Analogue of the Kubo Formula for Conductivity of Spatially Inhomogeneous Systems and Electric Fields.

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The average densities of currents and charges, induced by a weak electromagnetic field in spatially inhomogeneous systems, are calculated at finite temperatures. The Kubo formula for a conductivity tensor is generalized for spatially inhomogeneous systems and fields. The contributions containing electric fields and derivative from fields on coordinates are allocated. The Semiconductor quantum wells, wires and dots may be considered as spatially inhomogeneous systems.

I. INTRODUCTION

In connection with an increased interest to experimental and theoretical study of low dimensional semiconductor objects - quantum wells, wires and dots - a construction of the fundamental theory of interaction of electromagnetic fields with spatially inhomogeneous systems becomes actual.

R. J. Kubo [1] obtained the formula for the conductivity tensor \( \sigma_{\alpha\beta}(\omega) \), applicable in a case of spatially homogeneous systems and electric fields \( E(t) \) independent of spatial coordinates. This formula takes into account exactly the interaction of current carriers with the medium. Consequently, it is a powerful tool for the solution of concrete conductivity problems in solids.

In present work we generalize the Kubo formula on a case of spatially inhomogeneous systems and fields. Previously we calculate average densities of currents and charges induced by electromagnetic field.

Kubo [1] used the interaction operator of current carriers with the electric field as

\[
U_K = - \sum_i e_i r_i E(t),
\]

(1)

where \( e_i \) and \( r_i \) are the charge and radius - vector of \( i \)-th particle, respectively, \( E(t) \) is the time-dependent, but spatially homogeneous electric field. However, it follows from the Maxwell equations that the time-dependent electric field necessarily depends and on coordinates, so the use of Eq. (1) is always a certain approximation, if the field \( E \) depends on \( t \). In spatially inhomogeneous systems the dependence of fields on coordinates can be essential.

Our task consists in taking into account of heterogeneity of systems and in obtaining of additional terms in the Kubo formula containing derivatives from electric field on coordinates.

The operator of interaction of an electromagnetic field with a system of charged particles is expressed through the vector \( A(r, t) \) and scalar \( \varphi(r, t) \) potentials (see, for example, [2], page 68), but it is not expressed through electric \( E(r, t) \) and magnetic \( H(r, t) \) fields, except of individual cases as, for example, a constant electric field. Accordingly and operators of densities of currents \( j_i(r, t) \) and charges \( \rho_i(r, t) \) in linear approximation on vector and scalar potentials are not expressed through \( E(r, t) \) and \( H(r, t) \). However, average values \( \langle j_i(r, t) \rangle \) and \( \langle \rho_i(r, t) \rangle \) should be expressed through fields, as the observable values. At finite temperatures \( T \) an average value is defined as [1,3,4]

\[
\langle \ldots \rangle = \frac{Sp\{\exp(-\beta \mathcal{H})\ldots\}}{Sp\{\exp(-\beta \mathcal{H})\}}, \quad \beta = \frac{1}{kT}, \quad (2)
\]

\( \mathcal{H} \) is the Hamiltonian without an interaction of particles with a weak electromagnetic field.

The expressions for average \( \langle 0 | j_1(r, t) | 0 \rangle \) and \( \langle 0 | \rho_1(r, t) | 0 \rangle \) for \( T = 0 \) (when average \( \langle \ldots \rangle \) passes in average \( \langle 0 | \ldots | 0 \rangle \) on the ground state \( | 0 \rangle \) are obtained in [5]. The present work is a direct continuation of [5]. The designations and many results of [5] will be used below.

The problem of an expression of average \( \langle j_1(r, t) \rangle \) and \( \langle \rho_1(r, t) \rangle \) through electric and magnetic fields is essential also because if to express average \( \langle j_1(r, t) \rangle \) through vector and scalar potentials, this average contains the contribution \(-e/mc \langle \rho(r) \rangle A(r, t)\), where \( e = e_i, m = m_i \) are the charge and mass of the particle, \( c \) is the light velocity, \( \rho(r) \) is the operator of the charge density in a zero approximation on fields (see Eq. (9) below). This contribution creates complexities at solutions of some concrete tasks, for example, about light reflection and absorption by semiconductor quantum wells. These complexities may be avoided if to express the average \( \langle j_1(r, t) \rangle \) and
\langle \rho_i(r, t) \rangle \text{ through electric fields and their derivatives on coordinates.}

The question on what kind of interaction to use - containing the vector potential or electric field - was discussed earlier in [6] with reference to a task about light scattering in bulk crystals. In [6] apparently for the first time the reception is used from the operators \( v_i \) of particles velocities to the operators \( r_i \) of coordinates according to a quantum ratio \( v_i = (i/\hbar)[H, r_i] \), due to which it is possible to pass from expressions containing vector potential to expressions containing electric fields. However, as we should solve other tasks about spatially - inhomogeneous systems, it is necessary again to come back to this theme.

Considering finite temperatures we use mathematical receptions offered in [1,3]. We compare our results with conclusions of [4] devoted to construction of the quantum theory of a spatial dispersion electric and magnetic susceptibilities. It is supposed below that there are no changes and currents on the indefinitely removed distances and that the fields \( E(r, t) \) and \( H(r, t) \) are equal 0 on times \( t \to -\infty \) what corresponds to adiabatic field switching.

II. THE SYSTEM HAMILTONIAN AND OPERATORS OF CURRENT AND CHARGE DENSITIES.

Let us consider a system of \( N \) particles with the charge \( e \) and the mass \( m \) in any arbitrary weak electromagnetic field, characterized by intensities \( E(r, t) \) and \( H(r, t) \). Let us introduce vector \( A(r, t) \) and scalar \( \varphi(r, t) \) potentials so that

\[
E(r, t) = -\frac{1}{c} \frac{\partial A(r, t)}{\partial t} - \text{grad} \varphi(r, t),
\]

\[
H(r, t) = \text{rot} A(r, t). \tag{3}
\]

