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Self-focusing of light in nematic liquid crystals as a method of investigation of the orienting effect of a free surface

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The huge optical nonlinearity of the mesophase of a nematic liquid crystal (NLC), recently predicted and observed by the self-focusing of light, and caused by reorientation of the NLC director under the influence of light fields, is discussed. A calculation is carried out of the nonlinear advance of phase and of the optical power of the nonlinear lens for a layer of NLC oriented by means of one or two surfaces. Proposed experiments would enable one to obtain quantitative information about the orienting action of a free surface. Methods of increasing the accuracy of the experiment are discussed. Expressions are also obtained for the power of the nonlinear lens in a number of specific problems on external self-focusing of light in NLC.

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1. INTRODUCTION

A huge optical nonlinearity of the oriented mesophase of a nematic liquid crystal (NLC) was recently predicted theoretically and observed experimentally.[1] This nonlinearity is caused by reorientation of the NLC director by the electric field of the light wave. In the experiment,[1] the original uniform planar orientation of the NLC was preserved because of the rigid orientation of the director on the rubbed surface of the cell walls. A suitable departure

$$\delta\mathbf{n}(\mathbf{r})=\mathbf{n}(\mathbf{r})-\mathbf{n}_0$$

of the director from the unperturbed direction lowers the energy of interaction with the light wave but leads to the appearance of a positive energy of nonuniform deformation

$$F[\mathrm{erg/cm^3}]\sim K(\nabla\delta\mathbf{n})^2,$$

where K is a Frank constant (see below). Minimization of the sum of these energies leads to a local equation for $\delta\mathbf{n}$, whose solution was carried out[1] with allowance for the rigid pinning of the director at the boundaries and gave a completely satisfactory agreement with experiment.

Papers of Mada[2,3] discuss theoretically a possible mechanism of the orienting effect of a free NLC surface (that is, for example, the boundary between the NLC and air). The point is that there is a preferred orientation of the NLC director with respect to such a free surface, and this orientation may be different for different specific shapes of the NLC (see Refs. 4 and 5). The degree of rigidity of the orientation along such a preferred direction can be characterized[2] by the orientation-dependent part of the surface energy density,

$$\Lambda[\mathrm{erg/cm^2}]\sim\sigma_a(\delta\mathbf{n})^2$$

(see below for a more exact definition). From the constants σ_a and K we can form a quantity of dimensions length, $l=K/\sigma_a$. If the total thickness L of the cell is much larger than l, i.e., if $L\gg K/\sigma_a$, then the effect of the surface may be considered to be practically a rigid pinning of the director. If, on the contrary, $L\ll K/\sigma_a$ (or equivalently, if $\sigma_a\to 0$), the free surface exerts no influence at all on the orientation of the director. Mada[2,3] notes that so far no methods are known for experimental measurement of the value of the orientation-

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dependent part of the surface energy, that is of the constant σ_a, and he also points out the importance of information about the value of this constant.

The present paper is devoted to calculation of the reorientation of the NLC director by a light field and of the corresponding nonlinear advance of phase of the light wave, for $0 \leq \sigma_a < \infty$. Measurement of this advance of phase in two experiments—with one free surface and without it (that is, in a cell closed on both sides)—makes it possible to isolate the orienting effect of a free surface and thereby to measure the constant σ_a.

2. SYSTEM OF BASIC EQUATIONS

We write the free energy F of unit volume of the NLC in the form[6]

$$F=\frac{1}{2}K_{11}(\operatorname{div}\mathbf{n})^2+\frac{1}{2}K_{22}(\mathbf{n}\operatorname{rot}\mathbf{n})^2+\frac{1}{2}K_{33}[\mathbf{n}\operatorname{rot}\mathbf{n}]^2-\frac{\varepsilon_a}{16\pi}(\mathbf{nE})(\mathbf{nE}^*). \tag{1}$$

Here K_{11}, K_{22}, and K_{33} are the Frank constants (in dynes), and $\varepsilon_a = \varepsilon_{\|} - \varepsilon_{\perp}$ is the anisotropy of the dielectric constant of the NLC at optical frequencies. We treat the value of ε_a and the modulus of the order parameter s as constants over the whole volume of the NLC. As is well known, departure of s and of ε_a from a constant value can occur only in surface layers of thickness of order 10^{-7} cm and therefore does not affect the optical properties at radiation wavelength $\lambda \sim 0.5 \cdot 10^{-4}$ cm.[7]

