REVIEW OF METHODS OF CALCULATING THE FIELD IN OPTICAL CAVITIES AND CHOICE OF CALCULATION METHOD FOR FREE-FLOW CHEMICAL LASERS

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1. INTRODUCTION

Of particular importance in the design of laser systems aimed at energy transmission over large distances is the task of shaping an output beam having a small angular divergence. It is known from the theoretical and experimental studies elucidated, for example in monographs [1, 2], that in a laser with a high-gain active medium it is advantageous to use unstable cavities that permit us, if the medium is of good quality, to obtain radiation having an angular divergence close to the diffraction limit [3-7]. This is ensured by a number of properties of an unstable cavity, which were pointed out already by Siegman [8]: 1) large mode volume; 2) natural selective discrimination of the angular modes; 3) possibility of using totally reflecting optical systems to extract the radiation and to organize the feedback.

Solution of the general problem of producing high-efficiency laser systems calls for research into the choice of the optimal cavity design, aimed also at studying the influence of the spatial inhomogeneity of the active medium on the character of the laser emission [9-18]. Understandably, in the general case it is more effective to carry out the investigation by numerical means. This reduces in essence to the self-consistent problem of the mutual influence of the field in the cavity and the physicochemical processes that form the active medium. In the case of a cw chemical HF laser, the pertinent calculations are made complicated by the multilevel character of the excitation of the working molecules, and also of the substantial role of the effects of mixing of a large number of chemically active jets.

Undoubtedly the most general and rigorous mathematical model for the calculation of the magnetic field in a cavity should be taken to be the system of Maxwell equations and, for an active medium, the Navier—Stokes system of equations with allowance for physicochemical kinetics. This method, however, is too complicated and laborious in practice. We must therefore choose simplified approaches by starting from the specific features of the problem.

The scientific literature has described by now a wide spectrum of computation methods that have become classical and are contained in textbooks and monographs [1, 2, 19-27]. The choice of the method must therefore be justified on the basis of the aims pursued and the problems to be solved.

An advantage of analytic methods [1, 2, 28-43] is that they make it possible to obtain the solution in the most general form and to understand its physical meaning. Final analytic solutions, however, are frequently attainable only in some particular or limiting cases. Therefore, if specific numerical results are needed, computer methods turn out to be more useful.

The known published numerous geometric-optics [1, 2, 20, 25, 44-56], ray-matrix [1, 23, 57-64], opticogeometric [65-70], etc., methods, including the eikonal method [21, 24, 71-72], while relatively simple and sufficiently effective for the solution of a definite group of problems, can nevertheless not represent in the general case completely the phase structure of the radiation field in a cavity with a free-flowing optically inhomogeneous medium. Principal attention is therefore paid in this review to the description and mutual comparison of various methods of wave optics [73-163] and also to methods of calculating active-medium characteristics [164-198], aimed at choosing a working method of solving complex comprehensive problems of the ratio of the parameters of a cw HF chemical laser with an unstable telescopic cavity, so as to improve the directivity pattern of its radiation.

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2. METHODS OF DESCRIBING AN ELECTROMAGNETIC FIELD

As noted in the Introduction, the most consistent approach to the study of the posed problem can be based only on wave-optics methods. They can be arbitrarily divided into two main groups: 1) methods using the solution of integral equations that serve as a scalar expression of the classical Huygens–Fresnel principle on the basis of the known Fresnel–Kirchhoff integral [1, 2, 73-99]; 2) methods using the solution of partial differential wave equations for the electromagnetic field [27, 100-153]. These two groups of methods, while outwardly different, are closely related, as indicated already in [31, 32], since all are different mathematical forms for expressing the physical nature of one and the same phenomenon. Let us consider briefly the gist of these methods and compare their main advantages and shortcomings, so as to make a well-founded choice of the working method.

2.1. Methods Based on the Fresnel–Kirchhoff Integral. An integral method was developed by Fox and Li and first used in a paper [73] that can be regarded as pioneering in investigations for the field structure in a cavity. According to this method, if the mirror dimensions greatly exceed the radiation wavelength (λ), and if the electric and magnetic field vectors vary in a plane almost perpendicular to the field propagation direction, the complex function of the field of a surface B illuminated by a surface A is expressed in terms of the surface integral

$$\mathcal{E}_B = \frac{ik}{4\pi}\int_A \mathcal{E}_A e^{-ikr}\frac{1+\cos\theta}{r}\,ds_a, \tag{1}$$

where $\mathcal{E}_{A,B}$ is the complex amplitude of the field on the corresponding surface, r is the distance between the radiation point and the observation point, θ is the angle between the vector $\vec{r}$ and the normal drawn to the surface of the point through the radiating point, $k = 2\pi/\lambda$ is the wave number, and ds_a is an element of the radiating surface. If the control surfaces are taken to be the cavity-mirror surfaces, one can expect the following static field distribution to set in after a certain number q of reflections from each of the mirrors

$$\mathcal{E}_q = (1/\gamma)^q G, \tag{2}$$

where G is the field distribution and does not vary from reflection to reflection, while γ is a complex constant independent of the coordinates. Substitution of (2) in (1) yields an integral equation of the form

$$G = \gamma\int_A KG\,ds_a \tag{3}$$

with a kernel $K = (ik/4\pi r)(1 + \cos\theta)e^{-ikr}$. The field distribution function G, which satisfies Eq. (3), is taken as the transverse mode of the cavity, defined on the mirror surface, while the complex coefficient γ, which incorporates the gain of the signal and the phase shift per pass, is called the propagation constant of this mode. The integral equation (3) is solved numerically by successive approximations, and this is the gist of the method of Fox and Li.

Undisputed advantages of the integral method are the simplicity and clarity of its mathematical formulation and the good adaptivity to arbitrary mirror configurations. The method has maximum economy from the point of view of consumed computer memory, since it requires knowledge of the field distribution only within the limits of the radiation-source aperture.

The integral method was widely used approximately up to the mid-1970s [73-80] as the only numerical method for the solution of cavity problems in a rigorous formulation, without the need for any significant simplifications. It gave way then to no less rigorous but more effective methods. The integral method is ineffective because it requires $\sim N^4$ computation operations for each transfer, from one surface to another, of a field described by an $N \times N$-point matrix of discrete values. Nonetheless, it continues to be used in recent work [37, 81-85] in cases when the use of other methods is difficult, and since its undisputed accuracy has caused it to be included among the standards.

