and also

$$g'_0 = \frac{9}{4}\left[\frac{1}{2} d_1 d_3 \sin(d_1, d_3) - \frac{1}{\sqrt{20}} d_1 d_4 \sin(d_1, d_4)\right];$$

$$g'_2 = \frac{9}{4}\left[\frac{1}{2} d_1 d_3 \sin(d_1, d_3) - \frac{1}{2}\sqrt{\frac{3}{5}} d_1 d_4 \sin(d_1, d_4)\right];$$

$$g'_6 = \frac{9}{4}\left[-\frac{1}{\sqrt{3}} d_1 d_3 \sin(d_1, d_3) + \frac{1}{2}\sqrt{\frac{3}{5}} d_1 d_4 \sin(d_1, d_4)\right];$$

$$g'_3 = g'_2 = -g'_4 = -g'_5;$$

$$g'_1 = g'_7 = g'_8 = g'_9 = 0.$$

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14

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EXTENSION OF THE BOGOLIUBOV-TIABLIKOV PERTURBATION METHOD TO A NON-STATIONARY CASE

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The perturbation theory in the second-quantization representation, developed by Bogoliubov and Tiablikov in the stationary case for use with the polar model of crystals, is generalized to include the case of perturbation by the electromagnetic field of a light wave. A general expression is derived for the deformed operator of the electric current density excited by the radiation perturbation. A possible application of the method in the theory of optical properties of cyrstals is indicated.

1. INTRODUCTION

THE perturbation-theory method of Bogoliubov and Tiablikov[1-3] is based on the introduction of an operator that projects an arbitrary wave function of the system of valence electrons of the crystal in the homopolar* functions of the problem. In this variant of the theory the mean value of the electric current produced in the crystal by a weak constant external field is non-vanishing only in third approximation. This makes the method unsuitable for the consideration of the electrical and optical properties of metals, and also for the consideration of the strongly excited "current" states of semiconductors within the framework of the polar model, although it does not diminish its usefulness for the description of the properties of crystals that are determined by exchange interactions, for example.

Nevertheless it seems to us that the Bogoliubov-Tiablikov method can be used for the treatment of the electrical and optical properties of electronic semiconductors at low temperatures. Here we have

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*By the homopolar states in the polar model of a crystal we mean states in which there is always one valence electron close to each lattice point of the crystal.

to do with weak electric fields and low frequencies of the optical spectrum. The point is that at low temperatures electronic semiconductors have practically the properties of insulators, which offers the possibility of confining ourselves in a certain approximation to the consideration of just the weakly polarized (quasi-homopolar) states of the crystal. Moreover the limitation of low frequencies ($\omega < \omega_0$, where ω_0 is the minimum angular frequency necessary for the appearance of "current" states) in the consideration of the optical phenomena assures the correctness of neglecting the effects of quantum transitions of the electronic system into the polar excited states of the semiconductor. Although the region of applicability of a method in which one considers only quasi-homopolar states of a crystal to the treatment of, for example, optical properties of crystals is very limited, it is well to begin the discussion of such properties in the framework of a many-electron theory with this simplest case. In the present paper we carry out the extension of the Bogoliubov-Tiablikov method to the non-stationary case of the alternating electromagnetic field of a light wave propagated in the crystal.

2. THE HAMILTONIAN OF THE SYSTEM OF ELECTRONS IN A CRYSTAL IN AN ELECTROMAGNETIC FIELD, IN THE SECOND-QUANTIZATION REPRESENTATION

Let us consider a simple atomic cubic crystal, in which there is at each lattice point a single electron, which is an s state. In what follows we shall neglect the thermal vibrations of the lattice ions.

As in Refs. 1 — 3, let us denote by the symbol $f = (f^1 f^2 f^3)$ the coordinates of any lattice point, and use the lattice constant a as unit of length. We denote the position coordinates of the j-th electron by $\mathbf{r}_j = (x_j y_j z_j)$ and its spin coordinate by s_j.

The atomic wave functions $\varphi_{f\sigma}(\mathbf{r}; s) = \varphi_f(\mathbf{r}) \times \delta(s - \sigma)$ (where $\sigma = \pm \frac{1}{2}$ is the spin quantum number) at two different lattice points are not strictly orthogonal, so that in the general case the system of functions $\varphi_{f\sigma}$ is not an orthogonal system and a rigorous application of the method of second quantization is not possible. It is always possible, however, as shown in Ref. 3, to introduce an equivalent system of new "quasi-atomic" functions $\Theta_{f\sigma}$ which are exactly orthogonal to each other

$$\Theta_{f\sigma}(\mathbf{r}; s) = \Theta_f(\mathbf{r})\, \delta(s - \sigma). \qquad (2.1)$$

This makes it possible to apply the method of second quantization.

