Errors in retrieving the parameters of spectral lines from the absorption spectra. Part 3. Effect of distortions introduced into the central part of an absorption line profile at its recording

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The error of retrieval of spectral line parameters has been studied based on numerical simulation for the conditions when no central part of the line profile is involved in the processing (strong absorption). The values of the random noise and the width of the spectral range taken for processing, at which the influence of the central part of the line profile on the parameters to be retrieved is low, have been estimated.

Introduction

In experimental recording of spectra, the central part of a profile of the strongest lines may be distorted or even fully excluded from processing because of strong absorption (optical depth > 4–5). Examples are the recent papers,[1–3] dealing with the experimental investigation of water vapor absorption by the Fourier transform spectroscopy. The extension of the dynamic range of measurements in order to cover the strongest lines in such cases can be uneconomic because of the need to made shorter experimental cells. The use of a buffer gas for the additional broadening and, correspondingly, the decrease of the absorption coefficient at the center of strong lines is eliminated when it is necessary to study self-broadening spectra. Nevertheless, as was shown, for example, in Ref. 3, the parameters of such (cut-off) lines can be retrieved from the fitting of the rest part of the line profile, without the use of the distorted central part. However, the errors of retrieval of parameters of such lines remain unstudied yet.

In Refs. 4 and 5, based on numerical simulation, we have studied the effect of the measurements noise, background, and the wing of a neighboring line on the error of retrieval of line position, intensity, and half-width from a fragment of the absorption spectrum or its frequency derivative. In this paper, we study the error of retrieval of spectral line parameters (position, intensity, and half-width) as a function of the width of the central part of the line profile, excluded from the fitting. Noise and the width of the spectral interval, included in the processing, are considered as a variable parameters.

1. Simulation of a spectral fragment

The absorption lines were placed at the centers of the corresponding spectral fragments modeled. The central frequency of the line was $\nu_0 = 7.5$ in conventional unit. The scale of the frequency axis corresponded to reciprocal centimeters. The line profile was assumed the Voigt. The calculations were performed for the line with the intensity $S = 1$, the Doppler half-width $\gamma_D = 0.022$ cm^{-1}, and two values of the Lorentz half-width $\gamma_L = 0.022$ and 0.5 cm^{-1}, corresponding to largely Doppler and Lorentz types of the line profile. The model fragment was calculated using uniform frequency interval $\Delta\nu = 0.01$ cm^{-1} (for $\gamma_L = 0.022$ cm^{-1}) and 0.1 cm^{-1} (for $\gamma_L = 0.5$ cm^{-1}), so that four and five points fell, respectively, within the line half-width.

Random noise of 0.5, 1, and 2% of the level of absorption at the line center was superimposed onto the model spectral fragment. The relative errors of retrieval of the intensity and the Lorentz half-width are given in fractions of unity, and the relative errors in the line position are given in fractions of the Lorentz half-width:

$$\delta\nu_0 = \frac{\nu_{0\,\mathrm{retr}} - \nu_{0\,\mathrm{mod}}}{\gamma_{L\,\mathrm{mod}}},$$

$$\delta S = \frac{S_{\mathrm{retr}} - S_{\mathrm{mod}}}{S_{\mathrm{mod}}},$$

$$\delta\gamma_L = \frac{\gamma_{L\,\mathrm{retr}} - \gamma_{L\,\mathrm{mod}}}{\gamma_{L\,\mathrm{mod}}}.$$

When retrieving the position of the absorption line, we calculated not only the relative error $\delta\nu_0$, but also the absolute error of retrieval of the line position $\Delta\nu_0$ in reciprocal centimeters.

2. Influence of the missing points on the quality of the line parameters retrieval

The model spectral fragment included 100 points, that is, it was about 25 line half-widths wide

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at $\gamma_L = 0.022$ cm^{-1} (half-width of the Voigt profile ≈ 0.04 cm^{-1}) and 20 half-widths at $\gamma_L = 0.5$ cm^{-1}. The processing involved consecutive removal of points from the central part of the profile, from 1 to 20, starting from the line center. The model spectral fragment, normalized to the value of the absorption coefficient at the line center k_{max}, for $\gamma_L = 0.5$ cm^{-1} (corresponding to the Lorentz profile) and 2% noise level is shown in Fig. 1 along with the numeration of points. The cut-off level y_{max} was determined with respect to the absorption at the line center: $y_{max} = 1$ corresponds to the full profile, $y_{max} = 0.8$ means that all (five) points with $k(\nu) > 0.8k(\nu_0)$ are removed, and so on. The line parameters were determined by the fitting of the Voigt profile to the model spectral fragment by the Levenberg-Marquardt method.