The complex amplitude $\mathbf{E}(\mathbf{r})$ of the electric field of a monochromatic light wave is connected with the real field-intensity vector by the relation

$$E_{\text{real}}(\mathbf{r},\ t)=0{,}5(\mathbf{E}e^{-i\omega t+i\mathbf{kr}}+\mathbf{E}^*e^{i\omega t-i\mathbf{kr}}).$$

The free energy Λ of unit surface must have the form of a function possessing a minimum at the value

$$\mathbf{ne}_z=\cos\theta_0,$$

where θ_0 is the most favorable value of the director angle, and where $\mathbf{e}_z$ is the normal to the surface. If, following Refs. 2 and 3, we retain only terms of no higher than the second order in $\mathbf{n}$, and if we furthermore exclude terms linear in $\mathbf{n}$ and $-\mathbf{n}$, the expression for the n-dependent part of the surface energy takes the form

$$\Lambda={}^1/_2\sigma_a(\mathbf{ne}_z)^2. \tag{2}$$

Then only two possible values are obtained for the most favorable angle: $\theta_0 = 0$ for $\sigma_a < 0$ and $\theta_0 = 90°$ for $\sigma_a > 0$. The energy is of course independent of the azimuth φ of the director orientation, because of the absence of a preferred direction.

We note that according to some experimental data,[4] the value of the angle of exit of the director at the surface may differ from the favorable one $\theta_0 = 0$ or $\theta_0 = 90°$. Mada[2,3] explains this fact on the basis of minimization of the total free energy $F+\Lambda$. Values of the favorable angle θ_0 different from 0 or 90° are obtained from the theory, with allowance for van der Waals interaction, only because of anisotropy of the dielectric properties of the medium with which the nematic is in contact.[3] In this connection there is all the more interest in a test of the consequences of the hypothesis expressed by equation (2).

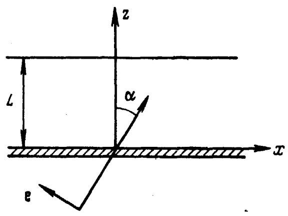

FIG. 1. Schematic representation of an experiment for observation of self-focusing in a plane cell with NLC. The polarization vector $\mathbf{e}$ of the light wave lies in the xz plane; the wave is propagating in the cell with wave vector $\mathbf{k}$. In the plane $z = 0$, the orientation of the director is prescribed by rubbing or appropriate treatment of the wall of the cell. The transparent material of the wall is hatched. The free surface of the NLC is in the plane $z = L$.

The total free energy of a NLC filling the region $0 \leq z \leq L$ (Fig. 1) will be

$$\Phi=\int_V F\,dV+\int_S \Lambda\,dS. \tag{3}$$

The variational equations have the form

$$\frac{\delta F}{\delta n_i}-\frac{\partial}{\partial x_j}\frac{\delta F}{\delta(\partial n_i/\partial x_j)}=0,\quad \left[\frac{\delta\Lambda}{\delta n_i}+\frac{\delta F}{\delta(\partial n_i/\partial z)}\right]_{z=L}=0.$$

3. LOCAL SOLUTION AND MINIMIZATION OF THE TOTAL ENERGY

We shall suppose that upon the NLC layer, of thickness L, there is incident an almost plane light wave, with a transverse inhomogeneity dimension a much larger than L; that is, $a \gg L$. We shall treat the effect in the first nonvanishing approximation with respect to $|\mathbf{E}|^2$, assuming the light field sufficiently weak. Furthermore, nonvanishing effects are obtained only for the extraordinary wave, whose polarization we shall suppose to lie in the xz plane. We shall consider two specific versions of the geometry of the experiment.