Suppose that an electromagnetic wave of frequency ω is propagated through the crystal. The vector potential $\mathbf{A}$ of this wave can always be chosen so that

$$\operatorname{div} \mathbf{A} = 0, \qquad (2.2)$$

and the scalar potential can be takn to be zero.[4]

Neglecting quantities of order A^2 and using Eq. (2.2), we can write the Hamiltonian in the second-quantization representation for a system of electrons in a crystal in an external electromagnetic field in the form (cf. Refs. 3 and 5)

$$\hat{H}(t) = \hat{H} + \hat{W}(t), \qquad (2.3)$$

where

$$\hat{H} = \hat{H}_0 + \varepsilon \hat{H}_1 + \varepsilon^2 \hat{H}_2, \qquad (2.4)$$

$$\hat{W}(t) = \sum_{ff'\sigma\sigma'} W(ff'; t)\, \hat{a}^+_{f\sigma} \hat{a}_{f'\sigma'}, \qquad (2.5)$$

$$W(ff', t) = \int \Theta_f(\mathbf{r}) \left[-\frac{ie\hbar}{mc} \mathbf{A}(\mathbf{r}; t)\, \nabla \right] \Theta_{f'}(\mathbf{r})\, d\mathbf{r}, \qquad (2.6)$$

$\hat{a}$ and $\hat{a}^+$ are the Fermi operators of second quantization, e is the absolute value of the electronic charge, and m is the mass of the electron.

The quantity ϵ in Eq. (2.4) is a small parameter (the non-orthogonality integral) with respect to which the Hamiltonian is expanded [see Ref. 3, Eq. (4.63)]. It must be kept in mind that each of the quantities $\hat{H}_0$, $\epsilon \hat{H}_1$, and $\epsilon^2 \hat{H}_2$ can also be expanded as a power series in ϵ. The way Eq. (2.4) is written means that such an expansion of $\hat{H}_0$ begins with a term of zeroth order of smallness, that of $\epsilon \hat{H}_1$ with a first order term, and so on, although each of these expansions contains also terms of higher orders.

In the second-quantization representation the Schrödinger equation for the system of electrons takes the form

$$i\hbar\, \partial C(\ldots n_{f\sigma} \ldots; t) / \partial t = \hat{H}(t)\, C(\ldots n_{f\sigma} \ldots; t), \qquad (2.7)$$

where $C(\ldots n_{f\sigma} \ldots; t) = C(n; t)$ is the wave function of the system and depends on the numbers of filled "quasi-atomic" states $\Theta_{f\sigma}$.

We assume as usual that for the visible and infrared regions the wavelength of the electromagnetic radiation is much larger than the dimensions of the "basic" domain in the crystal, so that the dependence of the vector potential on the coordinates can be neglected. Then Eq. (2.6) can be put in the form

$$W(ff'; t) = \frac{e}{mc} \mathbf{A}(t)\, \mathbf{I}(ff'), \qquad (2.8)$$

where $\mathbf{I}(ff')$ is as defined in Ref. 3 and is of first order in ϵ [cf. Eq. (4.41) and page 134 in Ref. 3], and

$$\mathbf{A}(t) = \mathbf{B}e^{i\omega t} + \mathbf{B}^* e^{-i\omega t}. \qquad (2.9)$$

Therefore Eq. (2.5) can be written in the following form:

$$\hat W(t) = \varepsilon \hat H_1'(t) = \frac{e}{mc}(\mathbf{A}(t)\,\mathbf{I}), \qquad (2.10)$$

where I is the operator of the total momentum of the system in the second-quantization representation [cf. Eq. (4.40) in Ref. 3].

