SCATTERING OF SUNLIGHT BY A BARIUM-ION CLOUD

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This paper presents some results of numerical simulations of the photoexcitation and glow of a spherical barium cloud illuminated with sunlight. It is shown that when the initial optical depth of a neutral cloud exceeds 10, *radiation transfer in one atomic (*553.5 nm*) and three ion (*455.4, 493.4, *and* 614.2 nm*) lines should be taken into account. The data obtained indicate that the processes of radiation transfer have a strong effect on the spatial distribution of ions in different states, on the angular dependence of the intensity of scattered radiation, and on the shape of the glow lines.*

INTRODUCTION

When performing active experiments on emitting barium into the upper atmosphere, the atomic cloud is formed due to the processes of gas-dynamic spread of the matter. The cloud is ionized under sunlight.[1–4] The ion component of the barium cloud also intensely absorbs the sunlight, what results in a redistribution of ions over the energy states. Excited ions emit radiation in the visible spectral region. This radiation is recorded optically. Analysis of the experimental spectroscopic data shows that barium clouds often are optically dense at the atomic transition with $\lambda = 553.5$ nm. The optical depth τ_0 of such clouds can be as large as 30 and even larger.[5,6] Simple estimates made in this work show that at optical depth larger than 10 a cloud becomes optically dense at other atomic and ion transitions as well. Therefore, the problem of the influence of radiation transfer, at all such transitions, on the dynamics of ionization and glow of a barium cloud is very important. Otherwise, the neglect of this factor may result in wrong conclusions when interpreting the experimental spectroscopic information.

ESTIMATES OF THE RATIO OF THE OPTICAL DEPTH

To estimate the ratio between the optical depths of a cloud at the ion transitions and the atomic ones with $\lambda = 553.5$ nm, let us describe the dynamics of its ionization in an optically thin cloud by the following expression[7]:

$$N_i(t) = N_0\,[1 - \exp\,(-\,t/\tau_{ph})]\ , \qquad (1)$$

where τ_{ph} is the characteristic time of photoionization, which is estimated, based on the experimental data, to be 20 – 30 s; N_0 is the initial density of particles (atoms); N_i is the concentration of photoions. The kinetics of photoexcitation of an ion cloud is described by the system of balance equations for the five-level model of an ion (Fig. 1). The processes of excitation and quenching of energy states by sunlight, as well as their spontaneous decay are taken into account. One differential equation in the set is replaced with the condition of conservation of the total number of ions. With a due regard for Eq. (1), this condition takes the following form:

$$N_1 + N_2 + N_3 + N_4 + N_5 = N_0\,[1 - \exp\,(-\,t/\tau_{ph})]\ . \qquad (2)$$

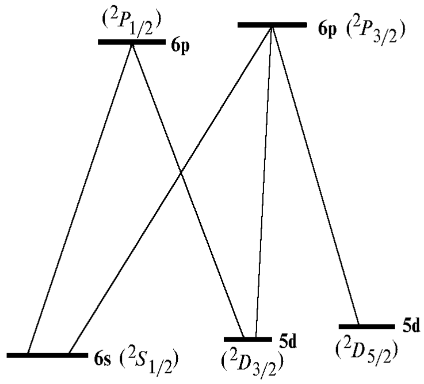

FIG. 1. Energy level diagram of the barium ion.

Let us consider the solution of the obtained Cauchy problem at $t \to \infty$, what corresponds to complete ionization of the atomic component of a cloud and achievement of a stationary mode of the photoexcitation

$$\mathrm{d}N_j/\mathrm{d}t \to 0\ ,\quad j = 1, 2, ..., 5, \quad N_i(t) \to N_0\ . \qquad (3)$$

The set of linear equations obtained in such a way can be easily solved for N_j. For the sunlight intensity[8] and population of the ground and metastable states of the barium ion, it takes the following values:

$$N_1(t)/N_0\,\big|_{t\to\infty} = 0.40867\ ,$$
$$N_2(t)/N_0\,\big|_{t\to\infty} = 0.26186\ , \qquad (4)$$
$$N_3(t)/N_0\,\big|_{t\to\infty} = 0.32946\ .$$