The fields are assumed classical, the gauge of potentials \( A \) and \( \varphi \) is any. For completeness of the task we shall admit, that the system of particles may be placed in the constant magnetic field \( H \) which may be strong. The vector potential \( A(r) \) corresponds to this field, so that \( H = \text{rot} A(r) \). The total Hamiltonian \( H_{total} \) is as follows

\[
H_{total} = \frac{1}{2m} \sum_i (p_i - \frac{e}{c} A(r_i))^2 + V(r_1, \ldots r_N) + e \sum_i \varphi(r_i, t), \tag{4}
\]

where \( P_i = -i\hbar(\partial/\partial r_i) \) is the generalized momentum operator, \( V(r_1, \ldots r_N) \) is the potential energy, including interaction between particles and an external potential. In Eq. (4) it is necessary to take into account noncommutativity of \( P_i \) and \( A(r_i) \), \( A(r_i, t) \). Let us allocate in Eq. (4) the energy \( U \) of the interaction of particles with electromagnetic field, including interaction with a strong magnetic field in the basic Hamiltonian \( H \)

\[
H_{total} = H + U, \tag{5}
\]

where the designations are introduced

\[
H = \frac{1}{2m} \sum_i p_i^2 + V(r_1 \ldots r_N), \quad P_i = P_i - \frac{e}{c} A(r_i), \tag{6}
\]

\[
U = U_1 + U_2,
\]

\[
U_1 = -\frac{1}{e} \int d^3r j(r)A(r, t) + \int d^3r \rho(r)\varphi(r, t),
\]

\[
U_2 = \frac{e}{2mc} \int d^3r \rho(r)A^2(r, t) \tag{7}
\]

The operators of densities of currents and charges are also introduced

\[
j(r) = \sum_i j_i(r),
\]

\[
\rho(r) = \sum_i \rho_i(r), \quad \rho_i(r) = e\delta(r - r_i).
\]

The operators \( j_i(r) \) and \( \rho_i(r) \) are connected by the continuity equation

\[
div j_i(r) + \dot{\rho}_i(r) = 0, \quad \dot{\rho}_i(r) = \frac{i}{\hbar}[H, \rho_i(r)], \tag{8}
\]

which will be used below. The operator \( U_2 \) is out of the frameworks of linear approximation on fields and is omitted below.

In the Heisenberg representation the additives to the operators of densities of currents and charges linear on potentials \( A(r, t) \) and \( \varphi(r, t) \) are equal

\[
\dot{j}_{\alpha}(r, t) = -\frac{e}{mc} \rho(r, t)A_{\alpha}(r, t)
\]

\[
+ \frac{i}{\hbar} \int_{-\infty}^{t} dt'[U_1(t'), j_{\alpha}(r, t)],
\]

\[
\dot{\rho}_i(r, t) = \frac{i}{\hbar} \int_{-\infty}^{t} dt'[U_1(t'), \rho_i(r, t)], \tag{9}
\]

where the subscript 1 means a linear approximation on fields, \( \rho(r, t), j(r, t) \) and \( U_1(t) \) are operators in the interaction representation, for example,

\[
\rho(r, t) = e^{i\hat{H}t/\hbar} \rho(r) e^{-i\hat{H}t/\hbar}, [F, Q] = FQ - QF \text{ is the commutator of the operators } F \text{ and } Q.
\]

By substituting Eq. (7) into Eq. (9) we obtain for \( U_1 \)
\[ j_{1\alpha}(r, t) = -\frac{e}{mc} \rho(r, t) A_{\alpha}(r, t) \]
\[ + \frac{i}{\hbar c} \int d^3r' \int_{-\infty}^{t} dt'[j_{1\alpha}(r, t), j_{\beta}(r', t')] A_{\beta}(r', t') \]
\[ - \frac{i}{\hbar c} \int d^3r' \int_{-\infty}^{t} dt'[\rho(r, t), j_{\beta}(r', t')] A_{\beta}(r', t') \phi(r', t'). \]
\[ \langle j_{1\alpha}(r, t) \rangle_{\mathcal{F}} = \frac{c}{\hbar} \int d^3r' \int_{-\infty}^{t} dt' \]
\[ \times \langle \{\rho(r, t, Y_{\beta\gamma}(r', t'))\} \rangle_{\mathcal{F}} \frac{\partial a_{\beta}(r', t')}{\partial r_{\gamma}'}, \]
\[ \text{where the designations are introduced} \]
\[ d(r) = r \rho(r), \quad Y_{\beta\gamma}(r) = r_{\beta} j_{\gamma}(r), \]
\[ a(r, t) = -c \int_{-\infty}^{t} dt' e(r, t'). \]

Let us transform the obtained expressions so that the transition to the Kubo formula for spatially homogeneous systems and electric field independent on coordinates would be seen clearly. We use the ratio [1,3]
\[ \frac{i}{\hbar} \langle [F(t), Q(t')] \rangle = \int_{0}^{\beta} d\lambda (\frac{dQ(t')}{dt'} F(t + i\hbar\lambda)), \]
true for any pair operators \( F \) and \( Q \). Using Eq. (19) we obtain from Eq. (13)
\[ \langle j_{1\alpha}(r, t) \rangle_{E} = \int d^3r' \int_{-\infty}^{t} dt' \int_{0}^{\beta} d\lambda \]
\[ \times \langle \{\partial d_{\beta}(r', t') \rangle \rangle_{\mathcal{F}} j_{\alpha}(r, t + i\hbar\lambda) E_{\beta}(r', t'), \]
\[ \text{It is possible to show that} \]
\[ \frac{\partial d_{\beta}(r, t)}{\partial t} = -r_{\beta} \frac{\partial j_{\alpha}(r, t)}{\partial r_{\alpha}}. \]

Substituting Eq. (21) in Eq. (20) and integrating on \( r' \) in parts we obtain
\[ \langle j_{1\alpha}(r, t) \rangle_{E} = \int d^3r' \int_{-\infty}^{t} dt' \int_{0}^{\beta} d\lambda \]
\[ \times \langle j_{\beta}(r', t') j_{\alpha}(r, t + i\hbar\lambda) \rangle E_{\beta}(r', t') \]
\[ + \int d^3r' \int_{-\infty}^{t} dt' \int_{0}^{\beta} d\lambda \]
\[ \times \langle Y_{\beta\gamma}(r', t') j_{\alpha}(r, t + i\hbar\lambda) \rangle \frac{\partial E_{\beta}(r', t')}{\partial r_{\gamma}'}. \]