1. Let the NLC layer have a planar orientation, and let $\sigma_a > 0$. In the plane $z = 0$, we shall suppose the director to be rigidly pinned in the direction of the x axis. Then $\mathbf{n}_0 = \mathbf{e}_x$, and in the approximation linear in $\delta\mathbf{n}(z) = \mathbf{n} - \mathbf{n}_0$ we have

$$-K_{11}\frac{d^2\delta n_z}{dz^2}=\frac{\varepsilon_a}{8\pi}(\mathbf{Ee}_x)(\mathbf{Ee}_z)', \tag{4a}$$

$$\left[K_{11}\frac{d\delta n_z}{dz}+\sigma_a\delta n_z\right]_{z=L}=0, \tag{4b}$$

$$\delta n_z(z=0)=0. \tag{4c}$$

The solution of equation (4a) under the boundary conditions (4b) and (4c) has the form

$$\delta\mathbf{n}=\mathbf{e}_z\delta n_z(z)=\mathbf{e}_z\frac{A}{2K_{11}}z\left(\frac{2+\xi}{1+\xi}L-z\right). \tag{5}$$

Here we have introduced the notation

$$A=\frac{\varepsilon_a}{8\pi}(\mathbf{Ee}_x)(\mathbf{Ee}_z),\qquad \xi=L\frac{\sigma_a}{K_{11}}.$$

It is easily verified that the solution (5) actually minimizes the total free energy (3).

2. Let the NLC layer be homotropically oriented, $\mathbf{n}_0 = \mathbf{e}_z$, and furthermore let $\sigma_a < 0$. Then the equation for

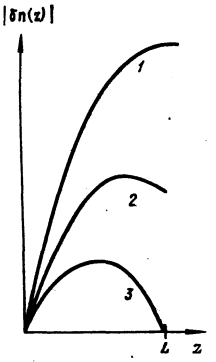

FIG. 2. Behavior of the perturbations $\delta n_x(z)$ and $\delta n_z(z)$ of the director in a cell of thickness L, in relative units, for various values of the parameter ξ: 1, $\xi=0$; 2, $\xi=1$; 3, $\xi=\infty$.

$\delta\mathbf{n}=\mathbf{e}_x\delta n_x(z)$ has the form

$$-K_{33}\frac{d^2\delta n_x}{dz^2}=\frac{\varepsilon_a}{8\pi}(\mathbf{E}\mathbf{e}_x)(\mathbf{E}^*\mathbf{e}_z), \qquad (6a)$$

$$\left[K_{33}\frac{d\delta n_x}{dz}+|\sigma_a|\delta n_x\right]_{z=L}=0, \qquad (6b)$$

$$\delta n_x(z=0)=0. \qquad (6c)$$

The solution of (6a) under the boundary conditions (6b) and (6c) has the form

$$\delta\mathbf{n}=\mathbf{e}_x\delta n_x(z)=\mathbf{e}_x\frac{A}{2K_{33}}z\left(\frac{2+|\xi|}{1+|\xi|}L-z\right). \qquad (7)$$

This solution also, of course, minimizes the total energy (3). Graphs of the functions $\delta n_x(z)$ or $\delta n_z(z)$ for parameter values $\xi=0$, $\xi=1$, and $\xi=\infty$ are shown in Fig. 2.

The case in which the director has rigid planar pinning on one surface and rigid homotropic on the other is considered in Appendix 1.

4. NONLINEAR ADVANCE OF OPTICAL PHASE, AND DISCUSSION OF EXPERIMENTAL POSSIBILITIES

The correction to the tensor dielectric constant because of the reorientation $\delta\mathbf{n}$ of the director is

$$\delta\varepsilon_{ik}=\varepsilon_a(n_{0i}\delta n_k+n_{0k}\delta n_i).$$

The change $\delta\mathbf{k}$ of the wave vector of the light wave, in the first order in $\delta\varepsilon_{ik}$, can be written in the form

$$\delta k=\frac{\omega^2}{2c^2k}e_i\delta\varepsilon_{ik}e_k,$$

where $\mathbf{e}$ is the unit polarization vector of the electric field.