Assuming the Doppler shape of a spectral line, we can find the ratio of the optical depth τ_j to τ_0:

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$$\frac{\tau_j}{\tau_0} = \left(\frac{\lambda_j}{553.5\text{ nm}}\right)^3 \frac{g_j^*}{3g_j} \frac{A_j}{A_{553.5}} \frac{N_j}{N_0}, \quad (5)$$

where λ_j is the wavelength of the ion line; g_j^* and g_j are the statistical weights of the upper and lower ion states, respectively; A_j and $A_{553.5}$ are the probabilities of decay of the excited states for the ion and atomic transitions; N_j is the population of the lower energy level of the ion transition considered. By substituting the parameters of corresponding transitions into Eq. (5), we obtain the following table of the ratios between the optical depths:

TABLE I.

Transition	λ_j, nm	N_j/N_0	τ_j/τ_0
$^2P_{3/2} \to {}^2S_{1/2}$	455.4	0.40867	0.152
$^2P_{1/2} \to {}^2S_{1/2}$	493.4	0.40867	0.077
$^2P_{3/2} \to {}^2D_{5/2}$	614.2	0.32946	0.031
$^2P_{1/2} \to {}^2D_{3/2}$	649.7	0.26186	0.019
$^2P_{3/2} \to {}^2D_{3/2}$	585.4	0.26186	0.004

The tabulated results allow the conclusion to be drawn that at $\tau_0 \geq 30$ the ion cloud becomes dense for sunlight at the wavelengths of 455.4, 493.4, and 614.2 nm. Consequently, when simulating the processes of cloud photoexcitation and glow, radiation transfer at these transitions should be taken into account.

Estimates of optical depths for the atomic transitions, in which the level $^1D_2$ is the lower one (such transitions are most intense), give the values 20 times smaller than τ_0. Such a ratio of the optical depths gives grounds to state that it is beyond reason to account for the radiation transfer at these spectral lines (as well as at other weaker lines) when simulating the process of photoionization of a barium cloud, because their contribution will be negligibly small.

STATEMENT OF THE PROBLEM AND THE METHOD OF SOLUTION

The physical and mathematical formulation of the problem corresponds to that made in Refs. 9 and 10. The main stages of the numerical method and the computational grid are described briefly in Ref. 10. The procedure of a search for a solution to the transfer equation for the selected direction of radiation propagation is based on the method of short characteristics.[11,12] The integral over angular and frequency variables was calculated with the help of the corresponding cubature formulas. This integral accounts for the contribution from the whole cloud into the rate of photoexcitation for the radiation coming to a given point of a medium. This sufficiently complicated quantization procedure for the frequency, angular, and spatial variables allows one to reduce the system of integro-differential equations to the Cauchy problem for a system of standard differential equations for the populations of energy levels of atoms and (or) ions in the considered nodes of the computational grid. Its dimensionality can be reduced significantly with regard for the cylindrical symmetry of the problem. We used IBM PC 486 to perform numerical calculations for different values of the initial optical depth τ_0 of the cloud. The computational FORTRAN 77 program accounts for radiation transfer at the chosen set of atomic and ion lines.

RADIATION TRANSFER AT THE ATOMIC TRANSITIONS

As was noted above, the estimates of the optical depths for the atomic transitions, except for the transition with $\lambda = 553.5$ nm, indicate that a cloud becomes optically dense for sunlight at these transitions at $\tau_0 \geq 30$. Therefore, in simulation of photoionization of a neutral cloud, it would be quite good to consider the processes of radiation transfer at these transitions. To find how strong is their influence upon the dynamics of ionization and glow at the line of 553.5 nm, we have performed corresponding numerical computations. The results obtained give grounds to state that, when included in the model, these transitions do not change markedly the populations of the states and the glow intensity at the line of 553.5 nm. Basically, these results confirm the conclusion about the exclusive influence of sunlight of the 553.5 nm wavelength on the radiative processes under study. This conclusion was first drawn from the simple estimates of the ratios between the optical depths.