In agreement with Eq.(15) the expression for \( \langle j_{1\alpha}(r, t) \rangle_{\partial E/\partial r} \) consists of two parts. We do not transform first of them, and in the second we integrate on \( t' \) in parts and afterwards use Eq. (19). It results in
\[ \langle j_{1\alpha}(r, t) \rangle_{\partial E/\partial r} = \frac{e}{mc} \langle d_{\beta}(r) \rangle \frac{\partial a_{\beta}(r, t)}{\partial r_{\alpha}} \]
\[ - \frac{1}{c} \int d^3r' \int_{0}^{\beta} d\lambda (Y_{\beta\gamma}(r') j_{\alpha}(r, t + i\hbar\lambda)) \frac{\partial a_{\beta}(r', t')}{\partial r_{\gamma}'} \]
\[ - \int d^3r' \int_{-\infty}^{t} dt' \int_{0}^{\beta} d\lambda (Y_{\beta\gamma}(r', t') j_{\alpha}(r, t + i\hbar\lambda)) \]
\[ \times \frac{\partial E_{\beta}(r', t')}{\partial r_{\gamma}'} . \]
Summing Eqs. (22) and (23) we see that last terms in the RHSs of both formulas are reduced. Total expression we break on two parts

\[ \langle j_{1\alpha}(r, t) \rangle = \langle j_{1\alpha}(r, t) \rangle^{(1)} + \langle j_{1\alpha}(r, t) \rangle^{(2)} \]  

(24)

so, that the first part contains an electric field, and the second contains a derivative from field on coordinates, i.e.

\[ \langle j_{1\alpha}(r, t) \rangle^{(1)} = \int d^3r' \int t' dt' \int_0^\beta d\lambda \times (j_\beta(r', t')j_\alpha(r, t + i\hbar \lambda))E_\beta(r', t'), \]

(25)

\[ \langle j_{1\alpha}(r, t) \rangle^{(2)} = \frac{e}{mc} (d_\beta(r)) \frac{\partial a_\beta(r, t)}{\partial r_\alpha} - \frac{1}{c} \int d^3r' \int_0^\beta d\lambda (Y_\beta(r')j_\alpha(r, i\hbar \lambda)) \frac{\partial a_\beta(r', t)}{\partial r_\gamma}. \]

(26)

It is obvious, that the splitting Eq. (24) does not coincide with splitting Eq. (12) convenient only at \( T = 0 \).

By similar way we obtain from Eqs. (14) and (16)

\[ \langle \rho_1(r, t) \rangle = \langle \rho_1(r, t) \rangle^{(1)} + \langle \rho_1(r, t) \rangle^{(2)}, \]

(27)

\[ \langle \rho_1(r, t) \rangle^{(1)} = \int d^3r' \int t' dt' \int_0^\beta d\lambda \times (j_\beta(r', t')\rho(r, t + i\hbar \lambda))E_\beta(r', t'), \]

(28)

\[ \langle \rho_1(r, t) \rangle^{(2)} = -\frac{1}{c} \int d^3r' \int_0^\beta d\lambda (Y_\beta(r')\rho(r, i\hbar \lambda)) \frac{\partial a_\beta(r', t)}{\partial r_\gamma}. \]

(29)

By obtaining Eqs. (24) - (29) we have reached our main goal: We have allocated the basic contributions with subscript (1) in average values of induced densities of currents and charges and also have shown that the additional contributions with subscript (2) contain derivatives from, electric field on coordinates. The sense of splitting on basic and additional contributions is that at solution of any tasks, in which the field \( \mathbf{E}(r, t) \) is spatially inhomogeneous, it is possible to estimate magnitudes of additional contributions and to determine: It is necessary to take them into account or it is possible to reject them. As well as in the case \( T = 0 \), obtained expressions contain the operators \( r_i \) of particle coordinates unlike initial Eqs. (10) and (11) which do not contain these operators.

IV. COMPARISON WITH RESULTS OF [4].

In [3,4] the expressions for values \( \{ j_1(r, t) \} \) are received at finite temperatures, but these expressions differ from deduced by us and above mentioned. Parallel we make similar calculations of the value \( \{ \rho_1(r, t) \} \), which was not considered in [1,3,4], but in the Maxwell equations it acts on the equal rights with average density of a current. Let us notice that in [1,3] it was considered homogeneous medium, in [4] - inhomogeneous. Solving the equation for the density matrix authors of [3] and [4] come to the formula, which may be obtained from Eq. (10), if in the RHS and in the LHS to realize averaging \( \langle \ldots \rangle \) determined in Eq. (2). It is obvious, that similar expression for \( \{ \rho_1(r, t) \} \) may be obtained by averaging both sides of Eq. (11).

Further the authors of [3] and [4] transform the expression for the average induced current density in such a manner that the electric field \( \mathbf{E}(r, t) \) appears in it and it contains the vector potential \( \mathbf{A}(r, t) \) simultaneously. By doing similar procedure in initial expression for the average induced charge density we obtain the result of a kind of Eq. (27), in which the contribution \( \{ \rho_1(r, t) \}^{(1)} \) is determined by Eq. (28) and the contribution \( \{ \rho_1(r, t) \}^{(2)} \) is equal

\[ \langle \rho_1(r, t) \rangle^{(2)} = \frac{1}{c} \int d^3r' \int_0^\beta d\lambda \rho(r', i\hbar \lambda) \times A_\beta(r', t). \]

(30)

For the contribution \( \{ j_{1\alpha}(r, t) \}^{(1)} \) from the RHS of Eq. (24) in [3,4] the result of Eq. (25) is obtained, as well as the expression

\[ \langle j_{1\alpha}(r, t) \rangle^{(2)} = -\frac{e}{mc} \rho(r)A_\alpha(r, t) \]

\[ +\frac{1}{c} \int d^3r' \int_0^\beta d\lambda \rho(r')j_\alpha(r, i\hbar \lambda) A_\beta(r', t). \]

(31)

The authors of [4] went further. With the help of Eq. (31) they have expressed the derivative from \( \{ j_{1\alpha}(r, t) \}^{(2)} \) through an electric field. Integrating this derivative on time we obtain

\[ \langle j_{1\alpha}(r, t) \rangle^{(2)} = -\frac{e}{mc} \rho(r) A_\alpha(r, t) \]

\[ +\frac{1}{c} \int d^3r' \int_0^\beta d\lambda \rho(r')j_\alpha(r, i\hbar \lambda) a_\beta(r', t). \]

(32)

and analogously

\[ \langle \rho_1(r, t) \rangle^{(2)} = \frac{1}{c} \int d^3r' \int_0^\beta d\lambda \rho(r', i\hbar \lambda) \times a_\beta(r', t). \]

(33)

Thus, the formulas for the additional contributions of two kinds are obtained: Eqs. (26) and (29), containing only derivatives of electric fields on coordinates, and Eqs. (32) and (33), containing the electric field itself.