It was used for extensive investigations of the mode structure of a field and of the influence exerted on the mode by various misalignments of the mirrors, both for stable [73-75] and unstable [76-80] cavities. Not being very effective, the integral method was used mainly in a two-dimensional formulation, but was used in [80] to calculate the mode structure

of a field in an empty three-dimensional unstable cavity. This method was even used in [75, 79] to solve the problem of self-consistency of the interaction of a field with an amplifying saturating medium.

An important trend in the development of the integral method was the Prony method, the gist of which was to expand the solution G of integral equation (3) in competing transverse modes G_k

$$G = \sum_k \gamma_k G_k, \tag{4}$$

each of which has its own propagation constant λ_k. This made it possible to investigate the behavior of the losses of each transverse mode separately, and to show that these modes replace one another alternately to assume the role of the fundamental highest-Q mode.

In the case of a cylindrical coordinate system the solution can be sought in the form of an expansion of the field in Bessel functions [88]. That paper contains an interesting reference to a report by Siegman [89], in which it is proposed to expand in Hankel rather than Bessel functions, since the former permit the use of the last Fourier transformation (FFT).

One of the most successful approximate methods of calculating the field in a cavity by solving an integral equation is assumed to be that developed by Paul Horwitz for an empty symmetric unstable cavity with rectangular mirrors. According to this paper, the integral equation (3), assuming the total-reflection mirror to be infinite, reduces to an equation of the form

$$\gamma v(x) = \sqrt{iN_f} \int_{-1}^{1} e^{-i\pi M N_f (y - x/M)^2} v(y)\, dy, \tag{5}$$

in which are used the traditional expressions introduced in Siegmann's papers on unstable cavities [45, 76]

$$v(x) = \mathfrak{G}(x) e^{i\pi N_{ef} x^2}; \quad N_{ef} = N_f \sqrt{g^2 - 1} = \frac{N_f}{2}\left(M - \frac{1}{M}\right);$$

$$M = \frac{\sqrt{g+1} + \sqrt{g-1}}{\sqrt{g+1} - \sqrt{g-1}}; \quad g \equiv 2g_1 g_2 - 1; \quad N_f = \frac{a^2}{\lambda L} / (2g_2);$$

$g_i = 1 - L/R_i$; R_i – mirror curvature radii.

The gist of the method is that the integrand in (5) is expanded in terms of the small parameter $\tau = (\pi M N_f)^{-1/2}$ in the limit as $N_f \to \infty$. The expansion extends to terms of order $1/N_f$ and includes, besides the term corresponding to the geometric-optics approximation, also the terms that describe the effects of diffraction by the edges of the feedback mirror. Although the method was developed for large Fresnel numbers, its results are in sufficiently good agreement with those obtained by direct solution of the integral equation even at low values of the Fresnel numbers, all the way to ~1.

The asymptotic method was further developed by Paul Horwitz himself, who somehow was unable to present a physical interpretation of his brainchild. This was accomplished later by Butts and Avizonis, as well as by others. In [91], for example, was considered a two-dimensional misaligned cavity; in [92] the Horwitz method was extended to include a three-dimensional symmetrical cavity; while in [93-96] the elements of this method were extensively used to develop a theory of an unstable cavity with an active medium. The interest attached to asymptotic theory at the present time [97] points to its large potential and promise, especially in calculations for large-aperture cavities.

An advantage of Horwitz's method is that the problem, typical of the eigenvalues of a matrix, which is a feature of the integral method, is replaced by the problem of finding the roots of the polynomial, so that the computation is substantially accelerated. A shortcoming of the method is that it is difficult to adapt to complicated boundary and intracavity conditions, since the analytic expressions become then too cumbersome and nonuniversal, and also that its results agree less with the "exact" solutions of the "brute force" methods, apparently because the asymptotic expansion is crude.

Noteworthy among the methods using expansion of the integrand of Eq. (3) is also a method proposed by Siegman and Sziclas [98] for unstable three-dimensional cavities (UTC). The expansion in this method is in Hermite–Gauss polynomials, which are eigenfunctions of the field in stable cavities [28-30]. The method was developed and used for a numerical calculation for a UTC with the free-flowing optically inhomogeneous medium of a CO_2 laser.

The speed of this method turned out to be approximately the same ($\sim N^3$ operations per field-propagation act) as of the method of direct integration of a parabolic wave equation, using the explicit difference schemes to be discussed below. It was therefore possible to determine by this method the mode structure of the field only for cavities with Fresnel numbers on the order of several units. For large Fresnel numbers, this method calls for retention of a large number of expansion terms and, apparently due to its sluggishness, cannot compete with the more consistent finite-difference method, judging from the exceedingly scanty number of succeeding publications, e.g., [99].

2.2. Methods Based on Solution of Wave Equations. Another trend in the evolution of methods of field calculation in cavities is based on describing the field by differential wave equations directly derived from suitably simplified electrodynamics equations [36, 100]. A direct solution of the Maxwell equations is very complicated and unjustified for cavity problems, in which one can successfully use what is known as the paraxial approximation [36]. This implies small angles of the beams with a certain general direction of their propagation, and also a large excess of all the linear dimensions of the optical system over the radiation wavelength.

Differential equations permit solution of the problem in the most general form, for example with allowance for the temporal nonstationarity and spatial distribution of the dielectric constant of the medium [101-108]. For stationary problems, however, most frequent use is made of a wave equation of the form [100, 114]

$$\pm i\frac{\partial \mathcal{E}^{\pm}}{\partial z} = \frac{\nabla_{\perp}^2 \mathcal{E}^{\pm}}{2k} \pm k\left(\frac{\Delta n}{n_0} - i\frac{g-\rho}{2k}\right)\mathcal{E}^{\pm}, \tag{6}$$

where $\mathcal{E}^{\pm}$ are the complex amplitudes of the field of the forward and backward waves; $\nabla_{\perp}$ is the Laplace operator with respect to the transverse coordinates; $\Delta n = n - n_0$ is the deviation of the refractive index from its mean value; g and ρ are the gain and absorption coefficient of the medium, respectively; and $k = 2\pi/\lambda$ is the wave number.

