The resulting system of equations is nonlinear and can be solved by both direct-search methods and the methods of nonlinear optimization.[4,5]

The direct-search method consists, essentially, in the search for minimum value of the discrepancy at the nodes of a computational grid in terms of the sought parameters:

$$\Delta \to \min\,,\ p_j = p_j^{\,0} + n\Delta p_j\,,\ n = 0,\ \ldots,\ n_{\max},$$

where $\{p_j^{\,0}\}$ and $\{\Delta p_j\}$ are the initial value and the grid step for each of the parameters.

The quality of the solution obtained by the direct-search method (and its different versions, such as, for example, random-walk method) depends on the step $\{\Delta p_j\}$ value, and the time needed for the search is determined by the accuracy of the initial approximation $\{p_j^{\,0}\}$.

The nonlinear methods are mostly based on the known approaches to minimization of nonlinear equations (for example, the Newton–Raphson, Levenberg–Marquardt, and other methods[4–7]). In the first case, the following equation is solved

$$p_{n+1} = p_n + B^{\mathrm{T}}[\nabla^2\chi(p_n)]^{-1};$$
$$\chi_i(p) = [y(x_i) - f(x_i,p)]^2, \qquad (4)$$

while the second case involves solution of the following equations

$$\delta p = (B^{\mathrm{T}}WB + \alpha I)^{-1}B^{\mathrm{T}}W\delta y\,, \qquad (5)$$

where $\delta p_j = p_j - p_j^{\,0}$; $\delta y_i = \tilde{y}_i - f(x_i,p_j)$, $i = 1, \ldots, N$; W is the matrix of the weighting coefficients determined by the measurement error; $B_{ij} = \dfrac{\partial f_i}{\partial p_j}$, $\alpha > 0$ is the parameter determined by the problem conditions; I is the unit matrix; T denotes transposition.

The method (4) works quite efficiently provided that the initial values of the parameters $\{p_j^{\,0}\}$ are close enough to the exact ones and the noise is low. If these conditions do not hold, then the Levenberg–Marquardt method (5) is applied.

The methods considered above are use the first and/or second derivatives of the discrepancy function. However, in practice their application is not always possible, depending on the function to be differentiated (for example, in the case with Galatry profile[8] or others). Good alternatives to these methods are the direct-search methods, which do not involve the information about the derivatives.

We have conducted the retrieval of the spectral line parameters from model spectra by five methods: fitting the Doppler profile parameters using the Origin software package (second-order nonlinear optimization method), using two modifications of the direct-search method, Newton–Raphson method (first-order nonlinear optimization method), and using RELIP software package developed by us.[9]

Since the model spectrum included the background component, it was taken into account in processing. Processing using the Origin software assumed the presence of a linear background, whose parameters were fit simultaneously with the profile parameters. In using both the direct-search method and the Newton–Raphson method, the background with linear and frequency squared behavior was first removed using the same procedure. Another procedure for prior removal of the linear background component was included into the RELIP software package.

If the derivative of the absorption spectrum was modeled, then integration was performed prior to fitting in the RELIP package, which caused large errors in the retrieval of the profile parameters. In other cases, the Doppler profile derivative was used as a model function in fitting.

Results and discussion

The first series of calculations was performed for the model function without the background. Figures 2 and 3 depict the relative errors of retrieval of the line position, halfwidth, maximum absorption coefficient, and intensity from the absorption spectrum and its derivative. Since in modeling we used the frequency in arbitrary units, the relative error of retrieval of the line position is given in percent of the halfwidth. The line intensity was not fit, but calculated using the retrieved values of k_{max} and γ.