Let us show how it is possible to pass from Eq. (26) to Eq. (32), and from Eq. (29) to Eq. (33). In last term
from the RHS of Eq. (26) we integrate on \( r'_\gamma \) in parts. Then we use the equality

\[
\frac{dY_{\beta\alpha}(r)}{dr_\gamma} = j_\beta(r) + r_\beta(\partial j_\gamma(r)/\partial r_\gamma)
\]

\[= j_\beta(r) - r_\beta \dot{\rho}(r). \tag{34} \]

Then from Eq. (26) we have

\[
\langle j_{1\alpha}(r,t) \rangle^{(2)} = \frac{e}{mc} \langle \dot{d}_\beta(r) \rangle \frac{\partial A_\beta(r,t)}{\partial r_\alpha} 
+ \frac{1}{c} \int d^3r' \int_0^\beta d\lambda(j_\beta(r')j_\alpha(r,i\hbar\lambda))a_\beta(r',t) 
- \frac{1}{c} \int d^3r'r_\beta \int_0^\beta d\lambda(\dot{\rho}(r')j_\alpha(r,i\hbar\lambda))a_\beta(r',t). \tag{35} \]

In the last term we use Eq. (19) and integrate on \( r' \). We obtain that this last term is equal

\[-\frac{ie}{\hbar c}\langle [j_\alpha(r), \sum_i r_i \beta a_\beta(r_i,t)] \rangle = -\frac{e}{mc} \langle [\dot{\rho}(r)]a_\alpha(r,t) \rangle 
+ \langle \dot{d}_\beta(r) \rangle \langle \frac{\partial A_\beta(r,t)}{\partial r_\alpha} \rangle. \tag{36} \]

By substituting it in Eq. (35) we come to result of Eq. (32), as it was required to prove. We transform similarly Eq. (29) for \( \langle \rho_1(r,t) \rangle^{(2)} \). The difference consists only that instead of Eq. (36) we have

\[-\frac{ie}{\hbar c}\langle [j_\alpha(r), \sum_i r_i \beta a_\beta(r_i,t)] \rangle = 0 \]

and from Eq. (29) we pass to Eq. (33).

Thus, comparing our results with results of [3] and [4], we have proved applicability of Eqs. (26) and (29) for the additional contributions in average values of the induced densities of current and charge containing only derivatives on coordinates from electric fields.

V. THE ANALYSIS OF THE FORMULAS FOR THE ADDITIONAL CONTRIBUTION TO THE AVERAGE DENSITY OF A CURRENT.

The value \( \langle j_{1\alpha}(r,t) \rangle^{(2)} \) is determined in three forms of Eqs. (26), (31) and (32). In [4] some properties of this value are listed. Let us continue its research and we shall obtain the fourth expression for \( \langle j_{1\alpha}(r,t) \rangle^{(2)} \) through derivatives of vector potential \( \mathbf{A}(r,t) \) on coordinates. In the second term of Eq. (31) for \( j_\beta(r') \) we use Eq. (34). It results in splitting of the second term into two parts: In first of them we integrate on \( r'_\gamma \) in parts, in the second we use the formula

\[
\frac{i}{\hbar}\langle [F,Q] \rangle = \int_0^\beta d\lambda \langle \dot{Q} F(i\hbar\lambda) \rangle, \tag{37} \]

which follows from Eq. (19) at \( t' = t \). By calculating the commutator we obtain

\[
\langle j_{1\alpha}(r,t) \rangle^{(2)} = \frac{e}{mc} \langle \dot{d}_\beta(r) \rangle \frac{\partial A_\beta(r,t)}{\partial r_\alpha} 
- \frac{1}{c} \int d^3r' \int_0^\beta d\lambda(j_\beta(r')j_\alpha(r,i\hbar\lambda)) \frac{\partial A_\beta(r',t)}{\partial r_\alpha}. \tag{38} \]

For reception one more - fifth - expression for the additional contribution to the density of a current we apply Eq. (34) to the value \( j_\alpha(r,i\hbar\lambda) \) from Eq. (31), and also following updating of Eq. (37)

\[
\frac{i}{\hbar}\langle [F,Q] \rangle = \int_0^\beta d\lambda \langle \dot{Q} F(i\hbar\lambda) \rangle. \tag{39} \]

It results in

\[
\langle j_{1\alpha}(r,t) \rangle^{(2)} = -\frac{e}{mc} \frac{\partial}{\partial r_\gamma} \left\{ \langle d_\alpha(r) \rangle A_\beta(r,t) \right\} 
+ \frac{1}{c} \frac{\partial}{\partial r_\gamma} \left\{ \int d^3r' \int_0^\beta d\lambda(j_\beta(r')Y_{\gamma\alpha}(r,i\hbar\lambda))A_\beta(r',t) \right\}. \tag{40} \]

From Eq. (40) it follows, that the integral on all space from \( \langle j_{1\alpha}(r,t) \rangle^{(2)} \) is equal 0 [4].

VI. THE TRANSITION TO EXPRESSIONS CONTAINING A MAGNETIC FIELD.

Let us obtain the sixth expression for \( \langle j_{1\alpha}(r,t) \rangle^{(2)} \), in which we shall introduce a magnetic field. Let us break Eq. (38) on two parts

\[
\langle j_{1\alpha}(r,t) \rangle^{(2)} = \langle j_{1\alpha}(r,t) \rangle^{(-)} + \langle j_{1\alpha}(r,t) \rangle^{(+)} \tag{41} \]

\[
\langle j_{1\alpha}(r,t) \rangle^{(\pm)} = \frac{e}{2mc} \langle d_\alpha \rangle \left( \frac{\partial A_\beta(r,t)}{\partial r_\alpha} \pm \frac{\partial A_\gamma(r,t)}{\partial r_\beta} \right) 
- \frac{1}{2c} \int d^3r' \int_0^\beta d\lambda(Y_{\beta\gamma}(r')j_\alpha(r,i\hbar\lambda)) 
\times \left( \frac{\partial A_\beta(r',t)}{\partial r_\gamma} \pm \frac{\partial A_\gamma(r',t)}{\partial r_\beta} \right). \tag{42} \]