Direct integration of the wave equations was used mainly in the two-dimensional [100, 109-114] formulation, but also in the three-dimensional one [27, 115-117], to investigate the influence of optical inhomogeneities and of active-medium (AM) saturation effects on the characteristics of the radiation field in the near and far zones. This method was used to investigate amplifying single-pass [100, 109] and multipass [113] systems, as well as UTC [110-112]. The appropriate method used together with the AM model: of a solid-state laser [111], of a fast-flowing medium of a CO_2 gasdynamic laser (GDL) [109, 117] with allowance for density discontinuities in the flow [116], and also of the quasi-two-dimensional multilevel medium of an HF cw chemical laser (CCL) [112, 113]. Use was made here of both simplified AM models [110, 111] and of models that take into account real pumping mechanisms [109, 112, 113, 116, 117]. Questions involving the correction of the phase front of a beam thermally spreading in an absorbing medium were considered in the framework of this method in [115].

In the papers cited above the field inside the cavity is represented as a rule by a superposition of two counterpropagating fields connected on the mirror surfaces with allowance for the laws of reflection and the change of the form of the wave front. The problem is solved as a rule by a method using the Fox–Li iteration scheme [73]. The parameters of the medium and of the field are made self-consistent in the approximation of relatively sparse thin layers, in which are concentrated all the properties of the AM, and the propagation of the field between the layers is assumed to be similar to its propagation in free space [116, 117], i.e., is described by a parabolic wave equation of the type

$$\left[2ik\left(\frac{\partial}{\partial z}\right) + \nabla_{\perp}\right]\mathcal{E}^{\perp}(x, y, z) = 0. \tag{7}$$

The description of the field in the cavity with the aid of differential equations makes possible the use of curvilinear spatial coordinates and of computation grids with variable

mesh, and also highlights the advantages of this method, such as rigor and generality of the approach, good adaptivity and flexibility of the numerical algorithms that realize it (in the sense of their possible application under a large group of boundary conditions), and effective use of a possible symmetry of the problem.

The speed of calculations in the integration of the wave equation is higher by an order of magnitude than when an integral equation is solved. Thus, for a single act of field propagation from layer to layer it is necessary to perform $\sim N^2 \times N_Z$ operations for one and the same matrix with $N \times N$ points. The number N_Z of trial steps needed for this purpose along the principal direction of radiation propagation depends on the distance between the layers and also on the employed finite-difference scheme.

The use of implicit schemes [112, 117] makes it possible to increase substantially the longitudinal pitch of the integration, and also to lower the sensitivity of the numerical algorithm to abrupt discontinuities of the field function on the edges of the mirrors, which calls frequently for artificial amplitude smoothing of the edges. The latter can lead to a substantial smoothing of the obtained solutions through suppression of the converging wave in the UTC. Finite-difference methods require also additional broadening of the computation grid to ensure correctness of the boundary conditions $\mathcal{E}(\pm\infty, z) = 0$.

The increased computation speed notwithstanding, complete realization of the method of numerical integration of the wave equation, just as of the integral method, requires high-power computation technology, not yet attainable here or abroad, and it is necessary to operate at the limit of the available resources. It is indeed the need to "extricate ourselves" on account of the great decrease of the number of computation points that explains the crude character of the three-dimensional solutions obtained in [116, 117] for large Fresnel numbers. Head-on numerical solutions of three-dimensional complex problems in the context of this method are therefore as yet difficult for technical reasons.

The large technical difficulties encountered in a direct numerical integration of wave equations have always served as a strong stimulus for the development of approximate solution methods. An exact solution of a wave equation is frequently sought only in the region near the cavity axis [28-30, 49], while the peripheral part is considered as a multipass amplifier, frequently in the geometric approximation (combined methods).

A simple and lucid diffraction method of calculating the mode structure of the field in an empty cavity was proposed already at the dawn of laser research by Vainshtein [19]. In this theory the cavity is regarded in the transverse direction as an open waveguide in which differently propagating modes (usually called waveguide functions, which are solutions of the wave equation for the field between infinite mirrors) are interconnected at the discontinuity point corresponding to the edge of the mirror. This method, quite extensively used in the 1960s in calculations for stable and planar cavities, for example in [118], was subsequently developed by Lyubimov et al. [119, 120] and also by Felsen et al. [121-123] as applied to unstable cavities. From among the later publications, in which the open-waveguide method was used (qausioptical approximation), one can cite a paper [124] devoted to an investigation of lens-like phase distortions of the field in a misadjusted cavity. A shortcoming of this method is that it is suitable for the calculation of only empty cavities, since it takes no account of the distribution of the gain over the volume of the active medium.

To solve wave equations, just as integral ones, one frequently resorts to a preliminary expansion of the field function in terms of some previously selected system of eigenfunctions, and a corresponding transformation operator is applied directly already to the expansion terms, followed by a reverse convolution into a single solution. While these methods may be no less accurate than direct integration methods, they must still be regarded as approximate, since one always encounters the problem of a reasonable limitation of the expansion spectrum. Included among these methods is that of Suchkov, used in papers cited above [101-107], according to which the solution of the nonstationary wave equation is sought in the form of a series of eigenfunctions that satisfy this equation and the boundary conditions, while for the complex amplitudes, which are time-dependent expansion coefficients, there is obtained a system of numerically solvable equations. Unfortunately, however, this method has so far been used only in a formulation that is one-dimensional in the coordinates.

