Dynamic scattering of x rays in disordered crystals: statistical theory

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The general problem of dynamic x-ray scattering (DXRS) in crystals with randomly distributed crystal-lattice defects is considered. The Dyson and Bethe-Salpeter equations describing the propagation of coherent and diffuse waves in a crystal are obtained. With the use of a diagram technique, expansions for the polarization operator $\hat{\Pi}$ and intensity operator $\hat{\Omega}$ are constructed in the form of diagrammatic series in the cumulant averages of the fluctuations of the order of the crystal lattice. Solutions of the Dyson equations are found and analyzed in detail in the case of practical interest of DXRS with $\tau \ll \Lambda$, where τ is the correlation length and Λ is the extinction length of the x rays in the perfect crystal. The results obtained are given in a form that permits a direct description of a diffraction experiment with a two- or a three-crystal x-ray spectrometer. The theory developed is compared with Kato's statistical theory of DXRS.

It is well known (see, e.g., Refs. 1–6) that dynamic x-ray scattering (DXRS) in single crystals possesses extremely high sensitivity to small local strains ($\sim 10^{-5}$–10^{-6}), which lead to the appearance of diffuse waves alongside the propagation of the coherent wave field in the ideal ("on the average") crystal lattice. Rigorous allowance for the interaction of the diffuse waves in the general case of a disordered crystal with randomly distributed structural defects is a complicated problem. On the other hand, the experimental x-ray diffraction methods that are used to study microscopic defects of a crystal structure, e.g., the method of the three-crystal x-ray spectrometer,[1-4] the inclination method, and certain others that permit one, in principle, to separate the coherent and the diffuse component of the DXRS, are far in advance of the possibilities of theoretical analysis of the results obtained. The point is that, until now, the mathematical difficulties have made it impossible to construct a systematic theory of DXRS in crystalline media with disorder arising from the random character of the distribution of the structural defects.

In the literature, two limiting cases of a general theory are well known: 1) a strongly broken crystal, when the characteristic size t of a crystallite is much smaller than the extinction length Λ of the x rays in the perfect crystal (here, the so-called kinematic approximation of the theory, first proposed by Krivoglaz,[7] is applicable); 2) a weakly broken crystal, when multiple scattering of the diffuse waves can be neglected.[8-10]

In Refs. 11 and 12 a generalization of the theory of Refs. 8 and 9 is constructed with the use of the microscopic (unaveraged) Takagi-Taupin equations for the amplitudes of the wave field in the disordered crystal. In Refs. 13 and 14 this approach is extended to the case of DXRS in layer-disordered crystals. To describe the statistical properties of the crystal lattice, the authors of Refs. 11–14 introduce a static Debye-Waller factor $E = \langle \exp\{i\mathbf{h}\cdot\mathbf{u}(\mathbf{R})\}\rangle$ and the two-coordinate correlation function

$$g_2(\mathbf{r}) = \langle \exp\{i\mathbf{h}(\mathbf{u}(\mathbf{r}+\mathbf{R}) - \mathbf{u}(\mathbf{R}))\}\rangle_c,$$

where $\mathbf{h}$ is the diffraction-scattering vector, $\mathbf{u}(\mathbf{r})$ is the random vector of the displacement of the crystal-lattice site at the point $\mathbf{r}$, and the symbol $\langle \ldots \rangle_c$ denotes statistical three-dimensional (in Refs. 13 and 14, two-dimensional) cumulant averaging over the disposition of the defects in the crystal. In addition, it is assumed that the interaction of the coherent and the diffuse waves is sufficiently weak, so that the correlation length of local distortions of the crystal lattice

$$\tau = \int_0^\infty g_2(r)dr/g_2(0)$$

is much smaller than the extinction length Λ (the so-called τ-approximation). For $\tau \lesssim \Lambda$, perturbation theory in the interaction parameter of the coherent and diffuse waves is inapplicable, and, generally speaking, we cannot neglect the contribution of the many-point correlations

$$g_n(\mathbf{r}_1; \mathbf{r}_2; \ldots \mathbf{r}_{n-1}) = \exp\{i\mathbf{h}[\mathbf{u}(\mathbf{r}_1+\mathbf{r}_2+\ldots+\mathbf{r}_{n-1}+\mathbf{R}) \pm \mathbf{u}(\mathbf{r}_2+\ldots+\mathbf{r}_{n-1}+\mathbf{R}) \pm \ldots \pm \mathbf{u}(\mathbf{R})]\}\rangle_c,$$

which are not taken into account *a priori* in the theories of Refs. 11–14.