Since \( \mathbf{H} = \text{rot} \mathbf{A} \), the value \( \langle j_{1\alpha}(r,t) \rangle^{(-)} \) is expressed through the magnetic field

\[
\langle j_{1\alpha}(r,t) \rangle^{(-)} = -\frac{e}{2mc} \langle \mathbf{H}(r,t) \times r \rangle \langle \rho(r) \rangle 
+ \frac{1}{2c} \int d^3r' \int_0^\beta d\lambda(\mathbf{H}(r',t) \times r')j_\beta(j_\beta(r')j_\alpha(r,i\hbar\lambda)), \tag{43} \]

and \( \langle j_{1\alpha}(r,t) \rangle^{(+)} \) may be expressed through the second derivatives from the vector potential on coordinates.
\[ \langle j_{1\alpha}(r, t) \rangle^{(+)} = -\frac{e}{2mc}(\rho(r)) r_\beta r_\gamma \frac{\partial^2 A_\beta}{\partial r_\alpha \partial r_\gamma} \]
\[ + \frac{1}{2c} \int d^3 r' r'_\beta r'_\delta \int_0^\beta d\lambda (j_\gamma(r')) j_\delta(r, i\hbar\lambda) \frac{\partial^2 A_\beta}{\partial r'_\alpha \partial r'_\gamma} \]
\[ \text{To deduce Eq. (44) from Eq. (42) we have acted as follows: In Eq. (42) we have used a ratio } \rho_{\beta}(r') = r'^{\beta} j_\gamma(r'), \text{ and for } j_\gamma(r') \text{ we have used Eq. (34). Further in the term, containing } \partial Y_{\delta}(r')/\partial r'_\delta, \text{ we integrated on } r'_\delta \text{ in parts and in the term, containing } d_\lambda(r'), \text{ we used Eq. (39), integrated on } r' \text{ and have calculated the commutator. It is possible to show that values } \langle j_{1\alpha}(r, t) \rangle^{(+)} \text{ and } \langle j_{1\alpha}(r, t) \rangle^{(-)} \text{ separately have properties}
\]
\[ \text{div } \langle j_1(r, t) \rangle^{(\pm)} = 0, \quad \int d^3 r \langle j_{1\alpha}(r, t) \rangle^{(\pm)} = 0. \] (45)

Let us show that the contribution \( \langle j_{1\alpha}(r, t) \rangle^{(+)\pm} \) may be expressed through the second derivatives from an electric field on coordinates. For this purpose we shall substitute the expression
\[ A(r, t) = a(r, t) - c \int_{-\infty}^t dt' \frac{\partial \varphi(r, t')}{\partial r} \] (46)
for the vector potential (following from Eq. (3)) in Eq. (42). Then in values \( \langle j_{1\alpha}(r, t) \rangle^{(\pm)} \) it is possible to allocate the contributions from scalar potential, to which we shall attribute index \( \varphi \), i.e.
\[ \langle j_{1\alpha}(r, t) \rangle^{(\pm)} = \langle j_{1\alpha}(r, t) \rangle^{(\pm)}_\varphi + \langle j_{1\alpha}(r, t) \rangle^{(\pm)}_\rho. \] (47)
At once we obtain that
\[ \langle j_{1\alpha}(r, t) \rangle^{(\pm)}_\rho = 0, \] (48)
and
\[ \langle j_{1\alpha}(r, t) \rangle^{(\pm)}_\varphi = \int_{-\infty}^t dt' \left[ -\frac{e}{m} \langle d_\beta(r) \rangle \frac{\partial^2 \varphi(r, t')}{\partial r_{\alpha} \partial r_\beta} \right] \]
\[ + \int d^3 r' \int_0^\beta d\lambda \langle Y_{\beta\gamma}(r') j_\delta(r, i\hbar\lambda) \rangle \frac{\partial^2 \varphi}{\partial r'_{\alpha} \partial r'_{\gamma}}. \] (49)
In the second term of Eq. (49) we integrate twice in parts, at first on variable \( r'_\nu \), then on variable \( r'_\beta \). Further we use the equation of a continuity Eq. (8) and Eq. (37). In a result we obtain that the second term from Eq. (49) is equal to the first with opposite sign and
\[ \langle j_{1\alpha}(r, t) \rangle^{(\pm)}_\varphi = 0. \] (50)
Taking into account Eqs. (48) and (50) we obtain from Eqs. (47) and (42)
\[ \langle j_{1\alpha}(r, t) \rangle^{(\pm)} = \langle j_{1\alpha}(r, t) \rangle^{(\pm)}_\varphi = \frac{e}{2mc} \left( -\frac{\partial a_\beta(r, t)}{\partial r_\beta} \pm \frac{\partial a_\alpha(r, t)}{\partial r_\alpha} \right) \]
\[ \frac{1}{2c} \int d^3 r' \int_0^\beta d\lambda \langle Y_{\beta\gamma}(r') j_{1\alpha}(r, i\hbar\lambda) \rangle \left( \frac{\partial a_\beta(r', t)}{\partial r'_\beta} \pm \frac{\partial a_\alpha(r', t)}{\partial r'_\alpha} \right). \] (51)

VII. THE EXCEPTION OF DIAGONAL ELEMENTS OF OPERATORS
\[ \mathbf{r}_i. \]
Eqs. (26) and (29) for the additional contributions in average induced densities of currents and charges, as against Eqs. (32) and (33), contain the operators \( \mathbf{r}_i \) of coordinates of particles. Really, the definitions Eq. (17) may be copied as
\[ \mathbf{d}(r) = e \sum_i \mathbf{r}_i \delta(r - \mathbf{r}_i), \] (53)
\[ Y_{\beta\gamma} = \frac{e}{2} \sum_i (\mathbf{r}_i \mathbf{\beta} \mathbf{\gamma} + \mathbf{r}_i \mathbf{\beta} \mathbf{\gamma}). \] (54)
But average magnitudes \( \langle \mathbf{j}_1(r, t) \rangle \) and \( \langle \rho_1(r, t) \rangle \) should not depend on a point of readout of coordinates \( \mathbf{r}_i \). It means that Eqs. (26) and (29) contain only non-diagonal elements of the operators \( \mathbf{r}_i \), and the diagonal elements may be excluded. Let us show that it is so indeed.