Thus for the case considered Eq. (2.7) is written as follows:

$$(\hat H_0 + \varepsilon \hat{\mathscr{H}}_1(t) + \varepsilon^2 \hat H_2 - i\hbar\partial/\partial t)C = 0, \qquad (2.11)$$

where we have introduced the notation

$$\hat{\mathscr{H}}_1(t) = \hat H_1 + \hat H_1'(t). \qquad (2.12)$$

3. DEFINITION AND PROPERTIES OF THE OPERATOR OF PROJECTION ONTO THE L-SPACE

In zeroth approximation Eq. (2.11) takes the form

$$(\hat H_0 - i\hbar\partial/\partial t)C = 0 \qquad (3.1)$$

with the stationary solution

$$C(n;\ t) = C(n)\exp\left[-\frac{i}{\hbar}Et\right], \qquad (3.2)$$

given that

$$\hat H_0 C(n) = EC(n). \qquad (3.3)$$

The eigenvalues E in Eq. (3.3) depend on the total occupation numbers N_f^0:

$$E = E(\cdots N_f^0 \cdots),\ N_f = \sum_{\sigma} n_{f\sigma} \qquad (3.4)$$

[cf. Eq. (4.69) in Ref. 3]. The eigenfunctions corresponding to Eq. (3.4) are written in the form

$$C_\psi(n) = \Psi(n)\prod_f \delta(N_f - N_f^0), \qquad (3.5)$$

where Ψ is an arbitrary function of the occupation numbers. Thus in zeroth order the energy levels of the system are degenerate, and in the case in question the part of the "index" of the degenerate state is played by the function Ψ itself, since the form of the eigenfunction C_ψ depends on the choice of this function. We shall assume that the system of the C_ψ is already orthonormal.

Bogoliubov[3] has shown that in the approximation of quasi-homopolarity the lowest eigenvalue of the operator $\hat H_0$ is given by

$$E_0 = E(\cdots 1 \cdots). \qquad (3.6)$$

Following Refs. 1 — 3, we shall call the subspace (manifold) of eigenfunctions

$$C_{0\psi} = \Psi(n)\prod_f \delta(N_f - 1), \qquad (3.7)$$

corresponding to the lowest eigenvalue E_0 (the exactly homopolar states) the L-space.

We introduce the operator $\hat P_\psi$ which projects an arbitrary wave function C (n; t) onto the axis $C_{0\psi}$ of the L-space:

$$\hat P_\psi C(n;\ t) = a_\psi(t)\,C_{0\psi}(n), \qquad (3.8)$$

where $a_\psi(t)$ is a coefficient independent of the variables n but in general dependent on the time t. We determine this coefficient from the condition that the difference between the function C (n; t) and its projection onto the axis $C_{0\psi}$ is orthogonal to this axis:

$$(C_{0\psi}^*[C - \hat P_\psi C]) = 0. \qquad (3.9)$$

From this, using Eq. (3.8) and the orthonormality of the $C_{0\psi}$, we get

$$a_\psi(t) = (C_{0\psi}^* C). \qquad (3.10)$$

We call the operator

$$\hat P = \sum_\psi \hat P_\psi \qquad (3.11)$$

the projection operator onto the entire L-space. Clearly we have the equation

$$\hat P C(n;\ t) = \sum_\psi a_\psi(t)\,C_{0\psi}(n), \qquad (3.12)$$

where $a_\psi(t)$ is defined by Eq. (3.10)

It is also not difficult to show that the projection operator has the following properties:

$$\hat P^2 = \hat P,\ \hat P^+ = \hat P,\ \hat P\frac{\partial}{\partial t} = \frac{\partial}{\partial t}\hat P; \qquad (3.13)$$

$$\hat P \hat H_0 = \hat H_0 \hat P = E_0 \hat P; \qquad (3.14)$$

$$\hat P(\hat H_0 - i\hbar\partial/\partial t) = (\hat H_0 - i\hbar\partial/\partial t)\,\hat P,\ \hat P(\hat H_0 - i\hbar\partial/\partial t)^{-1} = (\hat H_0 - i\hbar\partial/\partial t)^{-1}\hat P. \qquad (3.15)$$

The last equation is valid only in cases in which the inverse operator contained in it actually exists (which is true in our further considerations).

4. EXTENSION OF THE BOGOLIUBOV-TIABLIKOV PERTURBATION METHOD TO THE NON-STATIONARY CASE

An arbitrary function C (n; t) can be represented in the form

$$C = C_0 + C_1, \qquad (4.1)$$

where $C_0 = \hat{P}C$ is its projection onto the L-space and $C_1 = (1 - \hat{P})C$ is a function orthogonal to the L-space, i.e.,

$$\hat{P}C_1 = 0. \tag{4.2}$$

Substituting Eq. (4.1) into Eq. (2.11), multiplying the resulting equation from the left by the operator $\hat{P}$, and using the properties of this operator, we get:

$$\begin{gathered}(\hat{H}_0 + \varepsilon\hat{P}\hat{\mathscr{H}}_1(t)\hat{P} + \varepsilon^2\hat{P}\hat{H}_2\hat{P} - i\hbar\partial/\partial t)\hat{P}C \\ + (\varepsilon\hat{P}\hat{\mathscr{H}}_1(t) + \varepsilon^2\hat{P}\hat{H}_2)C_1 = 0.\end{gathered} \tag{4.3}$$