The present paper is an attempt to move in the direction of constructing a general statistical theory of DXRS in disordered crystals. Without loss of generality, we have kept the description (inherent to the theory of Refs. 11 and 12) of the disorder of the crystal lattice by means of the phase function $\exp\{i\mathbf{h}\cdot\mathbf{u}(\mathbf{r})\}$ of the random field of the displacements. In Sec. 1 we give a derivation of the microscopic equations for the matrix $\hat{G}(\mathbf{r}, \xi)$ of the Green functions of the theory of DXRS in a disordered crystal. In Secs. 2 and 3 we obtain exact integral equations for the coherent part $\hat{G}^{\text{coh}} = \langle \hat{G} \rangle$ of the Green function and for the matrix of the correlations of the Green functions

$$J(\mathbf{r}, \mathbf{r}'; \xi, \xi') = \langle \hat{G}(\mathbf{r}, \xi) \otimes \hat{G}^*(\mathbf{r}', \xi') \rangle$$

(the Dyson equation and the Bethe-Salpeter equation, respectively; the symbol $\otimes$ denotes the direct product of the matrices), describing the propagation of the coherent and the diffuse waves in the crystal. The diagram technique is presented, and rules for writing the matrix elements describing n-fold scattering of waves are formulated. For the polarization operator $\hat{\Pi}$ and intensity (energy) operator $\hat{\Omega}$, which are the kernels of the Dyson and Bethe-Salpeter integral equations, respectively, expansions are found in the form of diagrammatic series in cumulant averages $\langle \exp(i\mathbf{h}(\mathbf{u}_1 \pm \mathbf{u}_2 \pm \ldots \pm \mathbf{u}_n)) \rangle_c$, of the random phases corresponding to a given multiplicity of scattering of x rays by fluctuations of the order of the crystal lattice. We note that

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the idea of using the Dyson and Bethe-Salpeter equations in application to the present problem of DXRS in disordered crystals was first put forward in Ref. 15.

In Sec. 4, from the general equations of the statistical theory of DXRS, we obtain the corresponding equations in the τ-approximation, and give a comparison with the results of the theory of Kato.[11,12] The main differences of physical interest in comparison with Refs. 11 and 12 are the following: 1) The dispersion surface, determining the dispersion law $\omega(\mathbf{k}_0, \mathbf{k}_h)$ and hence the propagation of the coherent x-ray waves in the "on-average" perfect crystal, undergoes distortions and is broadened as a result of allowance for the fluctuations of the order, and the corresponding expressions for Re $\Delta\omega$ and Im $\Delta\omega$ are found; 2) it is shown that the correlation lengths appearing in the equations for the coherent and the diffuse waves coincide, i.e., $\tau_{\text{coh}} = \tau_{\text{dif}}$, and this ensures the correct passage to the limit of the kinematic approximation as $\tau \to 0$ (see, e.g., Ref. 16).

1. MICROSCOPIC EQUATIONS OF DXRS IN CRYSTALS WITH RANDOMLY DISTRIBUTED DEFECTS

In the analysis of DXRS in quasiperiodic media it is natural to start from the representation of the Green's function $\mathbf{G}(\mathbf{r}; \boldsymbol{\xi})$ in the form of a quasi-Bloch wave (see Refs. 13 and 14)

$$\mathbf{G}(\mathbf{r}; \boldsymbol{\xi}) = \exp(-i\mathbf{k}_0\boldsymbol{\xi}) \sum_{\mathbf{h}} \mathbf{G}_{\mathbf{h}}(\mathbf{r}; \boldsymbol{\xi}) \exp(i(\mathbf{k}_0+\mathbf{h})\mathbf{r}) \qquad (1)$$

($\mathbf{k}_0$ is the wave vector of the incident radiation, $\varkappa = |\mathbf{k}_0| = \omega/c$, and $\mathbf{h}$ is a reciprocal-lattice vector, multiplied by 2π), satisfying the inhomogeneous Maxwell equation

$$-\varkappa^{-2} \operatorname{rot}\operatorname{rot} \mathbf{G} + [1+\theta(\mathbf{r})\chi(\mathbf{r})]\mathbf{G} = 2i\varkappa^{-1}\mathbf{e}\delta(\mathbf{r}-\boldsymbol{\xi}) \qquad (2)$$

with a point source of radiation at the point $\boldsymbol{\xi}$. In (2) $\chi(\mathbf{r})$ is the complex electric susceptibility of the crystal, and the step function satisfies $\theta(\mathbf{r}) = 1$ if the point $\mathbf{r}$ lies inside the crystal and $\theta(\mathbf{r}) = 0$ if the point $\mathbf{r}$ lies outside the crystal; $\mathbf{e}$ is the polarization vector of the incident radiation.