Let us transform Eq. (54) so that the operator \( \mathbf{r}_i \mathbf{\beta} \mathbf{\gamma} \) stood only at the left
\[ Y_{\beta\gamma}(r) = -\frac{i\hbar}{2m} \delta_{\beta\gamma} \rho(r) + \sum_i \mathbf{r}_i \mathbf{\beta} \mathbf{\gamma}(r). \] (55)
Substituting Eqs. (53) and (55) in Eq. (26) we obtain
\[ \langle j_{1\alpha}(r, t) \rangle^{(2)} = \frac{i\hbar}{2mc} \int d^3 r' \int_0^\beta d\lambda \langle \rho(r') j_{1\alpha}(r, i\hbar\lambda) \rangle \]
\[ \times \text{div } \mathbf{a}(r', t) + \frac{e^2}{mc} \sum_i \langle \mathbf{r}_i \mathbf{\beta} \mathbf{\gamma} (r - \mathbf{r}_i) \rangle \frac{\partial a_\alpha(r, t)}{\partial r_\alpha} \]
\[ = -\frac{1}{c} \int d^3 r' \int_0^\beta d\lambda \sum_i \langle \mathbf{r}_i \mathbf{\beta} \mathbf{\gamma} (r') j_{1\alpha}(r, i\hbar\lambda) \rangle \]
\[ \times \frac{\partial a_\beta(r', t)}{\partial r'_\gamma}. \] (56)
First two terms in Eq. (56) we shall leave without changes, and in the last let us split the operator \( r_i \) in two parts:

\[
r_i = r_i^d + r_i^{nd},
\]

(57)

where superscripts \( d \) and \( nd \) mean diagonal and non-diagonal contributions, respectively. The operator \( r_i^d \) is determined through its matrix elements

\[
\langle n | r_i^d | m \rangle = \langle n | r_i | m \rangle \langle m | n \rangle,
\]

(58)

where \( |n\rangle \) are the eigen-functions of the Hamiltonian \( \mathcal{H} \). The commutativity property of \( \mathcal{H} \) and \( r_i^d \) is obvious. Let us consider the contribution from the operator \( r_i^d \). The commutativity property is obvious. Let us substitute in Eq. (60) Eq. (62) with the help of Eq. (37) turns in

\[
I_{\alpha}(r, t) = \frac{1}{c} \int d^3 r' \int_0^\beta d\lambda \sum_i \langle r_i^d \rho_i(r') j_\alpha(r, i\hbar\lambda) \rangle a_\beta(r', t).
\]

(59)

As the operator \( r_i^d \) commutes with the Hamiltonian \( \mathcal{H} \) it is possible to rewrite Eq. (59) as

\[
I_{\alpha}(r, t) = \frac{1}{c} \int d^3 r' \int_0^\beta d\lambda \sum_i \langle \rho_i(r') \rangle j_\alpha(r, i\hbar\lambda) a_\beta(r', t).
\]

(60)

Let us consider the contribution from the operator \( r_i^{nd} \) in the last term in Eq. (56) and designate this contribution as \( I_{\alpha}(r, t) \). We execute integration on \( r_i' \) in parts and use a continuity ratio of Eq. (8). We obtain

\[
I_{\alpha}(r, t) = \frac{1}{c} \int d^3 r' \int_0^\beta d\lambda \sum_i \langle \rho_i(r') \rangle j_\alpha(r, i\hbar\lambda) a_\beta(r', t).
\]

(61)

where

\[
I_{\alpha}'(r, t) = \frac{1}{c} \int d^3 r' \int_0^\beta d\lambda \sum_i \langle \rho_i(r') \rangle j_\alpha(r, i\hbar\lambda) a_\beta(r', t).
\]

(62)

and

\[
I_{\alpha}''(r, t) = \frac{1}{c} \int d^3 r' \int_0^\beta d\lambda \sum_i \langle \rho_i(r') \rangle j_\alpha(r, i\hbar\lambda) a_\beta(r', t).
\]

(63)

Integrating on \( r' \) and calculating the commutator we obtain the expression

\[
I_{\alpha}'(r, t) = -\frac{e^2}{mc} \sum_i (r_i\beta (r - r_i)) \frac{\partial a_\beta(r, t)}{\partial r_i\alpha},
\]

(65)

which is reduced with the second term in Eq. (56). There remains the value \( I_{\alpha}''(r, t) \), which we shall transform using the continuity equation of Eq. (8) and integrating on variable \( r_i' \) in parts. It results in

\[
I_{\alpha}''(r, t) = \frac{1}{c} \int d^3 r' \int_0^\beta d\lambda \sum_i \langle j_\gamma(r') \rangle j_\alpha(r, i\hbar\lambda) a_\beta(r', t)
\]

\[
\times r_i^{nd}(i\hbar\lambda) \frac{\partial a_\beta(r', t)}{\partial r_i\gamma}. \]

(66)

Using Eqs. (61), (65) and (66) we obtain the final expression for the additional contribution to the average induced density of a current not containing of diagonal matrix elements of the operator \( r_i' \):

\[
\langle j_\alpha(r, t) \rangle = \frac{i\hbar}{2mc} \int d^3 r' \int_0^\beta d\lambda \langle \rho(r') j_\alpha(r, i\hbar\lambda) \rangle
\]

\[
\times \text{div} a(r', t) + \frac{1}{c} \int d^3 r' \int_0^\beta d\lambda \sum_i \langle j_\gamma(r') \rangle j_\alpha(r, i\hbar\lambda)
\]

\[
\times r_i^{nd}(i\hbar\lambda) \frac{\partial a_\beta(r', t)}{\partial r_i\gamma}.
\]

(67)

Similarly we obtain

\[
\langle \rho(r, t) \rangle = \frac{i\hbar}{2mc} \int d^3 r' \int_0^\beta d\lambda \langle \rho(r') \rangle \text{div} a(r', t)
\]

\[
+ \frac{1}{c} \int d^3 r' \int_0^\beta d\lambda \sum_i \langle j_\gamma(r') \rangle \rho(r, i\hbar\lambda) r_i^{nd}(i\hbar\lambda)
\]

\[
- r_i^{nd}(i\hbar\lambda) \rho(r, i\hbar\lambda) \frac{\partial a_\beta(r', t)}{\partial r_i\gamma}.
\]

(68)

VIII. THE CONDUCTIVITY TENSOR.

Let us make the Fourier-transformation of an electric field

\[
E_\alpha(k, \omega) = \int d^3 r \int_{-\infty}^{\infty} dt E_\alpha(r, t) e^{-i(kr - \omega t)},
\]

(69)

\[
E_\alpha(r, t) = \frac{1}{(2\pi)^3} \int d^3 k \int_{-\infty}^{\infty} d\omega E_{\alpha}(k, \omega) e^{i(kr - \omega t)} + \text{c.c.}
\]

(70)

Average induced density of a current may be written down as
where $\sigma_{\alpha\beta}(\mathbf{k}, \omega | \mathbf{r})$ is the conductivity tensor dependent on spatial coordinates (this designation is borrowed from [8]).