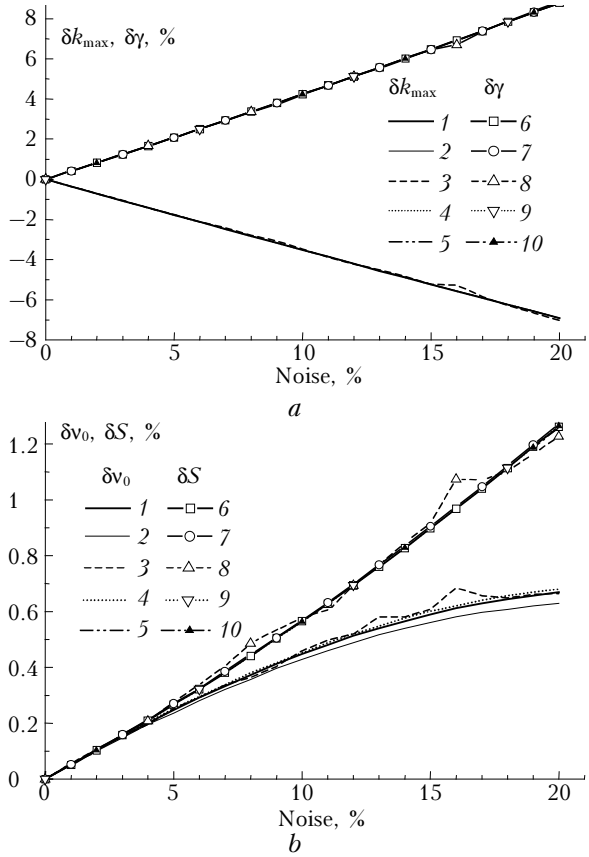

Fig. 2. Relative error of determination of the absorption coefficient at maximum (*1–5*) and halfwidth (*6–10*) (*a*); absorption line position (*1–5*) and intensity (*6–10*) (*b*) from the spectrum without background using the Origin software (*1*, *6*), two modifications of the direct-search method (*2*, *7*) and (*3*, *8*), Newton–Raphson method (*4*, *9*), the RELIP package (*5*, *10*).

It should be noted that RELIP package uses two methods for determination of spectral line parameters, namely, the random-walk method and the Levenberg–Marquardt method. The calculations were carried out using both of these methods, and in all the situations processed they gave the results identically accurate to the fifth or sixth significant decimal, therefore they are shown by the same line in Figs. 2 and 4. In Fig. 3 the results of fitting with the RELIP package are not shown.

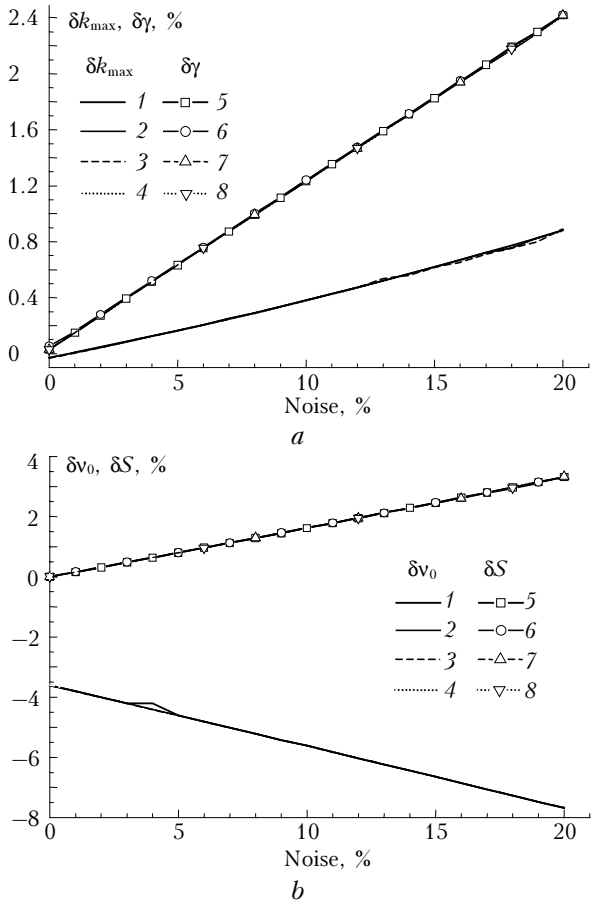

Fig. 3. Relative error of determination of the absorption coefficient at maximum (*1–4*) and halfwidth (*5–8*) (*a*); absorption line position (*1–4*) and intensity (*5–8*) (*b*) from the derivative of the spectrum without background using the Origin software (*1*, *5*), two modifications of the direct-search method (*2*, *6*) and (*3*, *7*), and the Newton–Raphson method (*4*, *8*).