In going over from (2) to a system of equations for the components of the Green's function (1), we shall assume that the disorder of the crystal lattice is described by a slowly varying (on the scale of the lattice constant) random function $\mathbf{u}(\mathbf{r})$ describing the displacement field. In this case, $\chi(\mathbf{r})$ at a point $\mathbf{r}$ of the distorted crystal can be assumed to be equal to the susceptibility at the point $\mathbf{r} - \mathbf{u}(\mathbf{r})$ of the perfect crystal; in other words, in our case,

$$\chi(\mathbf{r}) = \sum_{\mathbf{h}} \chi_{\mathbf{h}} \exp\{i\mathbf{h}(\mathbf{r}-\mathbf{u}(\mathbf{r}))\}, \qquad (3)$$

where $\chi_{\mathbf{h}}$ are the Fourier components of the electric susceptibility of the perfect crystal.

Let the crystal as a whole be oriented close to one Bragg reflection with diffraction vector $\mathbf{h}$ (the so-called two-wave approximation: $\mathbf{k}_h = \mathbf{k}_0 + \mathbf{h}$, $|\mathbf{k}_{\mathbf{h}}| = |\mathbf{k}_0|$). Substituting (1) into (2) and using (3) to separate groups of terms that have the same exponential factors, we arrive at the following system of equations for the π and σ components G_0 and $G_{\mathbf{h}}$ of the Green's function $\mathbf{G}$:

$$\begin{aligned}
&\varkappa^{-2}\Delta G_0 + 2i\varkappa^{-2}(\mathbf{k}_0\nabla)G_0 + \theta(\mathbf{r})[\chi_0 G_0 + C\chi_{-\mathbf{h}}e^{i\mathbf{h}\mathbf{u}(\mathbf{r})}G_{\mathbf{h}}] \\
&\quad = 2i\varkappa^{-1}\delta(\mathbf{r}-\boldsymbol{\xi}), \\
&\varkappa^{-2}\Delta G_h + 2i\varkappa^{-2}(\mathbf{k}_h\nabla)G_{\mathbf{h}} + \theta(\mathbf{r})[\chi_0 G_{\mathbf{h}} + C\chi_h e^{i\mathbf{h}\mathbf{u}(\mathbf{r})}G_0] = 0,
\end{aligned} \qquad (4)$$

where the polarization factor satisfies $C = 1$ for the σ polarization $[\mathbf{e}\times(\mathbf{k}_0\times\mathbf{k}_h) = 0]$ and $C = \cos(2\vartheta)$ for the π polarization $[\mathbf{e}\cdot(\mathbf{k}_0\times\mathbf{k}_h) = 0]$; ϑ is the Bragg angle.

We introduce an oblique-angled system of coordinates, with the s_0 axis along the vector $\mathbf{k}_0$, the s_h axis along the vector $\mathbf{k}_{\mathbf{h}}$, and the y axis perpendicular to the s_0, s_h plane. In this coordinate system Eqs. (4) take the following form:

$$\begin{aligned}
&\frac{\partial G_0}{\partial s_0} - \frac{i}{2\varkappa}\frac{\partial^2 G_0}{\partial y^2} - \theta(\mathbf{r})\left(i\frac{\chi_0\varkappa}{2}G_0 + i\frac{\chi_{-\mathbf{h}}\varkappa C}{2}e^{i\mathbf{h}\mathbf{u}}G_{\mathbf{h}}\right) \\
&\quad = \delta(s_0-\xi_0)\delta(s_h-\xi_h)\delta(y-\xi_y), \\
&\frac{\partial G_{\mathbf{h}}}{\partial s_h} - \frac{i}{2\varkappa}\frac{\partial^2 G_{\mathbf{h}}}{\partial y^2} - \theta(\mathbf{r})\left(i\frac{\chi_0\varkappa}{2}G_{\mathbf{h}} + i\frac{\chi_{\mathbf{h}}\varkappa C}{2}e^{-i\mathbf{h}\mathbf{u}}G_0\right) = 0.
\end{aligned} \qquad (5)$$

In the derivation of (5) it has been taken into account that the characteristic scales of the variation of the components G_0 and $G_{\mathbf{h}}$ are much greater than the wavelength of the radiation. We note that, in contrast to the Takagi-Taupin equations usually used in the theory of DXRS, in (5) we have kept the terms with the derivative $\partial^2/\partial y^2$, corresponding to emergence of the scattered radiation from the diffraction plane $(\mathbf{k}_0, \mathbf{k}_h)$.