Using Eqs. (25) and (67) for basic and additional contributions, respectively, into the average induced density of a current, we obtain

$$\sigma_{\alpha\beta}(\mathbf{k}, \omega | \mathbf{r}) = \sigma_{\alpha\beta}^{(1)}(\mathbf{k}, \omega | \mathbf{r}) + \sigma_{\alpha\beta}^{(2)}(\mathbf{k}, \omega | \mathbf{r}),$$

where

$$\sigma_{\alpha\beta}^{(1)}(\mathbf{k}, \omega | \mathbf{r}) = \int d^3r' \int_0^\infty dt \int_0^\beta d\lambda \langle j_{\beta}(\mathbf{r} - \mathbf{r}', -i\hbar \lambda) \rangle \times j_{\alpha}(\mathbf{r}, t) e^{-i(k\mathbf{r} - \omega t)},$$

$$\sigma_{\alpha\beta}^{(2)}(\mathbf{k}, \omega | \mathbf{r}) = \frac{i\hbar k_\alpha}{2m\omega} \int d^3r' \int_0^\beta d\lambda \langle \rho(\mathbf{r} - \mathbf{r}', -i\hbar \lambda) j_{\alpha}(\mathbf{r}) \rangle + \frac{e^2}{\hbar \omega} \int d^3r' \int d\lambda \langle \rho(\mathbf{r} - \mathbf{r}', -i\hbar \lambda) j_{\alpha}(\mathbf{r}') \rangle \sum_i j_{i\gamma}^{(n)}(\mathbf{r} - \mathbf{r}', -i\hbar \lambda) r_i^{nd} - r_i^{nd}(-i\hbar \lambda) \times j_{i\gamma}(\mathbf{r} - \mathbf{r}', -i\hbar \lambda) j_{\alpha}(\mathbf{r}).$$

In the case $T = 0$ instead of Eq. (72) we have

$$\sigma_{\alpha\beta,0}(\mathbf{k}, \omega | \mathbf{r}) = \sigma_{\alpha\beta}^{(1)}(\mathbf{k}, \omega | \mathbf{r}) + \sigma_{\alpha\beta}^{(2)}(\mathbf{k}, \omega | \mathbf{r})$$

where

$$\sigma_{\alpha\beta}^{(1)}(\mathbf{k}, \omega | \mathbf{r}) = \frac{e^2}{m\omega} \sum_i \langle 0|j_{\alpha}(\mathbf{r})\rangle r_i^{nd} - r_i^{nd}\rho_i(\mathbf{r} - \mathbf{r}') j_{\alpha}(\mathbf{r}, t)|0\rangle,$$

$$\sigma_{\alpha\beta}^{(2)}(\mathbf{k}, \omega | \mathbf{r}) = \frac{e^2}{m\omega} \sum_i \langle 0|j_{\alpha}(\mathbf{r})\rangle r_i^{nd} + \frac{e^2}{m\omega} \sum_i \langle 0|j_{\alpha}(\mathbf{r})\rangle r_i^{nd} - r_i^{nd}\rho_i(\mathbf{r} - \mathbf{r}') j_{\alpha}(\mathbf{r}, t)|0\rangle,$$

IX. THE APPROXIMATION OF A SPATIALLY HOMOGENEOUS ELECTRIC FIELD.

In some cases it is possible to neglect the contributions to average values of the induced densities of currents and charges containing derivatives from electric field on coordinates, i. e. to believe

$$\mathbf{E}(\mathbf{r}, t) \simeq \mathbf{E}(t),$$

as it is made, for example, in [1] though, strictly speaking, spatially homogeneous field $\mathbf{E}$ may be only time-independent. In approximation Eq. (79) the Fourier-transformation is

$$E_\alpha(\omega) = \int_{-\infty}^\infty dt e^{i\omega t} E_\alpha(t).$$

Then it is possible to write down

$$\langle j_{\alpha}(\mathbf{r}, t) \rangle_\hbar = \frac{1}{2\pi} \int_0^\infty d\omega \sigma_{\alpha\beta}(\omega | \mathbf{r}) E_\beta(\omega) e^{-i\omega t} + c.c.,$$

where the subscript $\hbar$ means a spatially homogeneous field. It is easily to see that

$$\sigma_{\alpha\beta}(\omega | \mathbf{r}) = \sigma_{\alpha\beta}(\mathbf{k} = 0, \omega | \mathbf{r}).$$

Then with the help of Eqs. (72)-(74) we obtain

$$\sigma_{\alpha\beta}(\omega | \mathbf{r}) = \int_0^\infty dt \int_0^\beta d\lambda \langle J_\beta(-i\hbar \lambda) j_{\alpha}(\mathbf{r}, t) \rangle e^{i\omega t},$$

where

$$J_{\alpha} = e \sum_i \mathbf{r}_{i\alpha}$$

is the current operator.

Eq. (83) is the generalization of the Kubo formula for the spatially inhomogeneous medium when the conductivity tensor depends on $\mathbf{r}$.