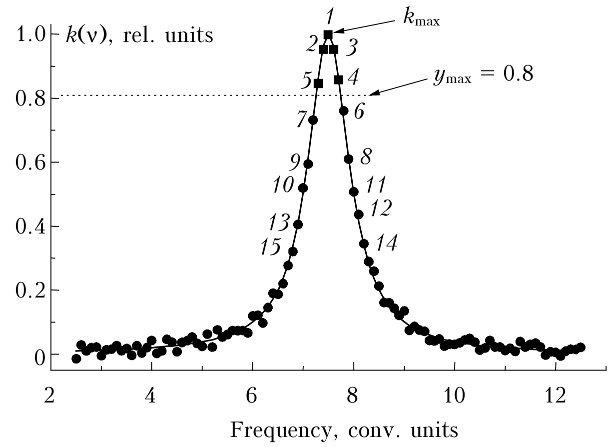

Fig. 1. Model spectral fragment for the Lorentz line profile with 2% random noise.

The errors of retrieval of line parameters versus cut-off level for the largely Doppler and Lorentz profiles are shown in Figs. 2 and 3. It can be seen that the errors of retrieval of line parameters are proportional to the level of the measurement noise and only weakly depend on the cut-off level, until it is lower than the half-maximum of the line. A stronger cut-off leads to a sharp increase of the errors. Thus, the error of retrieval of the line position from the spectral fragment with 2% noise for the Doppler profile cut-off at the level of $0.7k_{max}$ does not exceed 0.001 cm^{-1} and triples with the cut-off at the level of $0.25k_{max}$. For the Lorentz profile under the same conditions, the error of retrieval of the line position is much higher; it amounts to 0.01 cm^{-1} with cut-off at the level of $0.7k_{max}$ and triples at the level of $0.2k_{max}$.

As the line profile is cut off, a tendency to the underestimation of the line intensity and overestimation of the half-width arises, and the errors in determination of these parameters for narrower lines are much higher. Thus, we obtained a threefold as high relative error in the retrieved intensity and almost fourfold higher error in the half-width for the profile with the half-width $\gamma \approx 0.04$ cm^{-1} ($\gamma_D = \gamma_L = 0.022$ cm^{-1}) as compared to $\gamma \approx 0.5$ cm^{-1} ($\gamma_D = 0.022$ cm^{-1} and $\gamma_L = 0.5$ cm^{-1}). This is likely connected with the smaller number of points in the central part for the largely Doppler profile with $\gamma_D = \gamma_L = 0.022$ cm^{-1} (4 points at the line half-width, the fragment as wide as 25 half-widths) as compared to the Lorentz profile with $\gamma_L = 0.5$ cm^{-1} (5 points at the line half-width, the fragment as wide as 20 half-widths): in the first case, only 12 points lie above the 20% level, while in the second case they are 20.