As already noted, the method of expansion in Hermite–Gauss polynomial proposed by Siegmann and Sziclas, is not widely used. On the other hand, their other attempt [125] to develop an effective method of the UTC field calculation was indeed brilliantly successful and revo-

lutionized the development of cavity calculations. We refer here to the method of expanding the field function in plane waves and using for this purpose the FFT procedure [199-202], which made it possible to lower by one more order of magnitude the number of computation operations needed to implement a single act of field transport over an arbitrary distance, to a value $\sim N^2 \log_2 N$ for a two-dimensional $N \times N$ matrix. Postponing the detailed description of this method, we note that its high efficiency attracts great attention to this day [126-153]. A characteristic feature of its use is the ever greater complexity of the problems that it can treat, i.e., the shift of the center of gravity to investigations, jointly with the cavity, of such processes and phenomena which are either complicated problems by themselves, or place the cavity under conditions that are extremal for the calculations. All this is made possible by the fact that the calculation of the radiation-transport itself ceases to be decisive in the sense of the consumed time. Therefore, in addition to traditional calculations of the mode structure of empty UTC and those filled with ideal active medium [125, 127, 132, 136, 149, 150, 153], which have more readily a control-and-test character, UTC with more realistic AM models are considered, with account taken of the characteristic features of free-flow gas media of CO_2 lasers [125, 130] and, in particular, HF-CCL [131-135]. Also investigated was the effect exerted on the operation of a UTC by such perturbing factors as its misalignment [127] and distortion of the field on mirrors with nonideal surfaces [136], the presence in AM of large-scale [125, 131, 132] and small-scale periodic [126, 128, 129] and random [142, 148] phase inhomogeneities, as well as various methods for their compensation, including the use of intracavity adaptive optics [137, 138, 152] and the use of pseudowave front reversal (pseudo-WFR) methods [145-148]. The FFT method was used to study cavities with strong configuration of the mirrors [151] or of the cavity itself [137, 138, 152], while in [141] the FFT method was invoked to solve problems involving visualization of the flux by the phase-contrast method.

The FFT method, however, is likewise not free of shortcomings of its own. Its precision, while not worse than that of the integral method, calls for sufficient accuracy in its use, dictated by the singularities of the discrete Fourier transformation. It is possible, for example, to use in the calculations only a rectangular uniform grid and vary the number of its nodes only by multiplying by an arbitrary power of the number 2. This entails the same dependence of memory and computer-processing time loss on the dimensionality of the problem, and comes particularly into play if many computation points must be used. A rectangular grid hinders the exact description of curvilinear boundaries, for example of round mirrors [125, 132] or apertures in them [151]. The method can likewise not be regarded as effective when it comes to a field-function definition region that must include appreciable "empty" protective sidebands, where there is practically no field, but which are essential to ensure calculation accuracy and sufficient resolution of the space–frequency spectrum of the radiation. Attempts are therefore made to use other Fourier-transform algorithms, for example the continuous one [150], which makes it possible to obtain, on account of the nonuniform distribution of the computation points, the same accuracy with a smaller number of points, but at the expense of the operating speed.

A shortcoming of the FFT method, more accurately of all the wave-optics methods, is the rather crude simulation of the interaction of the field with the AM in the approximation of large-mesh amplitude–phase screens. Indeed, on the one hand each screen should have a sufficiently detailed distribution over the transverse coordinates (in principle, the same as the field itself) and, on the other hand, the very number of the screens should be sufficient to follow up with specified accuracy the variation of the field as it goes through an extended amplifying or inhomogeneous medium. Just as in any other numerical method, the accuracy problem can in principle be solved by increasing the number of computation points, but since the calculation of the functions of these screens consumes the bulk of the computer time and memory, it becomes necessary, even if the FFT method is used, to employ all the possibilities, and sometimes also forego accuracy within reasonable limits so as to reduce the number and sizes of the screens to a minimum determined by the technical characteristics of the employed computation technique.

Concluding the survey of methods of computing the field in a cavity, we wish to note two more nontraditional methods, discrete-ray [154] and statistical [155-163]. The only publication in which the first of these methods was used, in a three-dimensional formulation, to compute the field in the cavity of an optically pumped solid-state laser, attests to the fact that it did not attract much attention, being apparently too unwieldy. It is curious nonetheless, since it is similar to the method of "large particles" in gasdynamics, i.e.,

it uses Lagrange variables to describe the generated radiation. To this end, the active body of the cavity is broken up into $N_\varphi \times N_r$ parts in cross section and N_z parts in length. The noise radiation of each elementary volume at the generation frequency is simulated by rays uniformly distributed over a unit sphere. Each ray consists of N_f averaged "photons," constituting radiant-energy fractions that propagate in the direction of the corresponding ray, and characterized by an initial energy and coordinates and directions vector. It is assumed that the "photons" move for some time t without interacting with one another and with the medium, after which their new coordinates are determined and the average energies of the "photons" landing in one and the same elementary volume are given, with allowance for the properties of the medium and for the boundary conditions. The averaged characteristics of the "photons" should, by assumption, correspond to the parameters of the radiation field in the corresponding region of the active medium at the current instant of time. The process is then repeated. We see that the method is suitable for optically dense media and for nonstationary processes. It is, however, very cumbersome and laborious, inasmuch as sufficient accuracy of the local parameters calls for sufficiently extensive statistics of the "photons" in each elementary volume, the number of which must also ensure the required accuracy of the spatial distribution of the local parameters.

The second of the above methods is aimed mainly at determining the radiation directivity pattern of a cavity with a medium containing small-scale phase inhomogeneities. It is based on averaging over the realizations of these inhomogeneities and on a determination of what is known as the field coherence (correlation) function, knowledge of which suffices to determine the angular distribution of the laser-emission intensity. After its publication [155, 156] the statistical method was developed by Lyubimov [157-160] for the calculation of the modes in an unstable cavity. A generalization of this method to include spatial confinement of light beams, and the determination of the validity limits of the geometric approximation to determine the coherence function of the field in an unstable cavity was carried out by Sherstobitov et al. [161-163]. The statistical approach should apparently be regarded as the most promising way of finding and analyzing the laws governing the establishment of coherent radiation in cavities, under the condition that it take into account also temporal nonstationarity of optical inhomogeneities [43].

2.3. Fast-Fourier-Transform Method. We present in this section a brief exposition of the methodological part of the known paper of Sziclas and Siegmann [125], in which the FFT method is described in detail. Its complete analog can also be regarded to be the method part of [132].

Figure 1 shows schematically a UTC and the associated coordinate frame, as well as its main geometric parameters. We assume the X axis is directed along the AM stream, and the Z axis is directed along the optical axis of the cavity, from the convex to the concave mirror; in the case of a confocal cavity we have $z_0 = r/2$, where r is the curvature radius of the convex mirror.