Subtracting the two members of this equation from the equation which we had before multiplying by the operator $\hat{P}$, we find:

$$\begin{gathered}(\varepsilon\hat{\mathscr{H}}_1(t) + \varepsilon^2\hat{H}_2 - \varepsilon^2\hat{P}\hat{\mathscr{H}}_1(t)\hat{P} - \varepsilon^2\hat{P}\hat{H}_2\hat{P})\hat{P}C \\ + (\hat{H}_0 + \varepsilon\hat{\mathscr{H}}_1(t) + \varepsilon^2\hat{H}_2 - \varepsilon\hat{P}\hat{\mathscr{H}}_1(t) \\ - \varepsilon\hat{P}\hat{H}_2 - i\hbar\partial/\partial t)C_1 = 0.\end{gathered} \tag{4.4}$$

Since by Eq. (2.10) the perturbation by the light wave is of first order in ϵ, we can try to evaluate the function C_1 of Eq. (4.1) in the form of the series

$$C_1(n;\ t) = \varepsilon K(n;\ t) + \varepsilon^2 L(n;\ t) + \dots \tag{4.5}$$

Substituting Eq. (4.5) into Eq. (4.4), we get equations for the functions K and L; the solutions can be written in the form

$$K(n;\ t) = (\hat{H}_0 - i\hbar\partial/\partial t)^{-1}(\hat{P}\hat{\mathscr{H}}_1(t)\hat{P} - \hat{\mathscr{H}}_1(t))\hat{P}C(n;\ t),$$

$$\begin{gathered}L(n;\ t) = (\hat{H}_0 - i\hbar\partial/\partial t)^{-1}(\hat{P}\hat{H}_2\hat{P} - \hat{H}_2)\hat{P}C(n;\ t) + (H_0 - i\hbar\partial/\partial t)^{-1} \\ \times (\hat{P}\hat{\mathscr{H}}_1(t) - \hat{\mathscr{H}}_1(t))(\hat{H}_0 - i\hbar\partial/\partial t)^{-1}(\hat{P}\hat{\mathscr{H}}_1(t)\hat{P} - \hat{\mathscr{H}}_1(t))\hat{P}C(n;\ t).\end{gathered} \tag{4.6}$$

Generally speaking, the operator $(\hat{H}_0 - i\hbar\partial/\partial t)^{-1}$ does not always have a meaning. But in what follows we need only to know its effect on functions that depend exponentially on the time. In this case

$$(\hat{H}_0 - i\hbar\partial/\partial t)^{-1}e^{-i\Omega t} = e^{-i\Omega t}(H_0 - \hbar\Omega)^{-1}. \tag{4.7}$$

Since in fact $\hat{H}_0$ is not an operator, but a c-number, this expression always has a meaning except in the case $H_0 = \hbar\Omega$, which, as we shall see below, corresponds to a resonance. Consequently the calculations presented here hold for frequencies of the light that do not coincide with the proper frequencies of the system. Inclusion of damping makes it possible to consider the general case of arbitrary frequency of the incident light, as will be shown in a subsequent paper.

Using the properties of the projection operator (cf. Sec. 3), we can show without difficulty that

$$\hat{P}K = 0,\ \hat{P}L = 0. \tag{4.8}$$

Substituting (4.6) into (4.5), and then (4.5) into (4.3), and confining ourselves to the third approximation, we get

$$i\hbar\partial C_0(n;\ t)/\partial t = \tilde{H}(t)C_0(n;\ t), \tag{4.9}$$

where $\tilde{H}(t)$ differs from the corresponding expression for $\tilde{H}$ in Ref. 3 (cf. pp. 179 and 147) by the replacement of $\hat{H}_1$ by $\hat{\mathscr{H}}_1(t)$ and E by $i\hbar \times \partial/\partial t$.