DYNAMICS OF PHOTOEXCITATION OF THE ION CLOUD

Let us describe now the results of numerical simulation of the photoexcitation process as applied to the ion cloud. In this case, the radiation transfer is considered simultaneously at the atomic transition (553.5 nm) and three ion transitions (455.4, 493.4, and 614.2 nm).

Figure 2 shows the time behavior of the population of the ground and excited $^2P_{3/2}$ states of an ion, as well as the sunlight intensity at 455.4 and 614.2 nm at those boundary points on the dark side of the cloud, whose numbers coincide with the numbers of curves and correspond to Fig. 1 from Ref. 10. The behavior of the curves in Fig. 2*a* and *b* qualitatively follows the dynamics of changes in ions (cf. with Fig. 2*a* from Ref. 10).

However, two significant differences should be noted. First, the populations of the ground (Fig. 2*a*) and excited (Fig. 2*b*) states may strongly vary in value for different nodes of the computational grid (essentially at the end of the ionization process, when the optical depth of the ion cloud is maximum at the transitions under consideration). Second, their behavior may become non-monotonic with time, see, for example, curves *6* and *7* in Fig. 2*b* (the low maximum arises, which is caused by the competition between the processes of photon absorption and emission).

The calculated data show that population of the excited state $^2P_{3/2}$ depends on the coordinate to a greater degree than the population of the ground state and those of the metastable energy levels, though the overall ion density is the characteristic that is the least sensitive to it. From this it follows that the processes of sunlight transfer in the ion cloud result in a significant spatial inhomogeneity of ions in different states. At the same time, ions weakly depend on the spatial variable. So, this inhomogeneity is caused by the inhomogeneous ionization of the cloud due to the processes of sunlight absorption at 553.5 nm (Ref. 10).