In full accord with the procedures of the papers cited above, the inner volume of the cavity is segmented and the principle of separating the physical processes is used. The interaction of the UTC radiation field with the AM is modeled in the application of the thin active layers or amplitude–phase screens (APS), which are complex functions of the transverse coordinates and describe the integral action of the entire material layer that they replace. The APS have the form

$$F_z(x, y) = \left[\frac{\bar{g}(x, y)}{2} - ik\Delta\bar{n}(x, y)\right]\Delta z \qquad (8)$$

where $\bar{g}$ is the gain averaged over the thickness Δz of the AM, and $\Delta\bar{n}$ is the deviation of the refractive index from its mean value, likewise averaged over the active-layer thickness. The cavity mirrors can also be regarded as APS that take into account the curvature, shape, and reflectances of their surfaces.

The propagation of electromagnetic waves between the screens is regarded as similar to their propagation in free space. This means that the complex wave amplitude u(x, y, z) in the regions between the screens is a solution of the wave equation in the paraxial approximation [36]

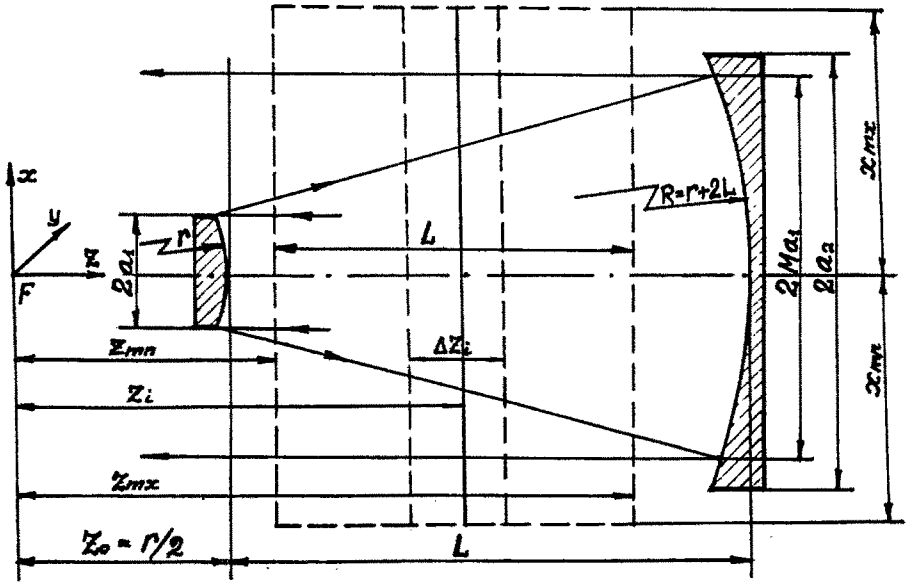


Fig. 1. Computation scheme for a UTC filled with an amplifying medium and with symmetric bilateral extraction of radiation.

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 2ik_0 \frac{\partial u}{\partial z}, \tag{9}$$

the solution of which can be written in the form of a product of a slowly varying traveling-wave complex amplitude $\mathcal{E}(x, y, z)$ and a rapidly oscillating factor

$$u(x, y, z) = \mathcal{E}(x, y, z) \exp\left\{i\omega t - ik_0 z\right\}, \tag{10}$$

where $k_0 = 2\pi/\lambda$ is the wave number and ω_0 is the cyclic frequency of the light.

Let $\mathcal{E}_0(x, y)$ be the field distribution in the plane of one of the screens. It can be represented by an integral over the spectrum of the spatial frequencies

$$\mathcal{E}_0(x, y) = \iint P_0(\nu_x \nu_y) \exp\left\{-i2\pi(\nu_x x + \nu_y y)\right\} d\nu_x d\nu_y. \tag{11}$$

The distribution over the spatial frequencies ν_x and ν_y is determined in turn by the expression

$$P_0(\nu_x, \nu_y) = \iint \mathcal{E}_0(x, y) \exp\left\{i2\pi(\nu_x x + \nu_y y)\right\} dxdy. \tag{12}$$

Each space–frequency component (ν_x, ν_y) corresponds to a plane wave

$$\exp\left\{-ik\vec{r}\right\} = \exp\left\{-i2\pi\nu_x x - i2\pi\nu_y y - ik_z z\right\}, \tag{13}$$

where $(2\pi\nu_x)^2 + (2\pi\nu_y)^2 + k_z^2 = k_0^2 = (\omega/c)^2$.

The component Z of the wave vector of each plane wave can be written in the Fresnel approximation:

$$k_z(\nu_x, \nu_y) = \sqrt{k_0^2 - (2\pi\nu_x)^2 - (2\pi\nu_y)^2} \approx k_{0,} - \pi\lambda(\nu_x^2 + \nu_y^2). \tag{14}$$

The space–frequency distribution in the plane of the next screen is defined as follows:

$$P_1(\nu_x, \nu_y) = P_0(\nu_x, \nu_y) \exp\left\{i\pi\lambda\Delta z(\nu_x^2 + \nu_y^2)\right\}, \tag{15}$$

where Δz is the distance between the considered screens. According to (11), the expression for the wave arriving at the next screen is

$$\mathcal{E}_1(x, y) = \iint P_1(\nu_x, \nu_y) \exp\left\{-i2\pi(\nu_x x + \nu_y y)\right\} d\nu_x d\nu_y, \tag{16}$$

and takes after the interaction with the screen the form

$$\tilde{\mathcal{E}}_1(x, y) = \mathcal{E}_1(x, y) \exp\left\{F(x, y)\right\} \tag{17}$$

We have left out of (15) and (16) the factor $\exp(-ik_0\Delta z)$, which is the same for all plane waves arriving at the screen. Expressions (11), (12), (15), (16) are Fourier transforms of the slowly varying complex amplitude of the field. They can be determined from the discrete values of the functions specified at the nodes of the spatial computation grid, using the FFT algorithm [199-202]. Proceeding in this manner from screen to screen we complete a full circuit of the cavity, requiring satisfaction, on the surfaces of the metallic mirrors, of the boundary conditions

$$\sqrt{r}\,\mathcal{E}^+(x, y) + \mathcal{E}^-(x, y) = 0, \tag{18}$$

where r is the mirror reflection coefficient; $\mathcal{E}^+$ is the complex amplitude of the incident wave, and $\mathcal{E}^-$ of the reflected. The procedure described is repeated until agreement, at the specified accuracy, is obtained for two successive field distributions or of the integral of its intensity in the plane of the initial (total-reflection) mirror.