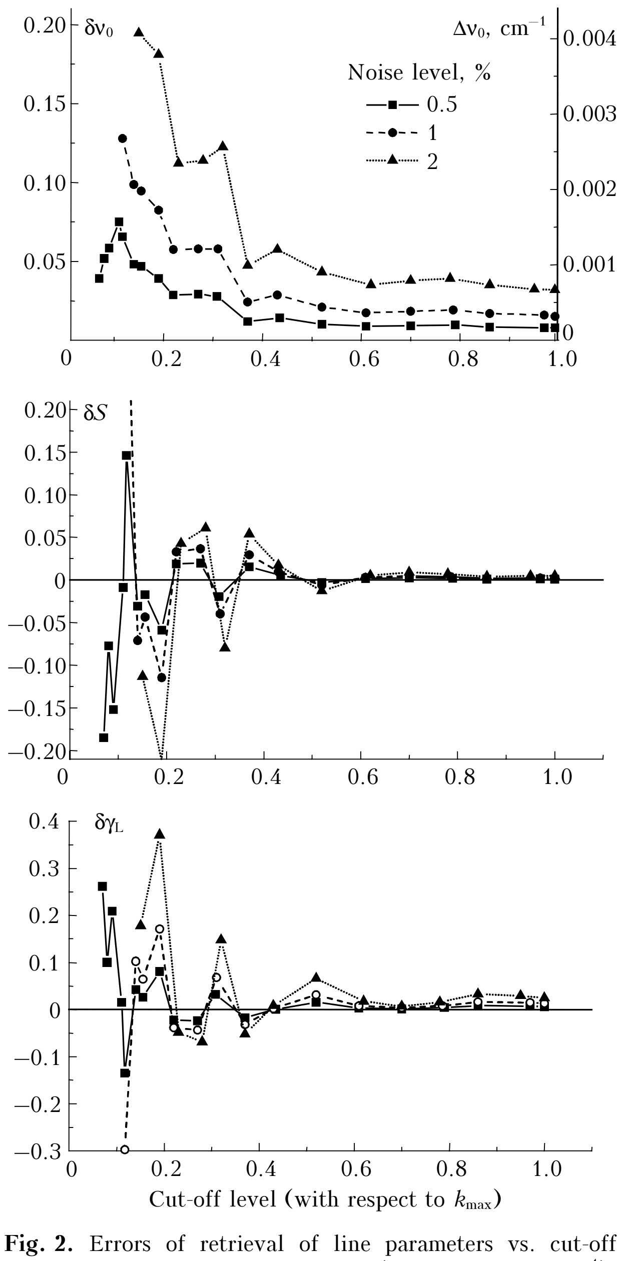

Fig. 2. Errors of retrieval of line parameters vs. cut-off level for the largely Doppler profile ($\gamma_D = \gamma_L = 0.022$ cm^{-1}).

However, it should be noted that the relative error of retrieval of line intensity from the spectral fragment corresponding to the Lorentz line profile, even when cut-off at the level of 0.2 k_{max}, did not exceed 6% with the noise not higher than 2%. This confirms the possibility of determining the intensity for cut-off lines with acceptable accuracy. With severe cutting-off of narrow lines, the half-width value obtained from the fitting can be considered only as approximate, because its relative error at the 2% measurement noise may reach 40%.