Using the properties of the operator $\hat{P}$ and of the Fermi operators, one can prove the following relations:

$$\hat{P}\varepsilon\hat{H}_1\hat{P} = 0,\ \hat{P}\varepsilon\hat{H}_1'(t)\hat{P} = 0. \tag{4.10}$$

Recalling Eq. (2.12), we can separate the operator $\tilde{H}(t)$ into a term depending on the radiation field and one independent of it. Keeping only terms linear in the radiation field amplitude and noting the relations (4.10), we represent $\tilde{H}(t)$ in the form:

$$\tilde{H}(t) = \tilde{H} + \Delta\tilde{H} + \tilde{W}(t), \tag{4.11}$$

where $\tilde{H}$ and $\Delta\tilde{H}$ agree with the corresponding notations in Ref. 3 (see page 179), differing from them only by the replacement of E_0 by $i\hbar\partial/\partial t$, and

$$\begin{gathered}\tilde{W}(t) = \varepsilon^3\hat{P}\{-\hat{H}_1'(t)(H_0 - i\hbar\partial/\partial t)^{-1}\hat{H}_2 - \hat{H}_2 \\ \times(H_0 - i\hbar\partial/\partial t)^{-1}\hat{H}_1'(t) \\ + \hat{H}_1'(t)(H_0 - i\hbar\partial/\partial t)^{-1}\hat{H}_1(H_0 - i\hbar\partial/\partial t)^{-1}\hat{H}_1 \\ + \hat{H}_1(H_0 - i\hbar\partial/\partial t)^{-1}\hat{H}_1'(t)(H_0 - i\hbar\partial/\partial t)^{-1}\hat{H}_1 \\ + \hat{H}_1(H_0 - i\hbar\partial/\partial t)^{-1}\hat{H}_1(H_0 - i\hbar\partial/\partial t)^{-1}\hat{H}_1'(t)\}\hat{P}.\end{gathered} \tag{4.12}$$

In obtaining Eq. (4.12) we have used the relations

$$\begin{gathered}\varepsilon^2\hat{P}\hat{H}_1'(t)(H_0 - i\hbar\partial/\partial t)^{-1}\hat{H}_1\hat{P} = 0; \\ \varepsilon^2\hat{P}\hat{H}_1(H_0 - i\hbar\partial/\partial t)^{-1}\hat{H}_1'(t)\hat{P} = 0,\end{gathered} \tag{4.13}$$

which can be proved without difficulty by using the symmetry properties of the matrix elements appearing in the expressions for $\hat{H}_1$ and $\hat{H}_1'(t)$.

Equation (4.9) is now written in the form

$$i\hbar\partial C_0/\partial t = [\tilde{H} + \Delta\tilde{H} + \tilde{W}(t)]\,C_0. \qquad (4.14)$$

The solution of this equation has the form

$$C_0(n;\ t) = C_0^0(n)\exp\left(-\frac{i}{\hbar}Et\right) + C_0'(n;\ t), \qquad (4.15)$$

where the first term corresponds to the solution of the stationary equation [with $\tilde{W}(t) = 0$] and C_0' is the part determined by the radiative perturbation. Since the operator $\tilde{W}(t)$ is of third order in ϵ, C_0' will also be of third order. According to Ref. 3 the energy E in Eq. (4.15) is given by

$$E = E_0 + \varepsilon^2 E_1 + \varepsilon^3 E_2 + \cdots, \qquad (4.16)$$

The first order term is absent from this expression, since in first approximation the Hamiltonian $\tilde{H} + \Delta\tilde{H}$ does not differ from the same operator in zeroth approximation.[3]

In the expression for the average value of the electric current of the system in the electromagnetic field

$$\mathbf{J} = \left(C^*\left|-\frac{e}{m}\,\hat{\mathbf{I}} - \frac{e^2N}{mc}\mathbf{A}(t)\right|C\right) =$$
$$= \left(C_0^*(n)\exp\left[\frac{i}{\hbar}Et\right] + C_0^{*\prime}(n;\ t) + C_1^*(n;\ t)\left|-\frac{e}{m}\,\hat{\mathbf{I}}\right.\right.$$
$$\left.\left.-\frac{e^2N}{mc}\mathbf{A}(t)\right|C_0(n)\exp\left[-\frac{i}{\hbar}Et\right] + C_0'(n;\ t) + C_1(n;\ t)\right) \qquad (4.17)$$

the terms containing C_0' and $\hat{\mathbf{I}}$ are of order ϵ^4 or higher (since $C_0' \sim \epsilon^3$ and $\mathbf{I} \sim \epsilon$), and the terms containing C_0' and $\mathbf{A}(t)$ are quadratic in the radiation field amplitude; therefore in calculating the current to third order we can neglect the terms in question. Then, recalling Eq. (4.5), we have

$$\mathbf{J} = \left(C_0^*(n)\exp\left[\frac{i}{\hbar}Et\right] + \varepsilon K^* + \varepsilon^2 L^* + \cdots\right.$$
$$\left.\cdots\left|-\frac{e}{m}\,\hat{\mathbf{I}}\right|C_0(n)\exp\left[-\frac{i}{\hbar}Et\right] + \varepsilon K + \varepsilon^2 L + \cdots\right). \qquad (4.18)$$

In the expression for the current operator in Eq. (4.17) we consider only the first term $-(e/m)\hat{\mathbf{I}}$, since the second term is not actually an operator and gives a trivial correction to the dielectric permeability of the crystal.