It is seen from Figs. 2 and 3 that in the absence of a background component all the methods used for determination of the parameters give close results. The error in retrieval of the line position does not exceed 0.5% of the halfwidth for the signal and 8% for the derivative even at 20-% noise level. Although the errors in determination of k_{max} and γ increase with the increasing noise and achieve 7–10% when the spectrum includes 20-% noise, the error in determination of the intensity is within 1–1.5%. This is connected with the fact that the errors in determination of k_{max} and γ have opposite signs, and thus these effects compensate each other. When analyzing the spectrum derivative, the accuracy in determination of k_{max} and γ is much higher than in the case of analyzing the spectrum itself. The errors in determination of all the parameters increase

depending on the noise level, and this increase is roughly linear.

Similar calculations were performed for the model signal with the linear background and with the removal of the linear background in processing. The results obtained are shown in Figs. 4 and 5.

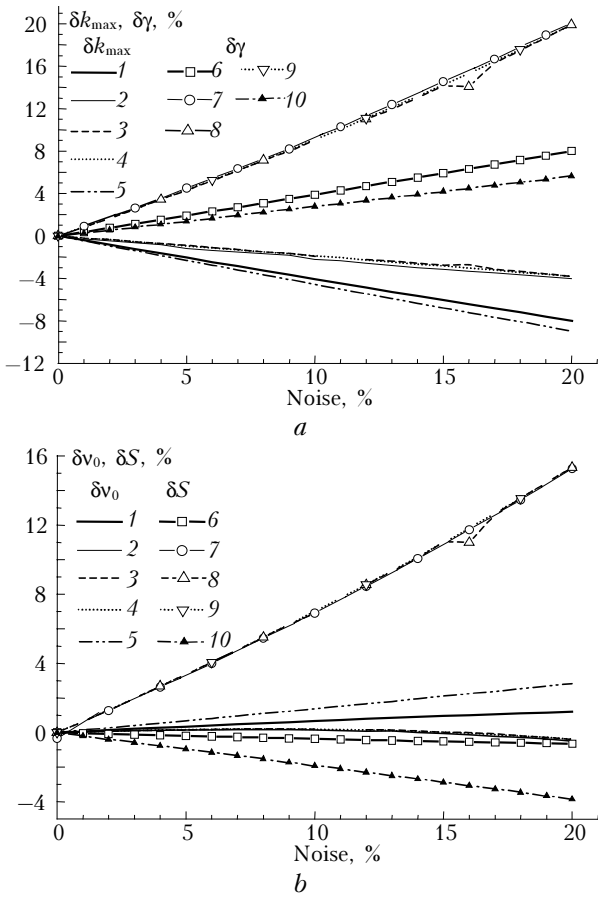

Fig. 4. Error in determination of the line parameters from the spectrum with linear background. Designations are the same as in Fig. 2.

It is seen from Figs. 4 and 5 that, although processing used the same background model as in simulation, the errors in determination of the line parameters increased, but kept the linear dependence on the noise level. The results obtained with the use of different processing methods differ. Since the results obtained using both the direct-search methods and the Newton–Raphson method are close and the same procedure was used to remove the background for them, the difference between the errors in determination of the line parameters is likely caused just by the incomplete removal of the background component. The results of retrieval of the line position and intensity from the spectrum turned out to be the best in applying the Origin software (that is, at simultaneous fitting of the line parameters and the background), although the accuracy of halfwidth determination is higher for the RELIP package, and the absorption coefficient at the line center is determined most accurately by other three methods.