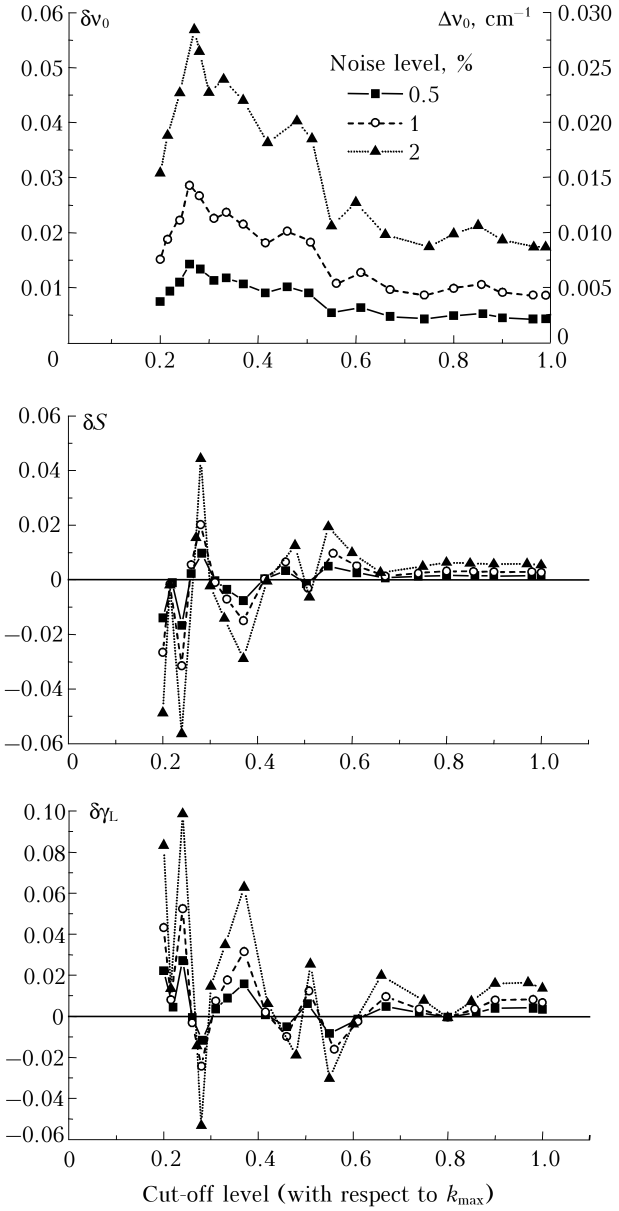

Fig. 3. Errors of retrieval of line parameters vs. cut-off level for the Lorentz profile ($\gamma_D = 0.022$ cm^{-1}, $\gamma_L = 0.5$ cm^{-1}).

3. Influence of the width of a fragment on the quality of the line parameters retrieval

It can be seen from Fig. 1 that, though the line wings do not reach zero, a significant part of the points falls within the line wings. For example, once 20 central points are removed (the whole fragment contains 100 points), the rest part includes the line wings at the level of 20% of the maximum, that is, in the model fragment only about 20% of points correspond to the central part. Figure 4 shows the dependence of the relative error of retrieval of line parameters on the width of the spectral fragment (in half-widths) for $\Delta\nu = 0.1$ cm^{-1}, $\gamma_L = 0.5$ cm^{-1} without removal of points from the central part of the profile.

It can be seen from Fig. 4 that the error of determination of the line position is independent of the fragment width, while the errors of determination of the half-width and intensity at the fragment widths smaller than 14 half-widths (7 half-widths on each side of the line center) begin to increase, as the width of the spectral interval involved in the processing decreases, at least at the measurement noise higher than 1%.

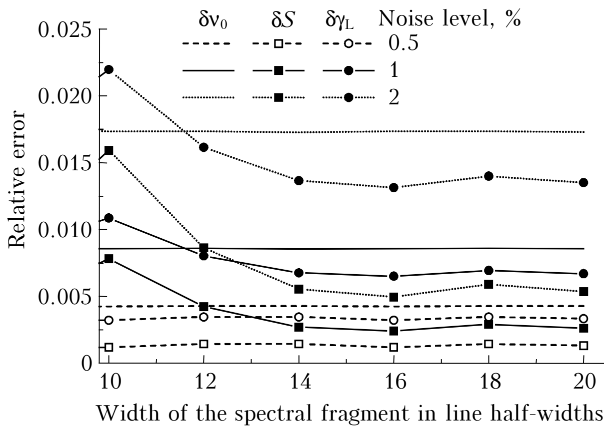

Fig. 4. Errors of retrieval of line parameters vs. width of the spectral fragment involved in the processing.

Such a dependence of the errors of retrieval of the line half-width and intensity on the width of the spectral interval was obtained in Ref. 5, where we have found that, depending on the method of consideration of the background component, the errors in the half-width and intensity increased for the fragments narrower than 8 or even 5–6 half-widths at a 5% measurement noise. However, these results were obtained for different line half-width, at a much higher density of points in the spectral fragment (in Ref. 5, 12 points fell within the line half-width, while in this work they are only five), and the background component, linearly dependent on the frequency.

The influence of the spectral fragment width on the errors of retrieval of line parameters is illustrated indirectly by the difference in errors obtained for the largely Doppler (Fig. 2) and Lorentz (Fig. 3) line profiles, whose fragments amounted to 25 and 20 half-widths, respectively. However, it is possible that not only different width of the fragments, but also different types of profiles have led to the difference in this case.

Figure 5 shows the error of retrieval of line parameters as a function of the cut-off level for the fragments 10, 15, and 20 half-widths wide at the 1% noise.