Since the path traversed by the wave in the medium is $L/\cos\alpha$ (where α is the angle of refraction; see Fig. 1), the correction to the phase of the light wave is $\delta\varphi=L\delta k/\cos\alpha$. Taking also $\mathbf{e}\approx\mathbf{e}_x\cos\alpha+\mathbf{e}_z\sin\alpha$, we get

$$\delta\varphi=\varepsilon_2^{\text{eff}}\frac{\omega}{4c(\varepsilon_e)^{1/2}}\frac{L}{\cos\alpha}|E|^2. \qquad (8)$$

Here for planar orientation

$$\varepsilon_2^{\text{eff}}=\frac{\varepsilon_a^2\sin^2\alpha\cos^2\alpha L^2}{24\pi K_{11}}\left(1+\frac{3}{1+\xi}\right) \qquad (9)$$

and for homotropic orientation

$$\varepsilon_2^{\text{eff}}=\frac{\varepsilon_a^2\sin^2\alpha\cos^2\alpha L^2}{24\pi K_{33}}\left(1+\frac{3}{1+|\xi|}\right). \qquad (10)$$

We have presented the result (8) in the form of an expression that contains an effective constant of nonlinearity $\varepsilon_2^{\text{eff}}$. An expression of the type (8) would be obtained if one were to take for the permittivity of a scalar medium

$$\varepsilon(|E|^2)=\varepsilon_0+0.5\varepsilon_2|E|^2,$$

as is done in nonlinear optics. In our case, the "constant" ε_2 itself depends on the thickness of the medium ($\varepsilon_2\sim L^2$). Here we assumed that the inhomogeneity dimension a of the field $|E|^2$ perpendicular to the beam was much larger than the value of $L/\sin\alpha$; that is, that $a\gg L/\sin\alpha$. The nonlinear-lens properties for self-focusing in a NLC, when $a\ll L/\sin\alpha$, are considered in Appendix 2.

It follows from (8)–(10) that the nonlinear advance of phase depends substantially on the parameter ξ. The case $\xi\to\infty$ corresponds to rigid pinning of the director even at a free surface. The other limiting case, $\xi\to 0$, corresponds to truly free orientation of the director on this surface. It is easy to verify that

$$\frac{\varepsilon_{2\,\text{pl}}(\xi=0)}{\varepsilon_{2\,\text{pl}}(\xi=\infty)}=\frac{\varepsilon_{2\,\text{hom}}(\xi=0)}{\varepsilon_{2\,\text{hom}}(\xi=\infty)}=4.$$

In other words, for the same thickness L, a layer of NLC with a single truly free surface shows four times as large a nonlinearity as a layer with two surfaces that rigidly pin the director.

A method of measurement of the effective constant ε_2, on the basis of the effect of external self-focusing of the light (according to measurement of the angular divergence of the beam in the far zone), was used experimentally and described earlier.[1] Also possible is direct measurement of the optical advance of phase, by known methods of interferometry that may give a quite high accuracy of measurement of the phase.

It is important to emphasize that measurements for two cases—with two rigidly pinning surfaces and with one—make it possible to isolate the effect of a free surface on the orientation of the NLC in the purest form; that is, without substantial influence of the errors in measurement of ε_a, α, $\varepsilon_e^{1/2}$, the total power of the light beam, and other absolute values.

Thus in the present paper there is presented a method of measurement of the influence of a free surface on the orientation of the NLC director, on the basis of a measurement of the nonlinear optical advance of phase. We emphasize that the apparatus required for these experiments reduces, except for the cell with the NLC, to an easily accessible low-power continuous laser, for example helium-neon. Also of interest is a test of the hypothesis of absolutely rigid pinning of the director on a rubbed surface. This method also permits investigation of the influence of surface-active substances and, generally, any liquids that can be brought into contact with the surface of a NLC.

In conclusion, the authors sincerely thank E.I. Kats, N.F. Phipetskii, A.V. Sukov, and Yu.S. Chilingaryan for valuable discussions.

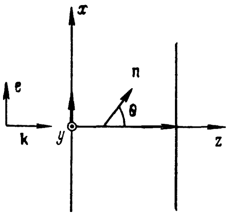

FIG. 3. Schematic diagram of self-focusing of light in a cell with NLC, with distorted director orientation. In the plane $z = 0$, the director $\mathbf{n}(\mathbf{r})$ is oriented along the x axis; in the plane $z = L$, along the z axis.

