

Fractal properties of the absorption spectra of gaseous atmospheric constituents

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The spectra of rotational-vibrational bands of main absorbing atmospheric molecules (H_2O , CO_2 , and O_3) are interpreted in terms of fractal analysis. The results demonstrate that these spectra possess non-trivial and rather individual multifractal characteristics. In particular, the spectrum of fractal dimensions is shown to be sensitive to molecular and isotopic content of a gas and to the type of a rotational-vibrational absorption band.

Introduction

Optical spectra bring information about the structure and internal motion of a quantum system, and every spectral line characterizes certain conditions for this motion. The study of individual spectral lines and characteristic series forms the basis for methods of spectral analysis.

At the same time, there is another approach to studying spectral properties of quantum systems "as a whole." It is based on the methods of statistical analysis^{1,2} (see also reviews 3–5, Ref. 6, and references therein). The reason for this approach is the complex, pseudo-random character of the spectrum of a quantum chaotic system (QCS). The statistical approach treats spectral manifestations of the quantum chaos as a property of the group of system states or, in other words, as a collective behavior of the groups of quantum ensemble's elements. Statistical criteria of the quantum chaos are represented in terms of distribution features of interlevel intervals. For regular quantum systems, distribution of interlevel intervals is Poissonian; at the same time, for QCS the Wigner distribution takes place. This leads, in particular, to small probability that one can find close levels in the QCS spectrum (the phenomenon of level repulsion).

The salient features of the structure of complex systems often can be expressed in terms of fractal geometry. In the simplest case, the distribution geometry for elements of the studied set is characterized by the Hausdorff–Besicovich dimension^{7,8} which can be treated as an indicator of singularity α : the distribution density for elements of a set inside some subset of diameter δ is proportional to δ^α . It is evident that the more irregular is the distribution of elements in the set, the smaller is α .

Application of methods of multifractal analysis is natural development of the idea to study fractal

properties with a complex structure. A multifractal is a more complicated object as compared to an elementary fractal.^{8,9} It is a set of elementary fractals organized in a multifractal by distribution of singularities of a certain measure generated by a given physical parameter. As it was mentioned in Ref. 10, multifractal analysis can yield non-trivial results as applied not only to self-similar objects and even not obligatorily to fractals.

In the case of a multifractal, the Hausdorff–Besicovich dimension is generalized by Renyi's dimension D_q , connected with "density" distribution of a certain physical parameter $\rho(x)$, as a measure on a geometrical support. Note that the choice of this physical parameter is decisive, as it determines the choice of the measure of the set and, correspondingly, its fractal properties.

An example of studying fractal properties of the spectrum of a quantum system is presented in Ref. 11, where fractal properties of the geometrical structure of arrangement of spectral series of the hydrogen atom are found. The used approach is based on selection of a test function whose Levy set (the set of self-similarity points) has the same distribution as the physical parameter described. However, this approach is restricted to the case of rather simple spectra and, besides, the Levy set brings information only about geometrical properties of the support for the distribution function of spectral lines.

If collective characteristics of the set of spectral lines of a molecule are close to each other in a certain sense, their fractal analysis is of interest. Some vibrational–electronic and rotational–vibrational bands can be the subjects of such analysis. In this paper an attempt is made of multifractal analysis of rotational–vibrational absorption spectra of main atmospheric molecules: H_2O , CO_2 , O_3 , and their isotopic species.

Formulation of the general approach to spectral analysis

The set of spectral lines evidently leads to the measure distribution necessary for applying the multifractal analysis. For instance, the number of absorption lines of a certain intensity per unit frequency interval can be taken as a “measure density” $\rho(x)$. However, in our opinion, it is more natural to take the “absorption density”, i.e., total absorption per unit frequency normalized to the total absorption all over the frequency range, as the “measure density”.