By means of the exponential substitution

$$\begin{aligned}
G_{0,\mathbf{h}} &= \bar{G}_{0,\mathbf{h}} \exp\left[i\frac{\chi_0\varkappa}{2}\left(\int_{\xi_0}^{s_0} ds_{0,1} + \int_{\xi_h}^{s_h} ds_{h,1}\right)\theta(\mathbf{r})\right] \\
&= \bar{G}_{0,\mathbf{h}} \exp\left[i\frac{\chi_0\varkappa}{2}(s_0-\xi_0+s_h-\xi_h)\right]
\end{aligned}$$

Eqs. (5) are transformed into

$$\begin{aligned}
&\frac{\partial G_0}{\partial s_0} - \frac{i}{2\varkappa}\frac{\partial^2 G_0}{\partial y^2} - i\sigma_{-\mathbf{h}}e^{i\mathbf{h}\mathbf{u}}G_{\mathbf{h}} = \delta(s_0-\xi_0)\delta(s_h-\xi_h)\delta(y-\xi_y), \\
&\frac{\partial G_{\mathbf{h}}}{\partial s_h} - \frac{i}{2\varkappa}\frac{\partial^2 G_{\mathbf{h}}}{\partial y^2} - i\sigma_{\mathbf{h}}e^{-i\mathbf{h}\mathbf{u}}G_0 = 0,
\end{aligned} \qquad (6)$$

where we have introduced the notation

$$\sigma_{\pm\mathbf{h}} = \frac{\varkappa}{2}\chi_{\pm\mathbf{h}}C\theta(\mathbf{r}) \qquad (7)$$

(here and below, we omit the tilde symbol when writing the components of the Green's functions).

The solutions of Eqs. (6) that have physical meaning are those having the form of retarded Green's functions $G_{0,\mathbf{h}}$, which satisfy the following boundary conditions on characteristics that follow directly from (6):

$$\begin{aligned}
&G_0(s_0; \xi_h+\Delta; \xi_0; \xi_h) = F_y(s_0-\xi_0, 0, y-\xi_y) \\
&\quad \times[\delta(\Delta) - \sigma^2(s_0-\xi_0)\theta(\Delta)]\theta(s_0-\xi_0), \quad \Delta \to 0, \\
&G_{\mathbf{h}}(s_0; \xi_h; \xi_0; \xi_h) = i\sigma_{\mathbf{h}}F_y(s_0-\xi_0, 0, y-\xi_y)e^{-i\mathbf{h}\mathbf{u}(s_0, \xi_h, \xi_y)}\theta(s_0-\xi_0), \\
&G_0(\xi_0; s_h; \xi_0; \xi_h) = F_y(0, s_h-\xi_h, y-\xi_y)\delta(s_h-\xi_h), \\
&G_{\mathbf{h}}(\xi_0; s_h; \xi_0; \xi_h) = i\sigma_{\mathbf{h}}F_y(s_0-\xi_0, 0, y-\xi_y)e^{-i\mathbf{h}\mathbf{u}(\xi_0, \xi_h, \xi_y)}\theta(s_h-\xi_h).
\end{aligned} \qquad (8)$$

Here the quantity $\sigma^2 = \sigma_{\mathbf{h}}\sigma_{-\mathbf{h}} = (\pi/\Lambda)^2$, $\theta(s)$ is the Heaviside step function, and the function $F_y(\mathbf{r}-\boldsymbol{\xi})$ has the form

$$F_y(\mathbf{r}-\boldsymbol{\xi}) = \frac{\varkappa}{[2\pi i(\mathbf{k}_0+\mathbf{k}_h)(\mathbf{r}-\boldsymbol{\xi})]^{1/2}} \exp\left[\frac{i\varkappa^2(y-\xi_y)^2}{2(\mathbf{k}_0+\mathbf{k}_h)(\mathbf{r}-\boldsymbol{\xi})}\right]. \qquad (9)$$

In the following it is convenient to go over to a matrix formulation of the theory and to introduce a 2×2 matrix of

components of the Green's functions, of which the first column is composed of the elements $G_{00} = G_0$ and $G_{h0} = G_h$ and the second is composed of the corresponding quantities G_{0h} and G_{hh} in the complementary DXRS geometry:

$$\hat{G} = \begin{pmatrix} G_{00} & G_{0h} \\ G_{h0} & G_{hh} \end{pmatrix}, \tag{10}$$

where the matrix $\hat{G}$ satisfies the equation [compare with (6)]

$$\hat{L}_r \hat{G}(\mathbf{r};\ \boldsymbol{\xi}) = \delta(\mathbf{r}-\boldsymbol{\xi})\hat{I}. \tag{11}$$

Here the matrix differential operator $\hat{L}_r$ is defined as

$$\hat{L}_r = \begin{bmatrix} \dfrac{\partial}{\partial s_0} - \dfrac{i}{2\varkappa}\dfrac{\partial^2}{\partial y^2} & i\sigma_{-h}e^{i\mathbf{hu}} \\ i\sigma_h e^{-i\mathbf{hu}} & \dfrac{\partial}{\partial s_h} - \dfrac{i}{2\varkappa}\dfrac{\partial^2}{\partial y^2} \end{bmatrix}, \tag{12}$$

and $\hat{I}$ is the 2×2 unit matrix.