APPENDIX 1

Propagation of light in a layer with distorted orientation

We consider a cell of NLC one wall of which prescribes a rigid planar orientation of the NLC director (in the direction of the x axis), the other wall a rigid homotropic orientation. The distortion of the director field within the volume of the cell can be described by the angle $\theta(z)$ that the director vector $\mathbf{n}$ makes with the normal to the cell plates (the z axis) at the point with coordinate z,

$$\mathbf{n}=\{n_x, n_z\}=\{\sin\theta_0(z), \cos\theta_0(z)\}$$

(see Fig. 3). On such a cell let there be incident, in the direction of the z axis, a light wave polarized along the x axis (a wave polarized along the y axis would pass through such a medium as it would through a homogeneous medium with index of refraction $\varepsilon_\perp^{1/2}$ and would not produce nonlinear effects).

The field in the NLC, in the approximation of geometric optics, will have the form

$$\mathbf{E}(z,t)=\mathbf{E}(z)\exp\left\{i\frac{\omega}{c}\varepsilon_\perp^{1/2}\int_0^z\frac{dz'}{[1-(\varepsilon_a/\varepsilon_\parallel)\sin^2\theta_0(z')]^{1/2}}-i\omega t\right\}, \quad (11)$$

$$\mathbf{E}(z)=\{E_x(z), E_z(z)\},$$
$$E_x(z)=A\varepsilon_{zz}^{1/4}, \quad E_z(z)=-(\varepsilon_{xz}/\varepsilon_{zz})E_x(z) \quad (12)$$

(a treatment of the geometric optics of anisotropic media will be found, for example, in Ref. 9). Here

$$\varepsilon_{xz}=\varepsilon_a\sin\theta_0(z)\cos\theta_0(z),$$
$$\varepsilon_{zz}=\varepsilon_\perp+\varepsilon_a\cos^2\theta_0(z)$$

are the components of the tensor dielectric constant of the NLC,

$$\varepsilon_{ik}=\varepsilon_\perp\delta_{ik}+\varepsilon_a n_i n_k.$$

To investigate the self-focusing of light in the scheme described (Fig. 3) and to estimate the magnitude of the nonlinearity, we take $K_{11}=K_{33}=K$ in formula (1) (the Frank constant K_{22} describes distortion of the twist type, which is absent in the geometry of our experiment). This approximation enables us to present in analytic form the basic results of the theory.

The equation for $\theta(z)$, describing the character of the director-field distribution in the presence of a strong light wave, takes the form

$$K\frac{d^2\theta(z)}{dz^2}=-\frac{\varepsilon_a}{16\pi}[\sin 2\theta(|E_x|^2-|E_z|^2)+\cos 2\theta(E_xE_z^*+E_x^*E_z)]. \quad (13)$$

Writing $\theta(z)=\theta_0(z)+\delta\theta(z)$, where $\delta\theta(z)$ is the perturbation of the director behavior by the light field, and using the expression (12) for the components of the field, we get, in the approximation linear in $\delta\theta$,

$$\delta\theta(z)=\frac{\varepsilon_\perp\varepsilon_\parallel^{1/2}|A|^2}{8\pi Kq^2}\left[K\left(\frac{\varepsilon_a}{\varepsilon_\parallel}\right)\frac{z}{L}-F\left(qz,\frac{\varepsilon_a}{\varepsilon_\parallel}\right)\right]. \quad (14)$$

Here $F(qz, \varepsilon_a/\varepsilon_\parallel)$ denotes the elliptic integral of the second kind, and $K(\varepsilon_a/\varepsilon_\parallel)=F(\pi/2, \varepsilon_a/\varepsilon_\parallel)$ is the complete elliptic integral. In the derivation of this formula it has also been taken into account that in the single-constant approximation, $\theta_0(z)=qz$ and that for our problem, $q=\pi/2L$.