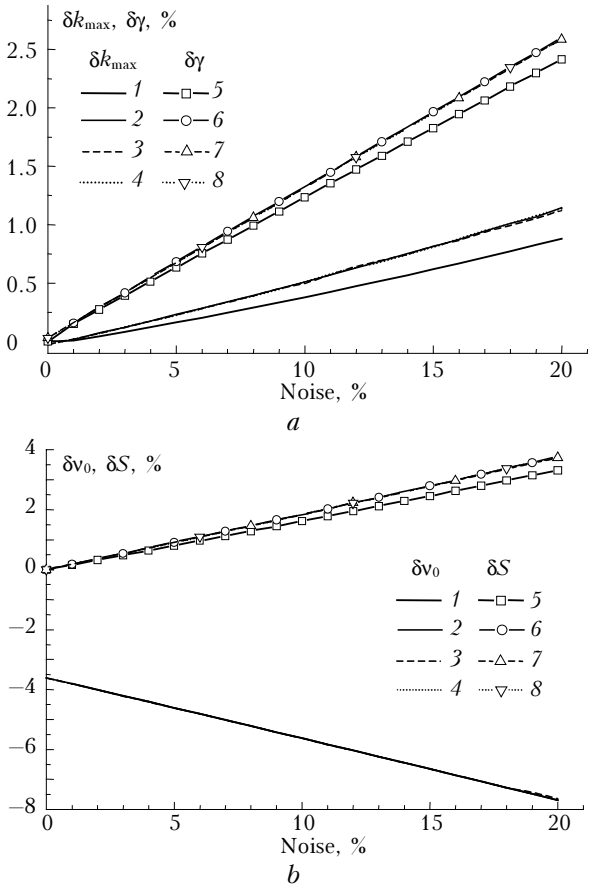

Fig. 5. Error in determination of the line parameters from the derivative of the spectrum with linear background. Designations are the same as in Fig. 3.

When using the spectrum derivative (Fig. 5), the contribution from the background component did not lead to a significant increase in the errors of determination of the line parameters. As in the case with the zero background, the largest error for the line position is 6–7% of the halfwidth, the errors of retrieval of the other parameters are within 2–3% even at 20-% noise level.

Since in experiments the source of the background is not always known, in the next series of calculations we have determined the line parameters by three of the methods listed above one of the direct-search methods, the Newton–Raphson method, and with the use of the Origin software) from the model spectra calculated for the linear, square, or zero background. In processing the background was assumed to be zero or having linear, or frequency squared behavior, regardless of the model spectrum used. The relative errors in the retrieval of the line parameters are shown in Fig. 6. It can be seen from Fig. 6 that with the unknown behavior of the background we can expect the error of 1% of the halfwidth in retrieval of the line position even at a 20-% noise level. The error in retrieval of k_{max} is within 8%, and the error in retrieval of the halfwidth in the worst case can exceed 20% (when neglecting the background component), but remains

within 5–7% in using the frequency squared behavior of the background component in processing.