In practice, fractal properties of the “absorption density” distribution on the set of N frequency intervals can be analyzed by the method of identical bins.¹² Let us divide the support of the set into equal frequency intervals (bins) of size δ normalized so that $\delta N = 1$. Then let us determine the moments

$$G_q(\delta) = \sum_{i=1}^N \rho_i^q,$$

where ρ_i is the absorption density in the i th bin, and summation is performed over all non-empty bins. Then, for not very small δ , we introduce the function

$$\tau(q) = \log G_q(\delta) / \log \delta,$$

which is related to the generalized Renyi dimension D_q as

$$\tau(q) = D_q(q - 1).$$

The singularity spectrum of the multifractal $f(\alpha)$ is related to the function $\tau(q)$ in the following way:

$$f(\alpha) = q \frac{d\tau(q)}{dq} - \tau(q),$$

where

$$\alpha = \frac{d\tau(q)}{dq}.$$

Let us illustrate this technique using as an example the test case permitting direct interpretation. Figure 1 shows the singularity spectrum for 500 equidistant lines of the same intensity. Since $\rho_i(\delta) \propto \delta$ in this case, the singularity spectrum must be the δ -function of unit amplitude at the point $\alpha = 1$.

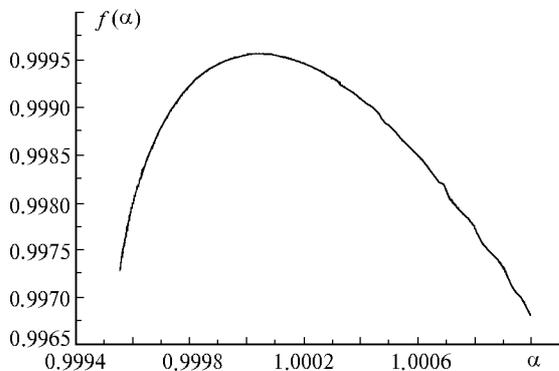


Fig. 1.

Fractal analysis of optical spectra

Let us consider the salient features of the singularity spectrum of main atmospheric molecules: H₂O, CO₂, and O₃. They are chosen because of the important role they play in the dynamics of atmospheric processes. For instance, atmospheric water vapor has the richest absorption spectrum in the visible and IR regions, carbon dioxide is one of the greenhouse gases, and the ozone layer protects the Earth from UV radiation.

Figure 2 shows the singularity spectra for different H₂O vibrational bands. One can see that the spectral functions of these bands differ significantly. It is interesting to analyze the influence of the isotopic composition of a gas on the singularity spectrum. Figure 3 shows the singularity spectra of the HDO molecule. One can see that the spectra of identical absorption bands but of different isotopic species differ markedly too.

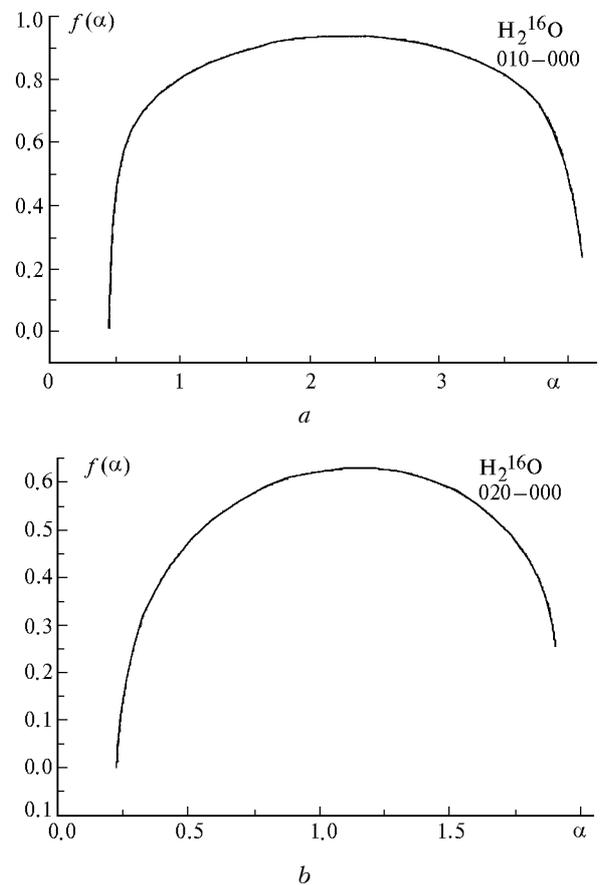


Fig. 2. Singularity spectrum for absorption density in the 010-000 (a) and 020-000 (b) bands of the main water vapor isotopic specie.