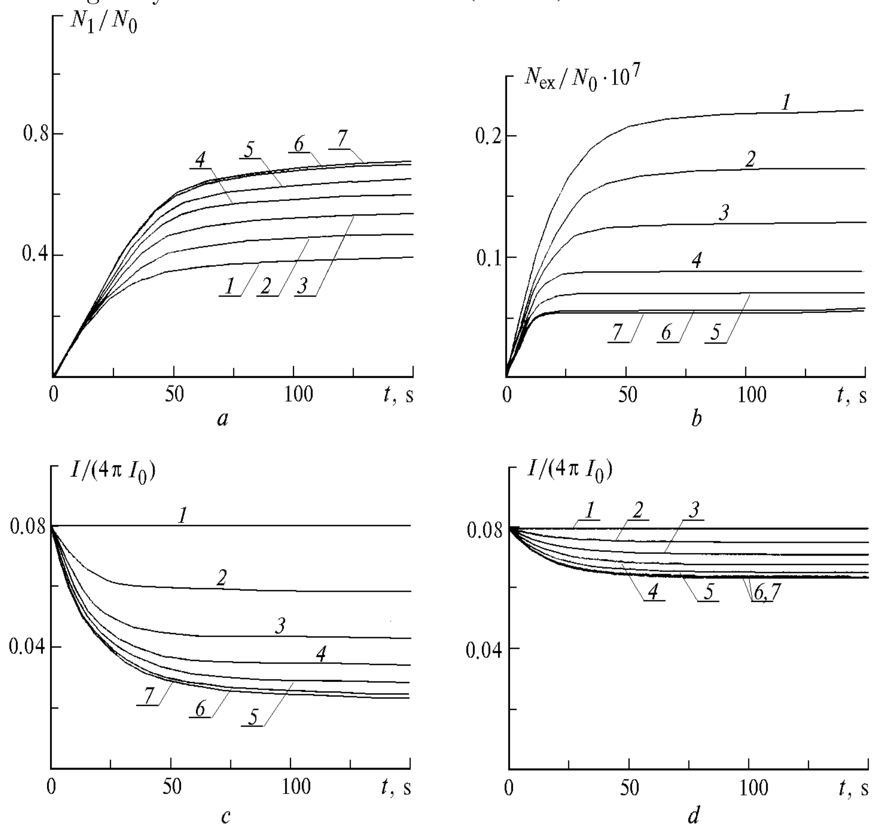


FIG. 2. Time behavior of the populations of the ground (a) and excited (b) states of the Ba *ion and the sunlight intensity in the lines of* 455.4 *(c) and* 614.2 nm *(d) at different boundary points on the dark side of the cloud.*

Thus, the radiation transfer in an ion cloud has a strong effect on the spatial distribution of ions being in different states. This is also confirmed by the computed results obtained in the case, when considering the radiation transfer only at the strongest ion transition with λ = 455.4 nm. The comparative analysis of these results with the results described above shows that the neglect of the radiation transfer processes at 493.4 and 614.2 nm with the same values of the initial optical depth τ_0 gives a significant error in the spatial distribution of ions in different states. The obtained populations may differ by a factor of two and even more. Therefore, when describing the processes of photoexcitation and glow of the ion cloud, the consideration may not be restricted to radiation transfer at only one most strong transition. This fact can be explained by small difference between the optical depths of the ion transitions as compared to the atomic ones.

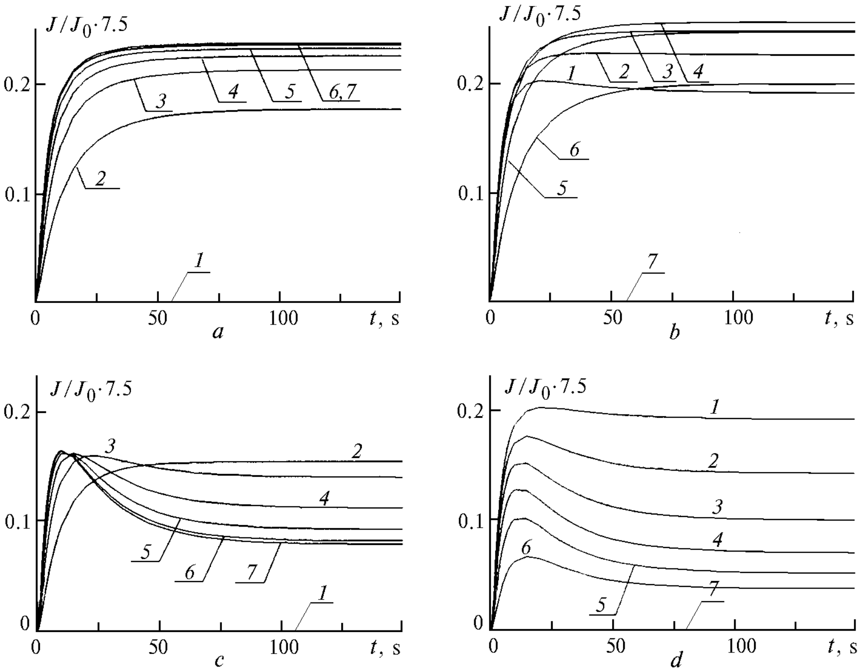
The intensity of sunlight passing through the cloud also strongly depends on the point of exit (Fig. 2*c*, *d*). This dependence is more pronounced for the line of 455.4 nm (Fig. 2*c*) than for the line of 614.2 nm (Fig. 2*d*). Such their behavior is caused by the fact that the cloud is optically more dense for radiation with λ = 455.4 nm than with λ = 614.2 nm. The intensity monotonically decreases with time in all the cases, and the rate of the decrease grows for the exit points which correspond to long optical paths. This decrease in the intensity with time is indicative of the monotonic grow of the optical depth of a path, what does not contradict the dynamics of photoionization of a neutral cloud. The data on the transmitted sunlight also indicate that, in contrast to the atomic cloud, there occurs darkening of the ion component (the radiation intensity decreases), rather than its clearing up.