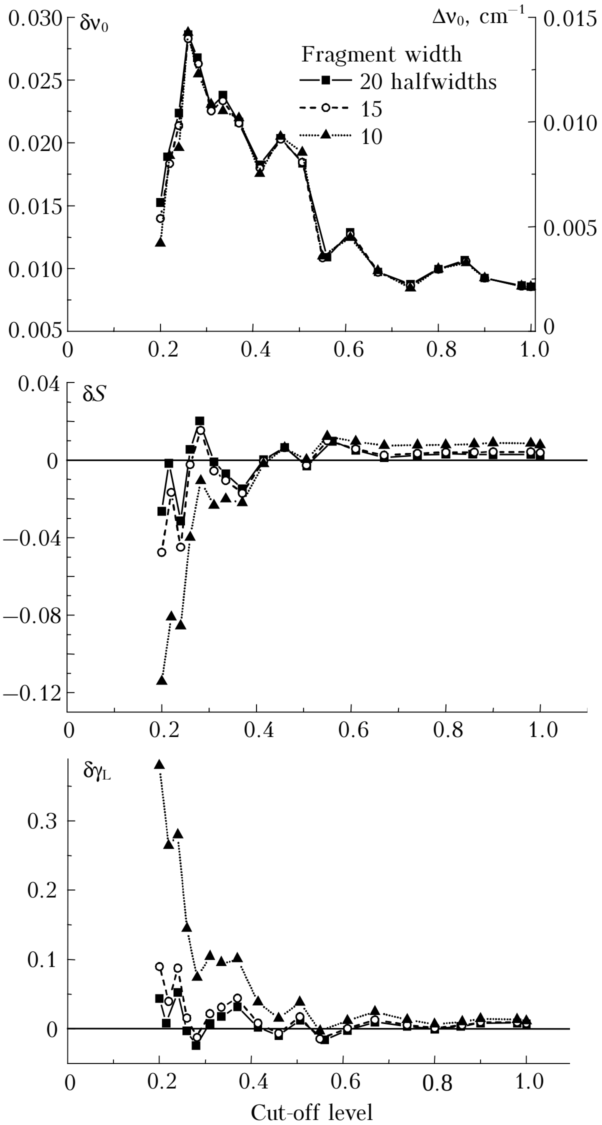

Fig. 5. Errors of retrieval of line parameters vs. cut-off level and the spectral fragment width for the Lorentz profile.

It can be noticed that if the line profile is cut off by more than a half, the tendency to overestimation of the half-width and underestimation of the intensity becomes much more pronounced as the width of the spectral fragment decreases. At the same time, the relative error of retrieval of the line intensity at the 1% measurement noise for the Lorentz profile remains no worse than 10% even with the fragment width of 10 half-widths and the cut-off level of $0.2k_{\max}$, although the error of determination of the half-width under these conditions increases almost up to 40%, that is, becomes close to the values obtained for the fragment twice as wide and with the twice as high random noise level.

Conclusions

The results of the calculations allow us to draw the following conclusions:

1. If the central part of the line profile is cut off by no more than a half, the errors in determination of line parameters are almost independent of the cut-off level and do not exceed 1–2% at the 2% noise level. If the most fraction of the central part of the profile is missing, the error in determination of line parameters begins to increase with the increase of the cut-off level, thus causing the systematic *underestimation* of the retrieved intensity and *overestimation* of the line half-width. At the 0.2 cut-off level, the error of retrieval of line parameters can reaches 10–12% even at the 1% noise.

2. The obtained relative errors of retrieval of line parameters for the Doppler profile are, on the average, 2 to 3 times higher than those for the Lorentz profile. This is likely attributed to the larger fraction of points in the central part (compared with the wing) for the Lorentz profile, than for the Doppler one.

3. The narrower is the spectral fragment used in processing, the higher is the influence of the central part of the line profile on the retrieval of line parameters. The optimal value, found in this work, amounted to 14–15 half-widths. If a narrower spectral fragment is used in the processing, the errors in retrieval of the line half-width and intensity increase sharply even with the undistorted central part of the line profile.

References

1. D. Belmiloud, R. Schermaul, K.M. Smith, N.F. Zobov, J.W. Brault, R.C. Learner, D.A. Newnham, and J. Tennyson, Geophys. Res. Lett. **27**, 3703–3706 (2000).
2. K.M. Smith, I.V. Ptashnik, D.A. Newnham, and K.P. Shine, J. Quant. Spectrosc. Radiat. Transfer **83**, 735–749 (2004).
3. I.V. Ptashnik, K.M. Smith, K.P. Shine, and D.A. Newnham, Quart. J. Roy. Meteorol. Soc. (2004), in press.
4. M.Yu. Kataev and O.Yu. Nikiforova, Atmos. Oceanic Opt. **16**, No. 11, 907–911 (2003).
5. M.Yu. Kataev and O.Yu. Nikiforova, Atmos. Oceanic Opt. **17**, No. 11, 852–860 (2004).