Using Eq. (4.7) and the identity

$$i\hbar\frac{\partial}{\partial t}C_0(n)\exp\left[-\frac{i}{\hbar}Et\right] = \exp\left[+\frac{i}{\hbar}Et\right]\left(E + i\hbar\frac{\partial}{\partial t}\right)C_0(n),$$

we can put Eq. (4.18) in the following form:

$$\mathbf{J} = -\frac{e}{m}(C_0^*(n)\,M(\hat{\mathbf{I}})\,C_0(n)), \qquad (4.19)$$

where

$$M(\hat{\mathbf{I}}) = \hat{P}\hat{\mathbf{I}}\hat{P} + D(\hat{\mathbf{I}}) + D^+(\hat{\mathbf{I}}) = D(\hat{\mathbf{I}}) + D^+(\hat{\mathbf{I}}), \qquad (4.20)$$

since $\hat{\mathbf{P}}\hat{\mathbf{I}}\hat{\mathbf{P}} = 0$, and

$$D(\hat{\mathbf{I}}) = \hat{P}\left\{-\varepsilon\hat{\mathbf{I}}\left(H_0 - E_0 - i\hbar\frac{\partial}{\partial t}\right)^{-1}\hat{\mathscr{H}}_1(t) - \varepsilon^2\hat{\mathbf{I}}\left(H_0 - E_0 - i\hbar\frac{\partial}{\partial t}\right)^{-1}(\hat{H}_2 - \hat{P}\hat{H}_2\hat{P}) + \varepsilon^2\hat{\mathbf{I}}\left(H_0 - E_0 - i\hbar\frac{\partial}{\partial t}\right)^{-1}(\hat{\mathscr{H}}_1(t)\right.$$
$$\left.-\hat{P}\hat{\mathscr{H}}_1(t))\left(H_0 - E_0 - i\hbar\frac{\partial}{\partial t}\right)^{-1}\hat{\mathscr{H}}_1(t) + \frac{\varepsilon^2}{2}\left[\left(H_0 - E_0 - i\hbar\frac{\partial}{\partial t}\right)^{-1}\hat{\mathscr{H}}_1(t)\right]^+\hat{\mathbf{I}}\left[\left(H_0 - E_0 - i\hbar\frac{\partial}{\partial t}\right)^{-1}\hat{\mathscr{H}}_1(t)\right]\right\}\hat{P}. \qquad (4.21)$$

In deriving this expression we have everywhere replaced E by E_0, in view of Eq. (4.16); that is, we have set

$$\varepsilon(H_0 - E_0 - \varepsilon^2 E_1 - i\hbar\partial/\partial t)^{-1} \approx \varepsilon(H_0 - E_0 - i\hbar\partial/\partial t)^{-1},$$

which is legitimate if we neglect in this expression all terms beginning from the third order of small quantities (which corresponds to the fact that in Eq. (4.21) terms beginning from the third order are dropped, because $\hat{\mathbf{I}} \sim \epsilon$).

From this it follows that in the approximation considered the absorption spectrum of the system of electrons in the crystal is a discrete one, since in this approximation the splitting-up of the energy levels into bands has practically no effect. Physically this means that the "pairs" and "holes" that appear under the action of the radiation field remain in bound states, and the absorption of light by the crystal is not photoelectrically active absorption, i.e., does not lead to the appearance of current states. It is only this sort of absorption of light that can be treated by the projection method, with the definition of the projection operator that we have given above.

From Eq. (4.20) we note that the operator $M(\hat{\mathbf{I}})$, like $\hat{\mathbf{I}}$ itself, is Hermitian. We call it the "deformed" operator for the current (in analogy with the usage in Refs. 1 – 3).

Thus, to determine the average value of the current (4.1), with C_1 given by Eq. (4.5), one needs only to find the projection of the wave function onto the L-space and the "deformed" current operator.