Further we shall consider a case of a spatially homogeneous medium in which any average values can not

$$[F, Q]_+ = FQ + QF$$

is the anti-commutator of two operators. It is possible to pass from Eq. (75) to Eq. (72) if in Eqs. (76) - (78) to replace averaging $\langle 0|\ldots|0 \rangle$ by $\langle \ldots \rangle$ and to use Eq. (37). *
Let us choose the vector potential as \( \vec{A}(\vec{r}) = \frac{1}{2}(\vec{H} \times \vec{r}) \). Then it is obvious from Eq. (44) that \( \langle j_1(\vec{r}, t) \rangle^{(+)} = 0 \) since it contains second derivatives from \( \vec{A}(\vec{r}) \) on coordinates. Thus, at \( \vec{H} = \text{const} \) in linear approximation on the field we managed to express the density of the induced current through the magnetic field intensity. Now we shall exclude diagonal matrix elements of the operators \( \vec{r}_i \) from expression for \( \langle j_1(\vec{r}, t) \rangle \) at \( \vec{H} = \text{const} \). For this purpose let us take advantage of Eq. (67) in which vector \( \vec{a}(\vec{r}, t) \) can be replaced by vector potential \( \vec{A}(\vec{r}, t) \), since the initial expression of Eq. (26) can be replaced by Eq. (38). By substituting Eq. (86) in Eq. (67) we obtain

\[
\langle j_{1\alpha}(\vec{r}, t) \rangle = \frac{-e^2}{2mc} \sum_i ((\vec{H} \times \vec{r}_i^{nd})_\alpha \delta(\vec{r} - \vec{r}_i)) \\
- \frac{ie}{2\hbar c} \sum_i \langle j_{\alpha}(\vec{r}) \rangle H_\beta (\vec{r}_i^{nd} \times \vec{r}_i^{nd})_\beta \\
+ \frac{e}{2c} \int_0^\infty d\lambda \sum_i \langle \vec{H} \times \vec{r}_i^{nd} \rangle_\beta v_{i\beta} j_{\alpha}(\vec{r}, i\hbar \lambda). \tag{87}
\]

Let us notice that the vector \( \vec{r}_i^{nd} \times \vec{r}_i^{nd} \neq 0 \) because projections \( r_{i\alpha}^{nd} \) with different subscripts \( \alpha \) do not commute among themselves, for example,

\[
(r_i^{nd} \times r_i^{nd})_z = [r_{ix}^{nd}, r_{iy}^{nd}]. \tag{88}
\]

XI. CONCLUSION.

Let us list the obtained basic results. It is shown that average values of densities of currents and charges induced by weak electromagnetic field at finite temperatures and spatially inhomogeneous systems are expressed through electric fields and their derivatives on coordinates. The contributions expressed through electric field were called "basic" and through derivatives - "additional".

For the "additional" contributions to average values of induced densities of currents and charges six pairs of various expressions are obtained. Two of these expressions for the density of a current coincide with the results of [4]. But the expressions from [4] contain electric fields or vector potentials, instead of derivatives from these values on coordinates, that complicates an estimation of value of the "additional" contributions. Generally speaking, integrating on \( \vec{r}' \) in parts it is possible to get rid of derivatives \( \partial E_\beta(\vec{r}', t)/\partial r'_z \) passing to the formulas containing only fields instead of derivative from them. However, the opposite procedure - transition from a field to derivatives - is not possible always. In the "basic" contributions the fields are always kept.

The sixth expression obtained in section VI for the "additional" contribution to average induced density of a current breaks up on two parts. First of them with an index (−) is expressed only through magnetic field \( \vec{H}(\vec{r}, t) \), the second with an index (+) - through the second derivative from an electric field on coordinates. The similar result is obtained for the average induced density of charge. If the "additional" contributions are expressed through derivatives from electric fields, the operators \( \vec{r}_i \) of coordinates of particles enter in the appropriate formulas necessary. It may seem that this result is absurd, since coordinate \( \vec{r}_i \) depends on a point of a beginning of readout. However, it appears that diagonal matrix elements \( \langle n_i|n_i \rangle \) do not enter into the average induced densities of currents and charges, that is shown in section VII, and the non-diagonal elements do not depend on a beginning point of readout.

In section VIII the "basic" and "additional" contributions are calculated in the conductivity tensor for spatially inhomogeneous systems and fields. In approximation, when the electric field is homogeneous in space, but time-dependent (section IX), the "basic" contributions are kept only. For this case for the conductivity tensor, dependent on frequency \( \omega \) and coordinates \( \vec{r} \), the modified Kubo formula is obtained which passes in the formula from [1] for spatially homogeneous systems.

At last, in section X the expression for the average induced density of a current is obtained in a case when a weak electromagnetic field is reduced to a constant magnetic field.

It follows from Eq. (74) that the "additional" contri-
butions in conductivity contain a factor \(k_r/\omega\). If a field \(\mathbf{E}(\mathbf{r}, t)\) is the plane wave extending with the light velocity \(c\) (at a monochromatic irradiation) or the wave packet (at a pulse irradiation), then \(k \simeq \omega/c\) and additional contributions contain in comparison with basic a small factor \(v/c\), where \(v\) is the speed of particles in system. However, this estimation is not correct always in case of spatially inhomogeneous systems, for example, in semiconductor quantum wells, wires or dots. It is possible to consider a field \(\mathbf{E}(\mathbf{r}, t)\) as an external or stimulating field only in the case of calculating the density of the induced current and charge in the lowest order on interaction of a field with system of charged particles. Such approximation is allowable in case of quantum wells under condition of \([9,10]\) \(\gamma_r \ll \gamma\), where \(\gamma_r (\gamma)\) is the radiative (non-radiative) broadening of electronic excitations.

Otherwise, when \(\gamma_r \gg \gamma\), it is necessary to take into account interaction of a field with particles in all orders of the perturbation theory, and then \(\mathbf{E}(\mathbf{r}, t)\) is the genuine field within the low dimensional object. This field already cannot be presented as a superposition of plane waves for which \(k = \omega/c\). For example, genuine field strongly varies within a quantum well along an axis \(z\), perpendicular to the well plane, if light is directed along an axis \(z\), and the frequency \(\omega\) is in a resonance with one of discrete energy levels of the electronic system excitations in a quantum well \([11,12]\). Then the values \(kd \simeq 1\), where \(d\) is the quantum well width, instead of small factor \(v/c\) appears the factor

\[ M \simeq \frac{v}{\omega d} = \frac{v \lambda}{2 \pi cd}. \]

If a wave length \(\lambda \gg d\) it can appear that the new factor \(M\) is greater than \(v/c\). In concrete cases one needs to estimate its value. In \([11,12]\) it was supposed that \(M \ll 1\) and the "additional" contributions to average induced densities of currents and charges (the case \(T = 0\) was considered) were neglected. By substituting the received expressions for average densities of a currents and charges in the Maxwell equations, basically it is possible to determine true fields inside and outside of low-dimensional semiconductor objects. Thus, it is possible to calculate factors of reflection and absorption of light by these objects (see, for example, \([11,12]\)).

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