The nonlinear advance of phase in the cell of thickness L, as follows from the expression (11), is

$$\delta\Phi=\frac{\omega}{c}\varepsilon_a(\varepsilon_\parallel\varepsilon_\perp)^{1/2}\int_0^L\frac{\sin qz\cos qz}{(\varepsilon_\perp+\varepsilon_a\cos^2 qz)^{3/2}}\delta\theta(z)\,dz. \quad (15)$$

Substituting in this formula the expression (14), we get for $\delta\Phi$

$$\delta\Phi=\frac{\omega}{c}\frac{\pi(\varepsilon_\parallel\varepsilon_\perp)^{1/2}P}{2cK_{11}q^3}\left[1-\frac{4}{\pi^2}\left(\frac{\varepsilon_\perp}{\varepsilon_\parallel}\right)^{1/2}K^2\left(\frac{\varepsilon_a}{\varepsilon_\parallel}\right)\right], \quad (16)$$

where $P=c(\varepsilon_\parallel\varepsilon_\perp)^{1/2}|A|^2/8\pi$ is the power density of the beam. Comparison of the value of $\delta\Phi$ with the value of the nonlinear advance of phase $\delta\Phi$ in the planar orientation of the cell, for $\xi\to\infty$ and $\alpha=45°$, gives $\delta\Phi/\delta\Phi_{pl}=2.2$ for the following NLC parameters: $\varepsilon_\perp=2.3$; $\varepsilon_\parallel=3.3$; $n_e=1.7$.

In the case of weak anisotropy, $\varepsilon_a/\varepsilon_\parallel\ll 1$, the expression (16) for the nonlinear phase advance reduces to the form

$$\delta\Phi=\frac{\omega}{c}\frac{\varepsilon_a^2|A|^2}{512Kq^3}.$$

This expression can also be derived directly from formula (13) and the equation

$$\delta\Phi=\omega\delta\varepsilon_{ik}e_ie_k/2n_ec,$$

by assuming that in the case of weak anisotropy $E_x\approx$ const and $E_z=0$. In this case the nonlinear advance of phase is about 2.15 times weaker than for planar orientation of an NLC layer ($\xi\to\infty$ and $\alpha=45°$) of the same thickness L.

APPENDIX 2

Nonlocality of response of NLC and its effect on optical nonlinearity

We consider the following experimental geometry (Fig. 4). The NLC director is directed along the z axis, and its orientation is maintained by an external magnetic field H, so that $\mathbf{n}_0\parallel\mathbf{H}$. A light wave is propagated along the x' axis, which makes an angle α with the x axis, and is polarized in the xz plane (the extraordinary wave). Here we shall consider propagation of a narrow beam; that is, of a beam for which the transverse inhomogeneity dimension a is much less than the thickness L of the NLC layer, or more accurately $a\ll L/\sin\alpha$ (Fig. 4). In this case the perturbation $\delta\mathbf{n}$ of the director field by the light wave will be a function of all the spatial coordinates, $\delta\mathbf{n}=\delta\mathbf{n}(\mathbf{r})$.

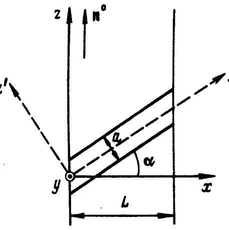

FIG. 4. The problem of the self-focusing of a beam with transverse dimension $a \ll L$. The coordinate systems are chosen as follows: the x axis is perpendicular to the cell plates; the y axis coincides with the y' axis and is perpendicular to the plane of the figure.

The equation that determines $\delta\mathbf{n} = \mathbf{e}_x \delta n$ in the single-constant approximation $K_{ii} = K$ has the form

$$\frac{\partial^2 \delta n}{\partial x^2} + \frac{\partial^2 \delta n}{\partial y^2} + \frac{\partial^2 \delta n}{\partial z^2} - p^2 \delta n = B|E(\mathbf{r})|^2, \qquad (17)$$
$$p^2 = \frac{\varkappa_a H^2}{K}, \quad B = \frac{\varepsilon_a \sin\alpha \cos\alpha}{8\pi K}.$$

Here $\varkappa_a = \varkappa_{\parallel} - \varkappa_{\perp}$ is the anisotropy of the magnetic susceptibility, $\mathbf{e}$ is the polarization vector of the electric field of the light wave, and $\mathbf{E} = \mathbf{e}E$. The expression (17) is obtained from the variational equations (3) with allowance in the free energy (1) for a term $F_H = -\varkappa_a (\mathbf{n}, \mathbf{H})^{2/2}$, which describes the orienting effect of the magnetic field.