5. DETERMINATION OF THE "DEFORMED" CURRENT OPERATOR

By the use of Eq. (2.12) we can make a separation of the expression (4.21) into two terms, as in Eq. (4.11); we thus obtain a current operator independent of the radiative perturbation (this part of the current is the same as given in Ref. 3 and is of no interest to us here), and a current operator dependent on the radiative perturbation. We give only the final result of the calculation of this second term, because of the cumbersome, though simple, manipulations required; for more detailed information the reader is referred to Ref. 5:

$$M(\hat{\mathbf{I}}) = \frac{e}{mc\hbar}\Big\{-\sum S_1(ff_1) + \sum S_5(ff_1f_2) + \sum S_1(ff_1)\,\hat{a}^{+}_{f\sigma}\hat{a}_{f\sigma_1}\hat{a}^{+}_{f_1\sigma_1}\hat{a}_{f_1\sigma} - \sum [S_5(ff_1f_2) + S_6(ff_2f_1) + S_5(f_2ff_1)]\,\hat{a}^{+}_{f\sigma}\hat{a}_{f\sigma_1}\hat{a}^{+}_{f_1\sigma_1}\hat{a}_{f_1\sigma}$$

$$+ \sum [S_7(ff_1f_2) + S_7\,(f_1ff_2)]\,\hat{a}^{+}_{f\sigma}\hat{a}_{f\sigma_2}\hat{a}^{+}_{f_1\sigma_1}\hat{a}_{f_1\sigma}\,\hat{a}^{+}_{f_2\sigma_2}\hat{a}^{+}_{f_2\sigma_1}\Big\}\,\mathbf{A}(t) + i\,\frac{e}{mc\hbar}\Big\{\sum [S'_{33}(ff_1f_2) - S'_{33}(f_1ff_2)]\,\hat{a}^{+}_{f\sigma}\hat{a}_{f\sigma_2}\hat{a}^{+}_{f_1\sigma_1}\hat{a}_{f_1\sigma}\hat{a}^{+}_{f_2\sigma_2}\hat{a}_{f_2\sigma_1}\Big\}\,\dot{\mathbf{A}}(t). \tag{5.1}$$

Here we have introduced the following notations*

$$\begin{aligned} S_5(ff_1f_2) &= S_2(ff_1f_2) + S_{31}(ff_1f_2) + S_4(ff_1f_2),\\ S_6(ff_1f_2) &= S_2(ff_1f_2) + S_{32}(ff_1f_2) + S_4(ff_1f_2),\\ S_7(ff_1f_2) &= S_2(ff_1f_2) + S_3(ff_1f_2) + S_4(ff_1f_2). \end{aligned} \tag{5.2}$$

$$\begin{aligned} S_1(ff_1) &= \frac{\omega(ff_1)}{\omega(ff_1)^2 - \omega^2}\,D(ff_1),\\ S_2(ff_1f_2) &= \frac{\omega(ff_1)\cdot\Lambda(ff_2)}{\hbar\omega(ff_2)\,[\omega(ff_1)^2 - \omega^2]}\,D(ff_1;\ f_1f_2),\\ S_3(ff_1f_2) &= \frac{[\omega(ff_1)\cdot\omega(f_1f_2) + \omega^2]\,\Lambda(ff_2)}{\hbar\,[\omega(ff_1)^2 - \omega^2]\,[\omega(f_1f_2)^2 - \omega^2]}\,D(ff_1;\ f_1f_2),\\ S_{31}(ff_1f_2) &= \frac{[\omega(ff_1)\cdot\omega(f_1f_2) + \omega^2]\,\Lambda_1(ff_2)}{\hbar\,[\omega(ff_1)^2 - \omega^2]\,[\omega(f_1f_2)^2 - \omega^2]}\,D(ff_1;\ f_1f_2),\\ S_{32}(ff_1f_2) &= \frac{V_{f_1f_2}(ff_2)\,[\omega(ff_1)\,\omega(f_1f_2) + \omega^2]}{\hbar\,[\omega(ff_1)^2 - \omega^2]\,[\omega(f_1f_2)^2 - \omega^2]}\,D(ff_1;\ f_1f_2),\\ S'_{33}(ff_1f_2) &= \frac{[\omega(ff_1) + \omega(f_1f_2)]\cdot[F(ff_1;\ f_2f_1) - F(ff_2;\ f_2f_2)]}{\hbar\,[\omega(ff_1)^2 - \omega^2]\,[\omega(f_1f_2)^2 - \omega^2]}\,D(ff_1;\ f_1f_2),\\ S_4(ff_1f_2) &= \frac{\omega(f_1f_2)\,\Lambda(ff_2)}{\hbar\omega(ff_2)\,[\omega(f_1f_2)^2 - \omega^2]}\,D(ff_1;\ f_1f_2). \end{aligned} \tag{5.3}$$

$$\omega(ff_1) = \Delta(ff_1)/\hbar, \tag{5.4}$$

$$\Lambda(ff_1) = L(ff_1) + \sum_{\substack{f''\\(\neq f)}} F(ff'';\ f_1f''), \quad V_{f_2f_1}(ff_2) = L(ff_2) + \sum_{f''} F(ff'';\ f_2f'')\,(1 - \delta_{f''f_2} + \delta_{f''f_1} - \delta_{f''f}). \tag{5.5}$$