Let us consider the salient features of fractal spectra of the same absorption band for two CO₂ isotopic species (Fig. 4). Here, the differences in the singularity spectra are also seen.

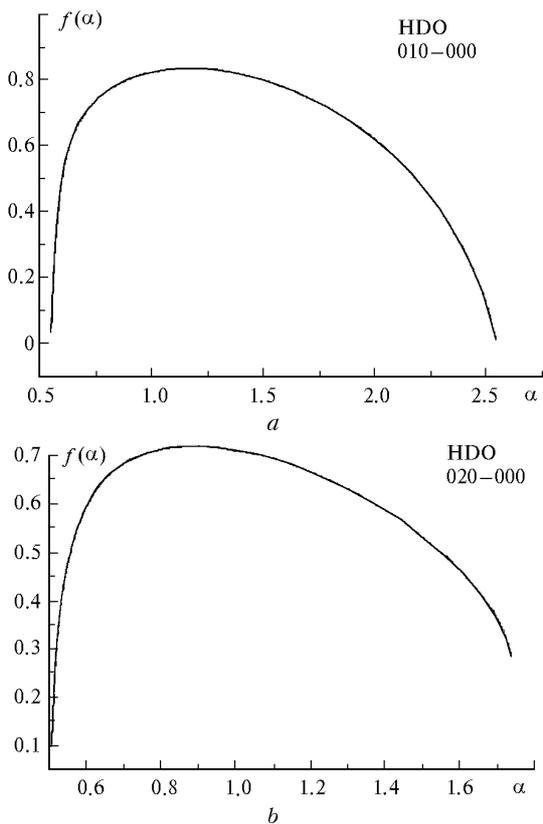


Fig. 3. Singularity spectrum for the absorption density in the 010-000 (a) and 020-000 (b) bands of the HDO isotopic specie.

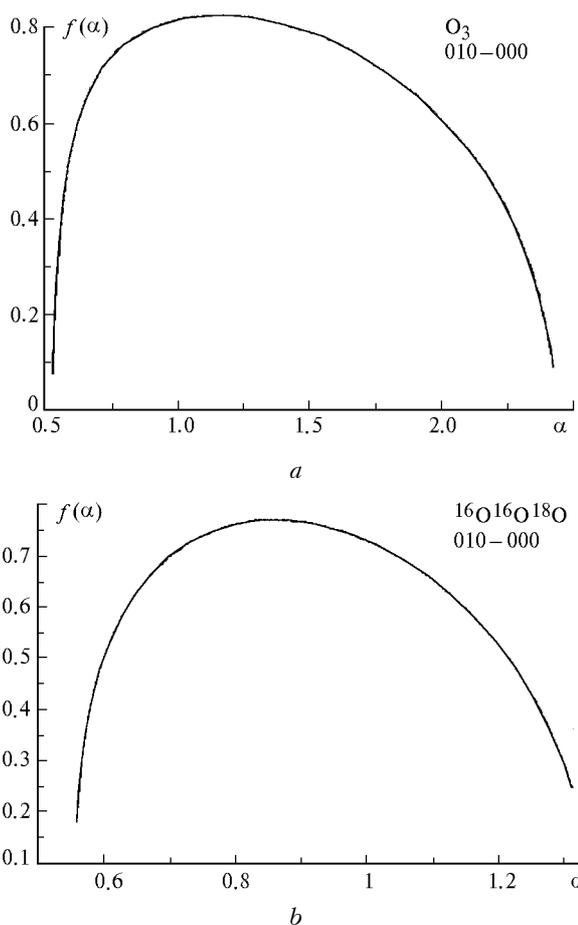


Fig. 5. Singularity spectrum for the absorption density in the 010-000 band of O_3 (a) and $^{18}O^{16}O^{18}O$ (b).