So, the processes of sunlight transfer in the ion cloud form some spatial distribution of ions in excited states. It is just this distribution that ultimately determines the cloud glow pattern.

GLOW OF THE ION CLOUD

Let us describe the glow dynamics of the ion cloud using the line of 455.4 nm as an example. Figure 3 presents the time behavior of the line intensity at different points and its brightness depending on the observation angle measured from the direction of sunlight propagation. The intensity of radiation scattered at an angle of 180° monotonically increases with time (Fig. 3*a*). It is always higher for the exit points which lie closer to the central cross section of the cloud, than for points which are far from it. For the same exit points, the intensity of radiation scattered at 90° (Fig. 3*b*) has the maxima (see curves *1*, *2*, and *3*). The position of the maximum shifts to shorter time with increasing optical depth of the path. When the radiation exits from the dark side of the cloud (scattering angles less than 90°), the line intensity varies non-monotonically with time, as for the zero angle (Fig. 3*c*). The exception is the curve *2* in Fig. 3*c*. The optical depth of the path is small for this curve, and, consequently, the influence of the radiation transfer processes is weak.

The behavior of the curves in Fig. 3*c* and *d* indicates that the intensity drops by the end of the excitation process, when its value becomes stationary. This is caused by the fact that the optical depth of the cloud becomes maximum by the end of the photoionization, and the glow intensity decreases because of the effects of radiation capture. It should be noted that the position of the intensity maximum for the ion lines shifts along the time scale with increasing optical depth of the path. However, the direction of this shift is opposite to that for the atomic lines. This is caused by the opposite change of the optical dense of the ion cloud, as compared to the atomic one, in the process of photoionization evolution.



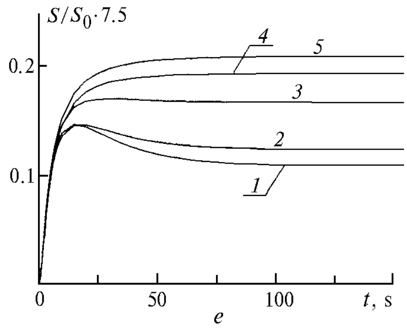


FIG. 3. Time behavior of the glow intensity at 180° *(a);* 90° *on the irradiated side of the cloud (b);* 0° *(c);* 90° *on the dark side of the cloud (d) at different boundary points; and the time behavior of the brightness of the* 455.5-nm *line (e):* 0° *(curve 1),* 45° *(curve 2),* 90° *(curve 3),* 135° *(curve 4), and* 180° *(curve 5).*

The intensity of radiation scattered at 493.4 and 614.2 nm behaves similarly. However, the effects associated with radiation propagation are less pronounced at 493.4 and 614.2 nm, because the optical depth of the cloud in the corresponding spectral ranges is less than at 455.4 nm. The contribution of these lines into the formation of the field of glow at the line of 613.2 nm is especially small, what is most clearly seen in the angular dependence of the intensity.

Figure 3*e* shows the dynamics of the glow brightness of the cloud in the 455.4 nm line at different scattering angles. As seen, the brightness changes non-monotonically for scattering angles from 0 to 90°. The maximum is observed, whose position shifts to shorter time with the decreasing scattering angle. At the scattering angles corresponding to the points of radiation exit on the irradiated side of the cloud, the brightness monotonically decreases with time, reaching its maximum at the end of the photoexcitation process. It is worth noting the fact that the brightness of glow at 455.4 nm takes a stationary value at the end of the process for all the scattering angles; and the greater is the scattering angle, the higher is this value.