We write equation (17) in the coordinate system $x'y'z'$ obtained by rotation of the x and z coordinate axes about the y direction through angle α. Taking into account that δn is independent of x', i.e., neglecting attenuation of the beam, we get

$$\frac{\partial^2 \delta n}{\partial y'^2} + \frac{\partial^2 \delta n}{\partial z'^2} - p^2 \delta n = B|E(\mathbf{r}')|^2. \qquad (18)$$

We consider first the case of propagation in the medium of a strip beam; that is, a beam of the form $|E|^2 = |E(z')|^2$. Then equation (18) can be written in the form

$$\frac{d^2 \delta n}{dz'^2} - p^2 \delta n = B|E(z')|^2. \qquad (19)$$

The solution of equation (19) has the form

$$\delta n(z') = -\frac{B}{2p} \int |E(z'')|^2 \times \exp(-p|z'-z''|)\, dz''. \qquad (20)$$

If the magnetic coherence distance $l_M = 1/p$ is much larger than the field inhomogeneity a, $l_M \gg a$, then from (20) there follows

$$\delta n(z') \approx -\frac{B}{2p} e^{-p|z'|} \int |E(z'')|^2 dz''.$$

Thus in the case $l_M \gg a$, the perturbation of the director field by the light wave is determined by the whole energy of the wave and is independent of the form of the light field $|E(z')|^2$. The value of $d^2\delta n/dz'^2$, which determines the focal length of the nonlinear lens for a paraxial beam, is

$$\frac{d^2 \delta n}{dz'^2} \approx B|E(z')|^2 - \frac{1}{2} B p e^{-p|z'|} \int |E(z'')|^2 dz''. \qquad (21)$$

The second term in (21) can be estimated as

$$\int |E(z'')|^2 dz'' \approx |E(z'=0)|^2 a,$$

and for small z' (for a Gaussian beam, $|z'| \sim a$) we can write

$$\frac{d^2 \delta n}{dz'^2} \approx B|E(z')|^2.$$

Thus for a paraxial beam, aberrationless self-focusing occurs when $|E|^2 = \text{const}$. It is not difficult, however, to obtain an exact expression for $\delta n(z)$ and therefore for $d^2\delta n(z)/dz^2$ in the case of a Gaussian beam, in explicit form, from the expression (20).

We shall discuss the nonlocal character of the response of a NLC under the action of a light wave of the more general form $|E|^2 = |E(y', z')|^2$.

The solution of equation (18) has the form

$$\delta n(\mathbf{r}') = -\frac{B}{4} \int |E(\mathbf{r}'')|^2 i H_0^{(1)}(ip|\mathbf{r}'-\mathbf{r}''|)\, d^2\mathbf{r}'',$$

where $iH_0^{(1)}(iz) = 2K_0(z)/\pi$ is a zero-order Hankel function of purely imaginary argument. Hereafter, since we are interested in the effect of the nonlocality of the response on the self-focusing of the light beam, we neglect the term $p^2\delta n$ on the left side of equation (18). As we have already seen in the treatment of the one-dimensional case, this may be done when the inhomogeneity dimension of the field is much smaller than the magnetic coherence distance. Thus for consideration of the self-focusing of a narrow light wave, we shall start from the equation

$$\frac{\partial^2 \delta n}{\partial y'^2} + \frac{\partial^2 \delta n}{\partial z'^2} = B|E(y', z')|^2, \qquad (22)$$

which is correct in the beam region.