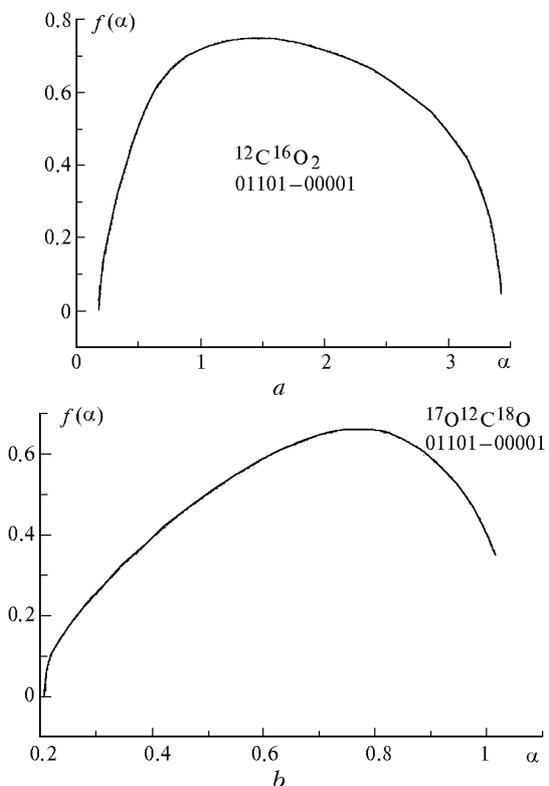


Fig. 4. Singularity spectrum for the absorption density in the 01101-00001 band of $^{12}C^{16}O_2$ (a) and $^{17}O^{12}C^{18}O$ (b).

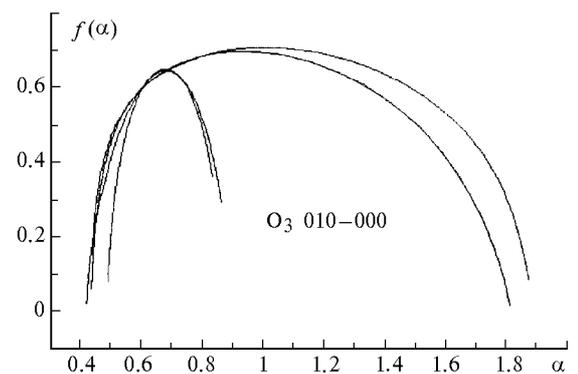


Fig. 6. Singularity spectrum for the absorption density in the 010-000 ozone absorption band divided into four equal frequency intervals.

The optical spectrum of the main absorption band of ozone is characterized by the far greater number of rotational lines (more than 7000) as compared to the spectra of the molecules considered above. The fractal spectrum of ozone is shown in Fig. 5. Analysis of self-similarity of the optical spectrum is also interesting. Figure 6 shows the fractal spectra of the main O_3 band

divided into four parts. One can see that the singularity spectrum is most variable in the area of large α , but the fractal spectra of two pairs practically coincide.

Conclusion

In this paper, the absorption density, i.e., total absorption per unit frequency normalized to the total absorption all over the frequency range, is used as a basis for multifractal analysis of optical spectra of gas molecules. In terms of fractal analysis, the absorption density is described by the singularity spectrum characterizing the collective properties of its distribution at the frequency axis.

The results of this work demonstrate that absorption spectra of rotational–vibrational bands of gas molecules possess non-trivial and rather specific multifractal characteristics. In particular, the singularity spectrum is shown to be sensitive to the molecular and isotopic composition of the gas under study and to the type of the rotational–vibrational absorption band.

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