The general solution of the DXRS boundary-value problem for a quasi-Bloch wave in a crystal,

$$E(\mathbf{r}) = E_0(\mathbf{r})e^{i\mathbf{k}_0\mathbf{r}} + E_h(\mathbf{r})e^{i\mathbf{k}_h\mathbf{r}} \tag{13}$$

can be written as $\left(\hat{E}(\mathbf{r}) = \begin{pmatrix} E_0 \\ E_h \end{pmatrix}\right)$

$$\hat{E}(\mathbf{r}) = \int \hat{G}(\mathbf{r};\boldsymbol{\xi})\hat{E}(\boldsymbol{\xi})\,d^2\boldsymbol{\xi}, \tag{14}$$

where the integration is performed over the entrance surface of the crystal, on which is specified the initial distribution

$$\hat{E}(\boldsymbol{\xi}) = \begin{pmatrix} E_0(\boldsymbol{\xi}) \\ 0 \end{pmatrix}$$

of the incident wave.

Thus, in the case of a plane wave incident on a plane-parallel crystal and with initial deviation $\mathbf{q}_0$ from an exact Bragg position [$E_0(\boldsymbol{\xi}) = \exp(i\mathbf{q}_0\cdot\boldsymbol{\xi})$], the general solution $\hat{E}(\mathbf{r})$ is determined by taking the Fourier transform of the Green's function:

$$\hat{E}(\mathbf{r}) = \frac{1}{\gamma_0}\hat{G}(\mathbf{r};\mathbf{q}_0).$$

Here we make the following comment. Equations (11)–(14) describe DXRS in a deformed crystal lattice with electric susceptibility (3) and with a random displacement field $\mathbf{u}(\mathbf{r})$ that depends, in principle, on the type and position of all the defects present in the crystal. The dynamical coefficients in the matrix operator $\hat{L}_r$ then differ from the corresponding quantities for the perfect crystal by random phase factors $\exp(\pm i\mathbf{h}\cdot\mathbf{u})$. It can be shown (see, e.g., Ref. 13) that in the case when the dynamical DXRS coefficients are modulated not only in phase but also in amplitude the microscopic equations (5) of the theory preserve their form with the following replacements:

$$\chi_0 \to \chi(\mathbf{r}),\quad \chi_{\pm h}e^{i\mathbf{hu}(\mathbf{r})} \to \chi_{\pm h}(\mathbf{r}),$$

where the relationship of the latter to the defect structure of the crystal is determined in the framework of a more general "rigid-ion" model (see, e.g., Ref. 7).

2. CALCULATION OF AVERAGES. COHERENT SCATTERING

According to the general principles of the statistical description of the propagation of wave fields in randomly inhomogeneous media, we go over from the microscopic equations (11), (12) to the matrix equation for the coherent (averaged) part $\hat{G}^{\mathrm{coh}}(\mathbf{r};\boldsymbol{\xi}) = \langle\hat{G}(\mathbf{r};\boldsymbol{\xi})\rangle$ of the Green's function.

To this end, we write Eq. (11) in integral form:

$$\hat{G}(\mathbf{r};\boldsymbol{\xi}) = \hat{G}^{(E)}(\mathbf{r};\boldsymbol{\xi}) + \int \hat{G}^{(E)}(\mathbf{r};\mathbf{r}_1)\hat{P}^{(E)}(\mathbf{r}_1)\hat{G}(\mathbf{r}_1;\boldsymbol{\xi})\,d^3\mathbf{r}_1, \tag{15}$$

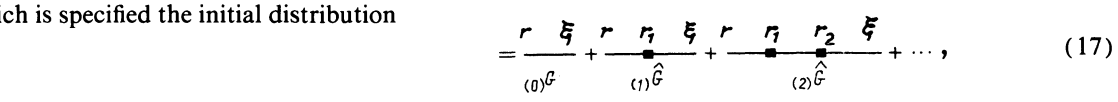
where the antidiagonal matrix $\hat{P}^{(E)}(\mathbf{r})$ has the following form:

$$\hat{P}^{(E)}(\mathbf{r}) = \begin{pmatrix} 0 & i\sigma_{-h}(e^{i\mathbf{hu}(\mathbf{r})}-E) \\ i\sigma_h(e^{-i\mathbf{hu}(\mathbf{r})}-E) & 0 \end{pmatrix}; \tag{16}$$

E is the static Debye-Waller factor, and $\hat{G}^{(E)}(\mathbf{r};\boldsymbol{\xi})$ is the Green's function for DXRS in the crystal with electric susceptibility averaged over the positions of the defects, i.e., $\hat{G}^{(E)}(\mathbf{r};\boldsymbol{\xi})$ satisfies (11) with $\exp(\pm i\mathbf{h}\cdot\mathbf{u})$ replaced by E in the operator (12). We shall assume that the expressions for $\hat{G}^{(E)}(\mathbf{r};\boldsymbol{\xi})$ are known from the theory of DXRS in perfect crystals.