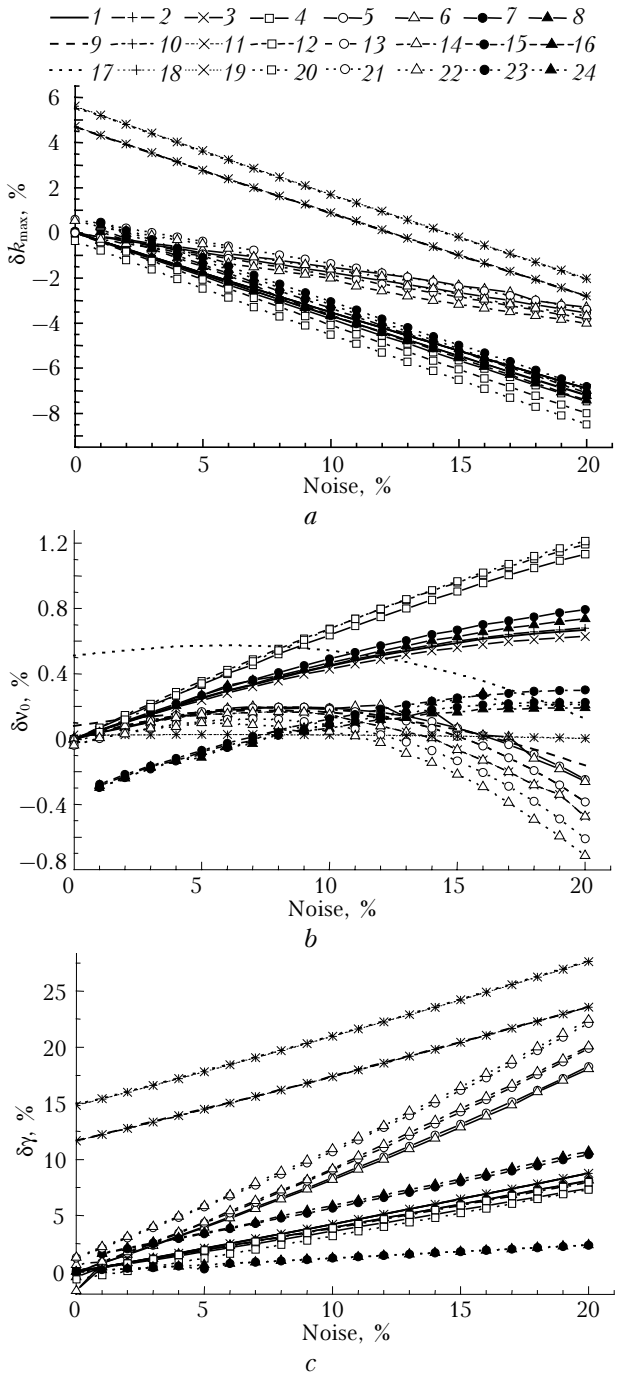

Fig. 6. Comparison of the errors in retrieval of the absorption coefficient at the line center (*a*), position (*b*), and halfwidth (*c*) of an absorption line in different situations: retrieval neglecting the background component (*1–3*, *9–11*, *17–19*), taking into account the frequency linear background (*4–6*, *12–14*, *20–22*) or squared background (*7*, *8*, *15*, *16*, *23*, *24*) from the model fragment of the spectrum with zero (*1–8*), linear (*9–16*), or frequency squared (*17–24*) background using the Origin software (*1*, *4*, *9*, *12*, *17*, *20*), by the Newton–Raphson method (*2*, *5*, *7*, *10*, *13*, *15*, *18*, *21*, *23*), and the direct-search method (*3*, *6*, *8*, *11*, *14*, *16*, *19*, *22*, *24*).

Conclusions

The results obtained have shown that the error in retrieval of the spectral line parameters nearly linearly depends on the noise level, at least, up to 20-% noise level when using both the absorption spectrum and its derivative.

The presence of even low (less than 8% of the maximum signal) background leads to an increase in the errors in determination of the spectral line parameters, but this increase is smaller if using the derivative rather than the absorption spectrum itself.

In analysis of the absorption spectrum, the prior removal of the background with the frequency squared behavior (even if its source is unknown) leads to a more accurate retrieval of the spectral line parameters.

All the results presented were obtained at zero background component in the model spectrum or the background of 8% of the maximum signal. The dependence of the error in retrieval of the spectral line parameters on different background characteristics will be studied in our following works. In addition, we plan to consider the effect of neighboring lines lying beyond the model fragment of the spectrum on the accuracy of determining the parameters of the line under study.

Acknowledgments

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