In addition we have introduced the tensor notations (i, k = x, y, z):

$$\begin{aligned} D(ff_1)_{ik} &= 2I_i(ff_1)\,I_k(f_1f),\\ D(ff_1;\ f_1f_2)_{ik} &= 2I_i(ff_1)\,I_k(f_1f_2). \end{aligned} \tag{5.6}$$

The quantity $\Delta(ff_1)$ in Eq. (5.4) represents the energy required for the production of a single pair with electron and "hole" at the points f and f_1. In the expression (5.1) the terms containing $S_1(ff_1)$ are small quantities of the second order, and all the other terms are of the third order. The interaction between the electrons affects only the third order terms, since these are the only ones that contain the interaction integrals.

As was shown in Ref. 3, when the only external electric field is one stationary in time, the "deformed" current operator is non-vanishing only in third order. In our case part of the "deformed" current operator produced by the radiation field is non-vanishing already in the second approximation.

By applying the method of approximate diagonalization to the operator (5.1) one can find the average value of the electric current density. Then, comparing this with the macroscopic expression for the electric current density in the crystal in the field of the light wave,

$$\mathbf{j} = \frac{\varepsilon - 1}{4\pi}\frac{\omega^2}{c^2}\,\mathbf{A}(t) - \frac{\sigma}{c}\,\dot{\mathbf{A}}(t), \tag{5.7}$$

one can derive the dispersion formulas for the dielectric permittivity $\epsilon = \epsilon(\omega)$ and electric con-

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*The summation is taken over all indices $f\sigma$ that appear under summation signs in Eq. (5.1), except indices f appearing equal in pairs.

ductivity $\sigma = \sigma(\omega)$. Using the connection between these quantities and the optical constants, it is then easy to find the dispersion formulas for the index of refraction $n = n(\omega)$ and the extinction coefficient $k = k(\omega)$. If in these calculations we keep the third order terms, we have a derivation of the dispersion formulas with approximate inclusion of the effects of interaction between the electrons.

This opens up possibilities for the development of a many-electron theory of the optical properties of crystals within the framework of the quasi-homopolar approximation.

The practical realization of this program encounters mathematical difficulties in connection with the diagonalization of the operator (5.1).

Using Tiablikov's method of approximate diagonalization,[2,3] which is correct for weak perturbations of the system, it is possible in principle to carry out the indicated program for some particular case, for example for a ferromagnetic crystal in a state close to saturation.

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15

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CONTRIBUTION TO THE THEORY OF ANTIFERROMAGNETISM AT LOW TEMPERATURES

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The energy spectrum of a uniaxial antiferromagnetic substance is obtained without the assumption of nominal magnetization of the spin sublattices in the ground state.

THE existing theory of antiferromagnetism[1] is based on the hypothesis (first proposed by Landau[2]) that an antiferromagnetic substance can be described in terms of two or more magnetic moments, which compensate each other in the absence of magnetic field. The construction of the microscopic theory of antiferromagnetism ordinarily begins with the Heisenberg model of exchange interaction and the assumption of a regular ordering of "left" and "right" spins in the ground state.[3,4]

As has been remarked by Landau, such an assumption is in contradiction with quantum mechanics: the spin component of an individual atom in a prescribed direction cannot have a definite value, because of the exchange interaction. On the other hand it appears that the experimental data do not contradict the results obtained by the use of this model.

The purpose of the present paper is to show that the energy spectrum of an antiferromagnetic substance, and thus all of its thermodynamic functions, can be obtained in a phenomenological way just from the assumption of two (or more) sublattices, without postulating nominal magnetization of each of the sublattices in the ground state.

1. The assumption of the existence of two (or several) sublattices can be reduced to the assumption that the state of an antiferromagnetic substance is characterized by the specification of two (or several) magnetic moments $\mathbf{M}_i(\mathbf{r})$ at each point. Here one picks out as the ground state the state with homogeneous values of each of the magnetic