We formally represent the exact solution of (15) for the Green's function in a disordered crystal in the form of the diagrammatic series

$$\hat{G}(\mathbf{r};\boldsymbol{\xi}) = \sum_{n=0}^{\infty} {}_{(n)}\hat{G}(\mathbf{r};\boldsymbol{\xi})$$



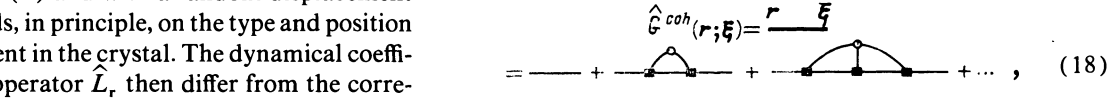
(17)

where the diagram ${}_{(n)}\hat{G}$ of order n corresponds to a $3n$-fold integral of the form

$$ {}_{(n)}\hat{G}(\mathbf{r};\boldsymbol{\xi}) = \int \hat{G}^{(E)}(\mathbf{r};\mathbf{r}_1)\hat{P}^{(E)}(\mathbf{r}_1)\hat{G}^{(E)}(\mathbf{r}_1;\mathbf{r}_2)\hat{P}^{(E)}(\mathbf{r}_2)\ldots \times\ldots\hat{P}^{(E)}(\mathbf{r}_n)\hat{G}^{(E)}(\mathbf{r}_n;\boldsymbol{\xi})\,d^3\mathbf{r}_1\,d^3\mathbf{r}_2\ldots d^3\mathbf{r}_n$$

with a certain specified realization of the "random" matrix $\hat{P}^{(E)}(\mathbf{r})$. In the expression (17) the horizontal lines correspond to the matrices $\hat{G}^{(E)}$, and the vertices ■ to the matrices $\hat{P}^{(E)}$; the multiplicity of the integrals over $d^3\mathbf{r}_i$ is equal to the number of vertices in the diagram.

Separating out in (17) the coherent part $\hat{G}^{\mathrm{coh}}$ of the Green's function, we arrive at the diagrammatic series



(18)

where the lines converging at a light circle denote that the matrices $\hat{P}^{(E)}(\mathbf{r})$ corresponding to the vertices should be averaged over the positions of the defects (we note that $\langle\hat{P}^{(E)}(\mathbf{r})\rangle = 0$.).

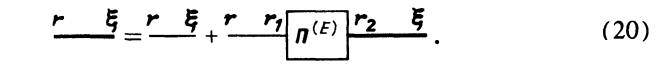
In the general case, a diagram of order n is determined by many-point correlation functions of the type

$$\langle\exp\{i\mathbf{h}(\pm\mathbf{u}_1\pm\mathbf{u}_2\pm\ldots\pm\mathbf{u}_n)\}\rangle \tag{19}$$

with an arbitrary combination of signs $\pm$ and arbitrary distances between the averaging points $\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_n$.

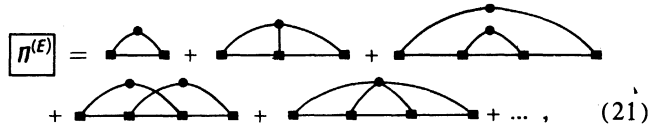
By going over to cumulant expansions of the averages

appearing in (18) (see Ref. 17), and regrouping the terms of the diagrammatic series, it is not difficult to show that the averaged Green's function satisfies the diagrammatic equation



(20)

Here, the polarization operator $\hat{\Pi}^{(E)}(\mathbf{r}_1;\ \mathbf{r}_2)$ is the sum of all the compact diagrams



(21)

where lines converging at a dark circle indicate that the matrices corresponding to the vertices form cumulant averages (we recall that a diagram is said to be compact if it is impossible to divide it into separate parts by cutting one $\hat{G}^{(E)}$ line.)

The diagrammatic equation (20) is none other than the integral Dyson equation (see, e.g., Refs. 18 and 19):

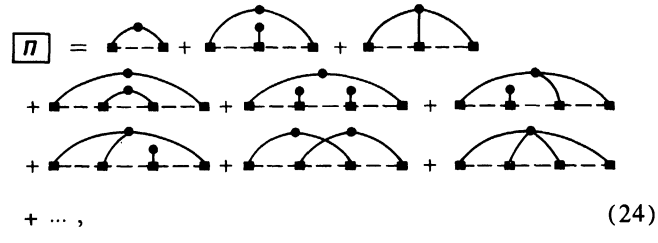
$$\hat{G}^{coh}(\mathbf{r};\xi)=\hat{G}^{(E)}(\mathbf{r};\xi)+\int \hat{G}^{(E)}(\mathbf{r};\mathbf{r}_1)\hat{\Pi}^{(E)}(\mathbf{r}_1;\mathbf{r}_2)\hat{G}^{coh}(\mathbf{r}_2;\xi)\,d^3\mathbf{r}_1\,d^3\mathbf{r}_2 \quad (22)$$

for the averaged Green's function in the theory of DXRS.