The important characteristic of the process of radiation scattering by the cloud is the angular dependence of radiation intensity, which is shown in Fig. 4 for the lines at 455.4 and 614.2 nm at different time. We can see from the comparison of the data shown in Fig. 4 that at practically all stages of ion photoexcitation, except only for the short initial interval (curve *1*, Fig. 4*a*), the scattering is anisotropic for radiation at 455.4 nm and practically isotropic at 614.2 nm (slight anisotropy is observed only by the end, curves *4* and *5*, Fig. 4*b*). It follows from Fig. 4*a* that anisotropy of scattering at 455.4 nm becomes more pronounced as photoexcitation of the ion cloud evolves (curves *2*–*5*, Fig. 4*a*). It is pertinent to note here that the anisotropy of scattering at 455.4 nm is lower than that in the atomic line of 553.5 nm wavelength. Besides, the frame-by-frame pattern of the anisotropy evolution for the ion lines looks like the back-time compared to that for an atomic line (compare Fig. 4*a* with Fig. 5 from Ref. 10).

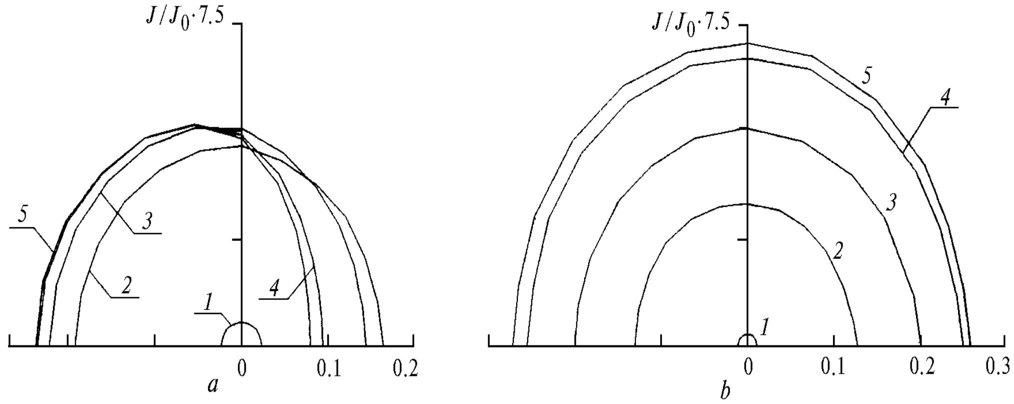
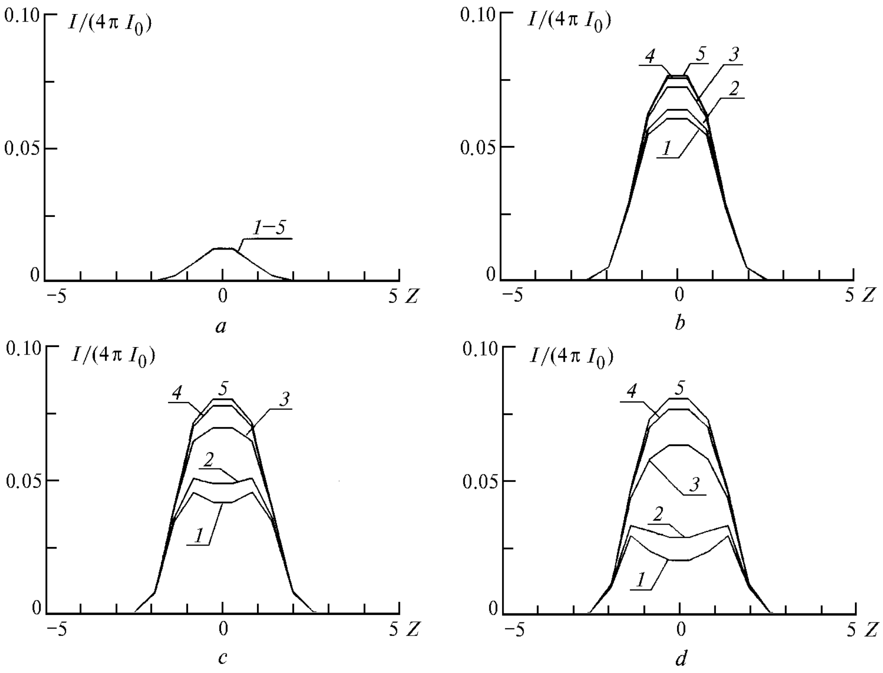