Let the light field have a radially symmetric form of $|E(y', z')|^2$. Then equation (22) in polar coordinates takes the form

$$\frac{d}{d\rho}\left(\rho \frac{dn}{d\rho}\right) = B\rho |E(\rho)|^2,$$

whence it follows that aberrationless self-focusing occurs when $|E(\rho)|^2 = \text{const}$. This corresponds to a light wave whose intensity is constant within a circle. Then the value of $d^2\delta n/d\rho^2$, which determines the focal length of the nonlinear lens, is

$$\frac{d^2 \delta n}{d\rho^2} = \frac{1}{2} B|E|^2. \qquad (23)$$

We shall make some numerical estimates of the focal length f of the nonlinear lens. In the paraxial approximation,

$$f^{-1} = \frac{2\pi}{\lambda} \frac{d^2 \delta\Phi}{d\rho^2},$$

where λ is the wavelength of the light in a vacuum and where $\delta\Phi$ is the nonlinear advance of phase,

$$\delta\Phi = \frac{\omega}{2cn_e} \frac{L}{\cos\alpha} 2\varepsilon_a \sin\alpha \cos\alpha \delta n.$$

Using equation (23), we get

$$\frac{1}{f} = \frac{\varepsilon_a^2 \sin^2\alpha \cos\alpha L |E|^2}{16\pi K n_e} = \frac{\varepsilon_a^2 \sin^2\alpha \cos\alpha L P}{2 n_e^2 c K},$$

where $P = cn_e|E|^2/8\pi$ is the power density of the beam. For $\varepsilon_a = 1$, $\alpha = 45°$, $L = 10^{-2}$ cm, $K = 4.5 \cdot 10^{-7}$ dyn, and $P = 1\ W/\text{cm}^2$, we get $f \approx 2.2$ cm.

[1)] Experiments on generation of the second harmonic of light in MBBA[8] indicate a possible nonequivalence of the directions **n** and -**n**. For simplicity, however, we adhere to the standard assumption[6] that they are equivalent.

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Characteristic features of the electron spectrum of metals with dislocations

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The theoretical data on the spectrum of electron states localized near edge dislocations are presented in a systematic manner and supplemented by new results. The following types of edge dislocations are considered: an isolated rectilinear dislocation, a dislocation dipole, a prismatic loop, and a segment of a bent dislocation of finite length. A detailed study is made of the problem of concentration broadening of the dislocation energy levels and bands in the case of random and quasiregular distributions of these various types of dislocations.

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INTRODUCTION

Distortions of the crystal lattice around dislocation lines create large-scale deviations of the crystal field from its periodic structure in a perfect crystal. In metals these distortions produce forces which act on conduction electrons and can sometimes alter significantly the nature of motion of these electrons. In the simplest cases it is found that electron excitations belonging to a continuous spectrum are scattered by dislocations exchanging energy and momentum: such processes give rise to a dislocation contribution to the electrical resistivity and to an electron contribution to the drag force exerted on dislocations. However, there can be situations in which the influence of dislocations on the electron motion is more fundamental, for example, an electron may become localized near a dislocation line. Localization is known to produce discrete levels in certain parts of the energy spectrum and such drastic changes in the structure of the electron spectrum may give rise to specific features in the thermodynamic and transport properties of a metal.

The concept of a dislocation covers a fairly wide class of different line defects of the crystal structure. The common feature of all of them is the presence of a core—representing a certain tube of radius of the order of the interatomic distance within which the deformation of the original lattice is of the order of unity—and an inhomogeneous field of elastic strains decreasing slowly away from the core. The shape of a dislocation line, microstructure of its core, and the actual law governing the decrease of the elastic field can differ considerably. This complicates greatly the formulation and solution of the quantum-mechanical problem of the interaction between electrons and dislocations. It is not possible to obtain a general solution of this problem applicable to all types of dislocation and in each case it is necessary to study much simpler specific models.

Many papers have been published on problems of this kind in the case of semiconductors and metals. Some of them deal with the conditions of formation and structure of electron states associated with dislocations[1-7]; others are concerned with the scattering of free electrons on dislocations and its influence on the electrical conductivity of a metal and on the dislocation mobility (the necessary references can be found in the monographs of Ziman[8] and Friedel[9] as well as in the review of Kaganov *et al.*[10]).

The main methodological difficulties are encountered in the analysis of changes in the electron spectrum due to dislocations. Kaner and Fel'dman[3] pointed out that an investigation of the spectrum of states localized at dislocations should include solution of problems of two types: 1) a calculation of the spectrum of an electron interacting with a single dislocation; 2) an analysis of the concentration broadening of levels or bands in such a spectrum due to the overlap of the long-range elastic fields of dislocations. In most cases, studies have been confined to the spectrum of an electron near