We shall show that the polarization operator $\hat{\Pi}^{(E)}$ does not depend on the choice of representation of the Green's functions on which the diagrammatic series (21) is constructed. In other words, the following identity holds:

$$\hat{\Pi}(\mathbf{r}_1;\ \mathbf{r}_2)\equiv\hat{\Pi}^{(E)}(\mathbf{r}_1;\ \mathbf{r}_2)|_{E=0}=\hat{\Pi}^{(E)}(\mathbf{r}_1;\ \mathbf{r}_2)|_{E\neq 0}, \quad (23)$$

where $\hat{\Pi}$ is defined as the complete sum of all compact diagrams [compare with (21)]:



(24)

where a dashed line corresponds to the Green's function

$$\hat{G}^{(0)}(\mathbf{r}-\xi)\equiv\hat{G}^{(E)}(\mathbf{r};\xi)|_{E=0}=F_y(\mathbf{r}-\xi)\begin{pmatrix}\delta(s_h-\xi_h)\theta(s_0-\xi_0) & 0\\ 0 & \delta(s_0-\xi_0)\theta(s_h-\xi_h)\end{pmatrix}. \quad (25)$$

In fact, taking into account the expansion of the Green's function $\hat{G}^{(E)}$ in powers of the matrix $\langle\hat{P}^{(0)}\rangle$:

$$\hat{G}^{(E)}(\mathbf{r};\xi)=\hat{G}^{(0)}(\mathbf{r}-\xi)+\int\hat{G}^{(0)}(\mathbf{r}-\mathbf{r}_1)\langle\hat{P}^{(0)}\rangle\hat{G}^{(0)}(\mathbf{r}_1-\xi)\,d^3\mathbf{r}_1+\int\hat{G}^{(0)}(\mathbf{r}-\mathbf{r}_1)\langle\hat{P}^{(0)}\rangle\hat{G}^{(0)}(\mathbf{r}_1-\mathbf{r}_2)\langle\hat{P}^{(0)}\rangle\hat{G}^{(0)}(\mathbf{r}_2-\xi)\,d^3\mathbf{r}_1\,d^3\mathbf{r}_2+\ldots \quad (26)$$

and the identity

$$\langle\hat{P}^{(E)}(\mathbf{r}_1)\otimes\hat{P}^{(E)}(\mathbf{r}_2)\otimes\ldots\otimes\hat{P}^{(E)}(\mathbf{r}_n)\rangle_c=\langle\hat{P}^{(0)}(\mathbf{r}_1)\otimes\hat{P}^{(0)}(\mathbf{r}_2)\otimes\ldots\otimes\hat{P}^{(0)}(\mathbf{r}_n)\rangle_c,\ n\geqslant 2 \quad (27)$$

(the symbol $\otimes$ denotes a direct product of matrices), we find $\hat{\Pi}^{(E)}(\mathbf{r}_1;\mathbf{r}_2)=\hat{\Pi}(\mathbf{r}_1;\mathbf{r}_2)$, which is what was to be proved.

It is easy to see that the Green's functions $\hat{G}^{(0)}$ appearing in the diagrammatic series (24) vary in the coordinate y over distances $\sim(\tau\lambda)^{1/2}\ll\tau$. It follows from this that the polarization operator $\hat{\Pi}$ and, correspondingly, the averaged Green's function $\hat{G}^{coh}$ can be represented as

$$\hat{\Pi}(\mathbf{r}_1;\ \mathbf{r}_2)=F_y(\mathbf{r}_1-\mathbf{r}_2)\hat{\Pi}(\mathbf{s}_1;\ \mathbf{s}_2), \quad (28)$$

$$\hat{G}^{coh}(\mathbf{r}_1;\ \mathbf{r}_2)=F_y(\mathbf{r}_1-\mathbf{r}_2)\hat{G}^{coh}(\mathbf{s}_1;\ \mathbf{s}_2). \quad (29)$$

The "two-dimensional" polarization operator $\hat{\Pi}(\mathbf{s}_1;\mathbf{s}_2)$ is determined by (24) with the simultaneous replacement $\mathbf{r}=(\mathbf{s},y)\to\mathbf{s}$, and the Dyson equation (22) takes the following form [$\xi=(\xi_0,\ \xi_h)$]:

$$\hat{G}^{coh}(\mathbf{s};\xi)=\hat{G}^{(E)}(\mathbf{s};\xi)+\int\hat{G}^{(E)}(\mathbf{s};\mathbf{s}_1)\hat{\Pi}(\mathbf{s}_1;\mathbf{s}_2)\hat{G}^{coh}(\mathbf{s}_2;\xi)\,d^2\mathbf{s}_1\,d^2\mathbf{s}_2. \quad (30)$$

Thus, the factorization of the dependence of the coherent Green's function (29) in the coordinate y makes it possible to reduce substantially the dimensionality of the general problem of coherent DXRS, and this corresponds to going over from the three-dimensional Dyson equation (22) to the two-dimensional Dyson equation (30).