FIG. 4. Angular dependence of the glow intensity at 455.4 nm *(a) and* 614.2 nm *(b) at the time:* 1 s *(curve 1),* 10 s *(curve 2),* 20 s *(curve 3),* 50 s *(curve 4), and* 100 s *(curve 5).*



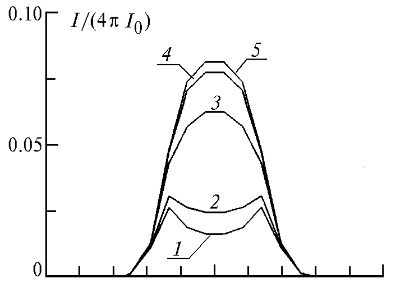


FIG. 5. The shape of the glow line at 455.4 nm *for different scattering angles:* 0° *(curve 1),* 45° *(curve 2),* 90° *(curve 3),* 135° *(curve 4), and* 180° *(curve 5);* $Z = (\nu - \nu_0)/\Delta\nu_D$ *at the time:* 1 s *(a),* 10 s *(b),* 20 s *(c),* 50 s *(d), and* 100 s *(e).*

Numerical simulation allows us to follow the dynamics of the glow line shape. This information is very useful, because it may tell something about the physical processes in such clouds. Figure 5 depicts the time behavior of the frequency dependence of the glow intensity at 455.4 nm for different scattering angles.

The results obtained evidence that the ion cloud is optically thin for 455.4-nm-wavelength radiation in the beginning of the photoionization process. This follows from the coincidence of the profiles of the glow lines for the scattering angles shown in Fig. 5*a*. This means that scattering at that time is isotropic at all frequencies of the absorption contour. As the ionization evolves, the lines corresponding to different scattering angles take different shapes.

This difference is most distinct at the central frequencies of the line profiles. For the scattering angles less than 90° we can see a dip at the central frequencies of the line profiles (curves *1* and *2*, Fig. 5*c* – *e*). This is a manifestation of the effect known as self-reversal of spectral lines. It is absent at other angles (curves *3* –*5*, Fig. 5). The appearance of the dip testifies that the medium is optically dense for radiation with a given frequency. The analysis of the line shape on the dark side of the cloud clearly shows that the ion cloud becomes denser as the photoionization evolves, because the dip becomes deeper. This circumstance can be used when constructing a qualitative pattern of the cloud density evolution.

The shapes of lines at 493.4 and 614.2 nm wavelengths change similarly in time. However, the above-described dependence is less pronounced for them than for the line of 455.4 nm wavelength due to small values of the medium optical depth at these wavelengths. As follows from analysis of the results obtained, the processes of radiation transfer at 455.4, 493.4, and 614.2 nm wavelengths are of a great importance in the formation of the glow line shape. Consequently, they govern the spatial distribution of excited ions and the radiation scattered by the cloud at these wavelengths.

In summary, let us formulate the main conclusions based on the results of computer simulation of the photoexcitation and sunlight scattering by a barium cloud.

1. The radiation transfer at the atomic Ba transitions, for which the level $^1D_2$ is the lower one, has practically no effect on the dynamics of cloud photoionization and glow at 553.5 nm.

2. The dynamics of photoexcitation and glow of the ion cloud at the initial value of its optical depth $\tau_0 \geq 10$ strongly depends on the processes of radiation transfer in the ion lines of 455.4, 493.4, and 614.2 nm wavelengths.

3. The anisotropy of sunlight scattering by the ion and atomic clouds evolves in the opposite directions with time.

4. Analysis of the shape of the ion lines' profiles confirms that the effects of radiation capture play a decisive part in the formation of spatial distribution of the excited ions, which determine the pattern of the cloud glow.

5. The results computed are in a close qualitative correspondence with the experimental data available.

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