Useful for the calculation of a spherically diverging wave is what is known as the lens or beam transformation of the coordinate frame, specified by the expressions

$$x'(x, z) = ax/z, \quad y'(y, z) = ay/z, \quad z'(z) = \frac{a^2(z - z_0)}{zz_0} \tag{19}$$

where a is an arbitrary scale factor. Choosing it in the form $a = z_0 + L$, we specify a coordinate transformation that converts divering or converging optical beams into equivalent collimated ones with the aperture of the beam exiting from the UTC (Fig. 2).

The wave function u(x, y, z) on the diverging section is transformed in accordance with the expression

$$v'(x', y', z') = zu(x, y, z) \exp\left\{i\frac{\pi}{\lambda z}(x^2 + y^2)\right\}. \tag{20}$$

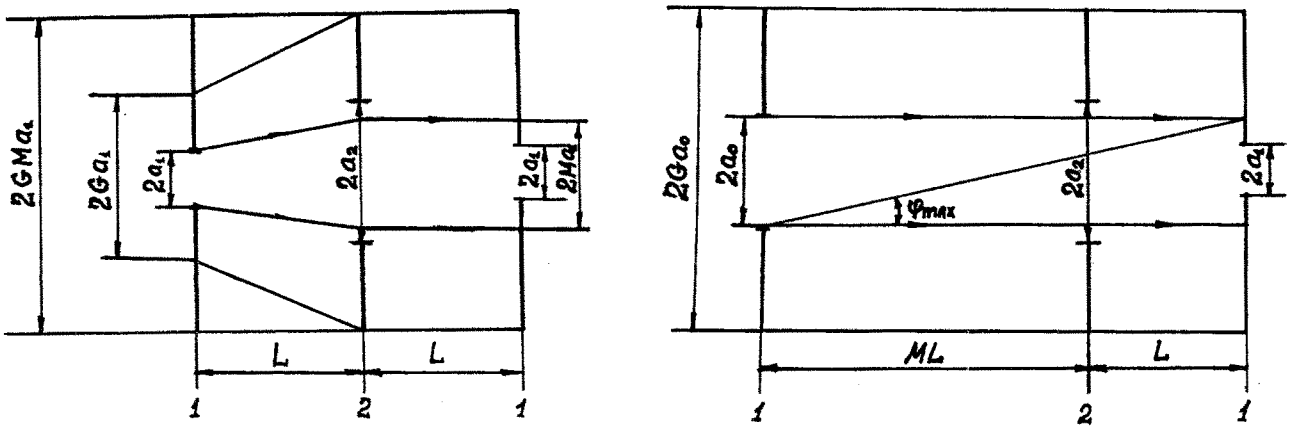
It is easy to verify that the transformed function v'(x', y', z') satisfies the same paraxial wave equation as the initial function u(x, y, z), but now already in a new coordinate space. Consequently, the same Fourier transforms (10)-(16) are valid for it, but in a new linearly diverging coordinate system. Note that the transformation of the wave function (20) takes automatic account of the surface curvature of the mirrors, so that the use of the coordinate transformation reduces the problem to a calculation of an equivalent cavity with planar mirrors. We get then a collimated Fresnel number connected with the traditional number by the relations

$$N = \frac{a^2}{\lambda L}, \quad N_{ek} = N\frac{M - 1}{2}, \quad N_k = N\frac{M^2}{M + 1} = N_{ek}\frac{2M^2}{M^2 - 1}, \tag{21}$$

where M is the coefficient of the geometric magnification of the UTC.

The transformation of the coordinates leads to the need for interpolating between coordinate grids having different scales. This increases insignificantly the volume of the computations, but, on the other hand, the coordinate transformation permits a more effective utilization of the computation grid, and, in particular, a more accurate description of the field distribution over the surface of a convex mirror.

Of great importance in calculations in which FFT is used are problems of false images, of the selection interval in the space–frequency region, and also of the limitation of the aperture of the discrete transformation. Since the use of the Fourier transform presupposes artificial periodic continuation of the field function to the outside of the region in which it is defined with respect to the transverse coordinates, a protective band must be introduced to limit the energy fraction that penetrates by diffraction into neighboring period,



a b

Fig. 2. Elementary optical scheme for the calculation of one cycle of field propagation in a UTC: a) without coordinate transformation; b) with coordinate transformation by a lens.

and vice vera. According to estimates [125] based on consideration of the residual integral of the Cornu spiral that describes diffraction by an abrupt edge of a uniformly illuminated slit of width $2a_0$, the dimension of the computation region should be $2Ga_0$, where the coefficient of the protective band is given by

$$G \geqslant 1 + (2\pi^2 \epsilon N_k)^{-1}, \tag{22}$$

in which ε is the permissible energy fraction penetrating from the considered period into its neighbor.

For a discrete Fourier transformation using a definiton region of width $2Ga_0$ in physical space, the selection in the space–frequency region is effected with an interval $\Delta\nu = 1/2Ga_0$. The largest spatial frequency for a discrete Fourier transform containing N_T points is then

$$\nu_{max} = \frac{N_T}{2}\Delta\nu = \frac{N_T}{4Ga_0}. \tag{23}$$

The number of computation points sufficient for a description of small-scale field pulsations on the edge of the exit aperture, and also to limit to a specified value ε the energy fraction cut off by the spatial-spectrum high-frequency part which becomes redistributed in the low-frequency region, is chosen on the basis of the following estimates. For a uniformly illuminated slit, the space–frequency spectrum described by the function

$$P(\nu) = 2a_0 \operatorname{sinc}(2\pi a_0 \nu), \text{ where } \operatorname{sinc}(x) = \frac{\sin(x)}{x}, \tag{24}$$

contains in the components $\nu > \nu_{max}$ an energy

$$\epsilon = \frac{1}{a_0}\int_{\nu_{max}}^{\infty} |P(\nu)|^2 \, d\nu \approx \frac{2G}{\pi^2 N_T}. \tag{25}$$

Hence

$$N_T \geqslant \frac{2G}{\pi^2 \epsilon}. \tag{26}$$

To take into account the small-scale field pulsations that are produced on the opposite side of the aperture through diffraction by the edge of the exit mirror after a complete circuit through the cavity (Fig. 2), it is necessary to limit the space–frequency spectrum at a frequency not lower than

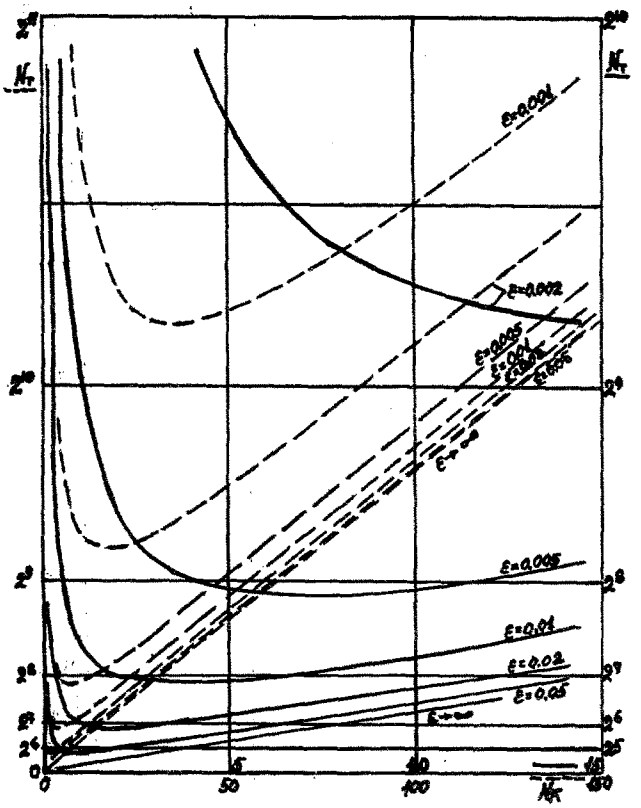


Fig. 3. Dependence of the required minimum of the computation point N on the Fresnel number N_k and on the permissible energy loss ε. Solid line) $0 < N_k < 15$, right-hand ordinate scale; broken line) $0 < N_k < 150$, left-hand ordinate scale.

$$\nu_{max} \geqslant \frac{2Ma_0}{\lambda L(M+1)}, \tag{27}$$

from which it follows that

$$N_T \geqslant 8GN_k \tag{28}$$

The estimate (26) is of great value for small Fresnel numbers, when a major role is played by diffractive spreading of the beam. Relation (28), on the contrary, points to the need of increasing the number of computation points for large Fresnel numbers. Figure 3 shows the total dependence of the needed number of points on the UTC collimated Fresnel number (21). It shows that for a given value of ε there exists an optimal interval of the numbers N_k within which the cavity problem can be solved using a definite minimum number N_T of computation points; it is also seen that for each N_k there exists a minimum N_T needed to obtain the slightest reliable solution at all.

Since the space–frequency spectrum of the Fourier expansion is limited, the weight of the high-frequency harmonics on its edges may be overestimated (the Gibbs effect). To suppress this purely mathematical effect one usually introduces smoothed edges of the aperture window in frequency space [125]. This may also be unnecessary, however, if the role of these small-scale pulsations is small.

3. METHODS OF SIMULATING AN ACTIVE MEDIUM

The determination of the spatial distributions of the amplifying and optical properties in the volume of an AM is the problem that determines the extent to which the simulation of the lasing process as a whole can be realistically simulated and can acquire the characteristic features of an actual type of laser. The choice of the mathematical model of an AM is therefore dictated, on the one hand, by the need for taking into account the various features whose influence on the radiation field is of fundamental character and, on the other hand, by the available mathematical resources that determine the possibility of an adequate

simulation of these processes. It is therefore necessary frequently to seek compromise solutions and it is permissible, in those cases when an exact determination of the energy parameters is unnecessary and their influence on the directivity pattern can be disregarded, to use simplified AM models in which the gain is determined from simple equations [65, 66, 71, 75, 79, 96, 128, 129, 142-148, 151] or from simplified model equations [110, 111].

Extensive use is made in cavity calculation of the model of an ideal or uniformly amplifying medium, where account is taken of the important effect of amplification saturation of the radiation, with a gain g(x, y, z) determined by Rigrod's formula [1, 2, 26, 164, 165]

$$g(x, y, z) = \frac{g_0}{1 + I_\Sigma(x, y, z)/I_0}, \tag{29}$$

where $I_\Sigma(x, y, z)$ is the distribution of the total intensity of the two opposing waves in the cavity, I_0 is the saturation intensity at which the gain decreases by one-half, and g_0 is the weak-signal gain.

Simultaneously with the simplified simulation of the AM gain, frequent use is made of the same model description of the phase inhomogeneities that result both from the nonuniform transverse distribution of the refractive index of the medium [1, 37, 40-43, 48, 50, 57, 58, 62-64, 71, 72, 81, 82, 98, 101, 104, 106, 109, 111, 116, 117, 124-126, 128, 129, 137, 139, 140, 142-148, 155-163], and from the nonideal character of the mirror surfaces or from the nonconfocal arrangement of the cavity [34, 39, 46, 51, 74, 78, 85, 91, 120, 124, 127, 133, 136, 151]. This approach can be regarded as fully justified for the determination of the angular divergence of the laser radiation in the case of a statistical distribution of the weak phase inhomogeneities, which are not connected in practice with the real distribution of the gain. It is possible to investigate in this manner hypothetical phase inhomogeneities, or else take them from experiment or determine them by separate rigorous calculations. The local value of the refractive index (n) in the case of a multicomponent gas medium can be easily determined from the known distributions of the gasdynamic parameters [21, 23]

$$n - 1 = \sum_{i=1}^{k} (n_i - 1) \frac{N_i}{N_L}, \tag{30}$$

where n_i is the refractive index of the i-th component, k is the number of mixture components, N_i is the number of particles of the i-th component per unit volume, and N_L is the Loschmidt number.

Choosing in the same manner in the simplified equations (29) the values of the parameters that determine the energetics, we can determine with sufficient accuracy the integral energy characteristics of the laser and the tendencies of their variation. In view, however, of the enhanced computation techniques and methods, it has become possible to carry out more interesting investigations of the field in a cavity with more realistic models. Therefore, the finite-difference method using implicit schemes, and especially the FFT method [98, 109, 116, 117, 125, 130-132], dealing with high-power CO_2 lasers, were followed by more complicated models of flow-through AM, with account taken of both the real pump velocity determined by the kinetics of the physicochemical reactions in the stream, as well as gasdynamic effects that influence the optical quality of such media.

In all gaseous AM, the medium of a chemical laser, particularly that of an HF-CCL, is distinguished by the exceptional variety of physicochemical processes that determine its properties and the complexity of the mathematical simulation [2]. In an analysis of systems of this type it is necessary to solve many problems connected with thermo- and gas-dynamics, with diffusion, with the chemical, relaxational, and laser kinetics, and sometimes also with turbulence. The calculation of the characteristics of the AM of a cw chemical HF laser is complicated mainly because of two circumstances: 1) all the kinetic processes in the cavity region evolve against a background of active mixing of reacting flows with variable gasdynamic parameters, and hence with variable flow velocities; 2) chemical excitation of the products of the reactions has a multilevel cascade character. Moreover, in the case of the solution of a cavity problem of this type the calculation must be carried out repeatedly during the entire iteration process. It is this which makes it necessary to choose a sufficiently accurate and at the same time effective method of simulating the principal processes in the AM of HF-CCL.

In this context, rigorous calculations based on a solution of a system of Navier—Stokes equations [166-170], which is by itself undoubtedly a most consistent but very complicated and time-consuming task, is simply unthinkable in the case of a cavity, in view of immense time consumption. Even the presently most effective algorithms, such as in [170], can hardly be routinely employed in diagnostic programs. They serve, therefore, at present as sort of accuracy standards and are used mainly for individual computations aimed at obtaining the most complete information on the characteristic features of the AM flow, which can subsequently already be used for the refinement of simpler AM models.

In the bulk of the investigations of HF-CCL, AM are used, therefore, two-dimensional and quasi-three-dimensional models involve the boundary-layer approximation, for example [131-133, 171-185]. This approach, based on a soluton of parabolic equations, is simplest to implement and allows at the same time for the transverse structure of the flow and the rate of mixing of the components. This permits a complete energywise calculation of HF-CCL with acceptable practical accuracy [131]. Even in this case, however, the most effective numerical methods that implement this approach [183-185] consume 5-10 min of EC-1045 computer time for one calculation of 5 cm of a laser region along the flow. Such an AM model for use in a cavity program is therefore suitable, at best, only for the design of a one-pass amplifier. Calculations for a two-dimensional cavity with allowance for lasing on the first two levels by means of this model require already one or several dozen hours.

Further simplification of the description of the AM model using one-dimensional equations [134, 135, 186-189], that can reflect only the role of kinetic processes but take no account of the finite rate of reagent mixing, is also unsuitable for the description of real laser systems, since the mixing factor is known to influence substantially the magnitude and the spatial distribution of the gain, and determines by the same token the energetics of cw chemical laser.

In [190] is proposed a quasi-two-dimensional AM model, frequently called also quasi-one-dimensional (owing to different interpretations of the prefix "quasi"), based on the "flame-front" concept. It is shown there, in particular, that allowance for the finite reagent mixing rate limits the energy characteristics of a chemical laser when the pressure is increased. A generalization of this model to include a multilevel emitting medium was carried out in [191-198]. Note that the quasi-two-dimensional approach developed in [193, 194] takes into account the thermal and gasdynamic phenomena in the stream. The first quantitative calculations of a continuous HF(DF) laser in the context of a quasi-two-dimensional model of an AM were made in [193, 195, 196].

The very same model was used to analyze the distinguishing features of an HF-CCL with an unstable cavity. Thus, a qualitative analytic model of an HF-CCL was developed in [52] on the basis of a two-level radiation scheme. A quasi-two-dimensional AM model was used in [61] to investigate, in the geometric approximation, the energetics of an HF-CCL with a cylindrical nozzle block. Effective geometric-optics methods of calculating HF lasers and amplifiers with UTC were developed on the same basis of a quasi-two-dimensional AM model in [67-70], including also a quasi-three-dimensional [69] cavity geometry. Finally, an approximate quasi-two-dimensional discription of an AM, in conjucntion with wave-optics methods, was used in [112, 113] for two-dimensional configurations of HF-CCL cavities.

It should be noted that quasi-two-dimensional models are not closed, since the diffusion mixing length must be determined from supplementary conditions [194]. However, after such a model is properly adjusted in accord with experimental results or rigorous calculations [61], it can be used repeatedly in calculations for variants with close mixing parameters, since they are practically independent of the radiation intensity. The use of a quasi-two-dimensional "flame-front" model can already shorten the computation time for one typical laser-zone variant to several dozen seconds, and to 6-10 sec if the numerical algorithm is well optimized. This, in turn, imposes practically no limitation on calculations for two-dimensional cavities and makes it possible to calculate, in reasonable time, three-dimensional cavity variants.

In simulation of the interaction of the field with the AM one uses as a rule the approximation of thin layers or of amplitude—phase screens (APS), which are characterized by parameters averaged over the layer thickness [75, 79, 98, 116, 117, 125-153]. The number of such layers frequently reduces to one, that is furthermore located in the plane of one of the mirrors [128, 129, 133, 134]. Such a scheme, strictly speaking, cannot provide a true picture of the radiation-field distribution in the cavity, since it ignores AM inhomogeneity

effects resulting from its interaction with the radiation, as well as effects connected with transformation of these inhomogeneities as the radiation is transported along the optic axis. If the AM layer is long enough, such effects can introduce into the field structure strong distortions that cannot be taken into account in the single APS approximation, especially in those cases when the inhomogeneity scale is small enough. More consistent in this case are therefore approaches that take into account the spatial distributions of the inhomogeneities in natural fashion [101-114], or those using several SPS [98, 116, 117, 125, 126, 131, 132].

As a result of the foregoing analysis of the wave methods of field calculation in laser cavities, we chose the method of expanding the field in plane waves with the aid of the FFT. In spite of its shortcomings, it ensures, when correctly applied, a high accuracy of the solution in a wide range of variation of the UTC parameters, and also a high computation speed. We propose to use it for calculations of HF-CCL jointly with the quasi-two-dimensional model of an active medium in the "flame front" approximation and of rotational equilibrium of the working molecule (direct calculations [134, 135, 198] have shown that under typical conditions of a "cold-reaction" cw HF laser allowance for the finite rate of the rotational relaxation decreases the laser power by not more than 20-30%).

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