In the case of DXRS in a crystal such that the Green's function $\hat{G}^{(E)}$ and polarization operator $\hat{\Pi}$ possess translational invariance, i.e.,

$$\hat{G}^{(E)}(\mathbf{s};\xi)=\hat{G}^{(E)}(\mathbf{s}-\xi),\quad \hat{\Pi}(\mathbf{s}_1;\ \mathbf{s}_2)=\hat{\Pi}(\mathbf{s}_1-\mathbf{s}_2)$$

(e.g., as is the case in Laue-diffraction geometry and with spatial uniformity of the distribution of defects), the exact solution of the Dyson equation (30) can be represented in the form of a double "inverse" Laplace integral:

$$\hat{G}^{coh}(s_0,s_h)=\frac{-1}{4\pi^2}\int_{a_0-i\infty}^{a_0+i\infty}\!\!\int\hat{G}^{coh}(p_0,p_h)e^{p_0s_0}e^{p_hs_h}dp_0\,dp_h$$
$$=\frac{-1}{4\pi^2}\int_{a_0-i\infty}^{a_0+i\infty}\!\!\int D^{-1}\begin{pmatrix}p_h-\Pi_{hh} & i\sigma_{-h}E-\Pi_{0h}\\ i\sigma_hE-\Pi_{h0} & p_0-\Pi_{00}\end{pmatrix}e^{p_0s_0}e^{p_hs_h}dp_0\,dp_h, \quad (31)$$

where the characteristic denominator D, the zeros of which are the poles of the Green's function $\hat{G}^{coh}(p_0,\ p_h)$ in reciprocal space, is equal to

$$D=(p_0-\Pi_{00})(p_h-\Pi_{hh})-(i\sigma_hE-\Pi_{h0})(i\sigma_{-h}E-\Pi_{0h}); \quad (32)$$

$\hat{\Pi}(p_0,\ p_h)$ is the two-dimensional Laplace transform of the polarization operator:

$$\hat{\Pi}(p_0,p_h)=\int_0^\infty ds_0\int_0^\infty ds_h\hat{\Pi}(s_0,s_h)e^{-p_0s_0}e^{-p_hs_h}.$$

In the general case the polarization operator $\hat{\Pi}$, as can be seen from (24), is an infinite series, each term of which corresponds to a certain multiplicity of the many-point cumulant averages. We show now that, if the condition $\pi\tau/\Lambda<1$ is fulfilled, the series (24) is asymptotic in this parameter. In fact, we consider an arbitrary compact diagram $_{(n)}\hat{\Pi}(\mathbf{s}_1;\mathbf{s}_n)$. The number of internal vertices in this diagram is equal to $n-2$, and the integration is performed over $2n-4$ internal variables s_0, s_h. Taking into account the explicit form of the Green's functions $\hat{G}^{(0)}$ (25), of which there are $n-1$, and the fact that the size of the range of integration over each internal variable is limited by the correlation length τ of the cumulant averages, we obtain the

following estimates:

$$|_{(3)}\hat{\Pi}(s_1; s_3)| \sim (\pi/\Lambda)^3 g_2(s_1, s_3),$$
$$|_{(n)}\hat{\Pi}| \sim |\pi\tau/\Lambda|^{n-3} |_{(3)}\hat{\Pi}|, \quad n>3, \tag{33}$$

while the first diagram of the series (24) does not contain internal vertices and has the form

$$_{(2)}\hat{\Pi}(s_1; s_2) \equiv \hat{\Pi}_\tau(s_1; s_2) = -\left(\frac{\pi}{\Lambda}\right)^2 g_2(s_1, s_2) \begin{pmatrix} \delta(s_{1,0}-s_{2,0})\theta(s_{1,h}-s_{2,h}) & 0 \\ 0 & \delta(s_{1,h}-s_{2,h})\theta(s_{1,0}-s_{2,0}) \end{pmatrix}. \tag{34}$$

The use in the Dyson equation (30) of the τ-approximation for the polarization operator (34) corresponds to all known formulations of statistical theory[11-14] in which coherent DXRS in crystals with randomly distributed defects is analyzed (for more detail, see Sec. 4).

In the practically interesting case of crystals with layer nonuniformity (e.g., heterostructures and superlattices), the macroscopic properties of the substance vary along the z direction (the normal to the crystal surface). In this case, from symmetry considerations it is clear that

$$\hat{G}^{(E)}(s; s_1) = G^{(E)}(x-x_1; z, z_1), \quad \hat{\Pi}(s; s_1) = \hat{\Pi}(x-x_1; z, z_1).$$

Fourier-transforming (30) in the coordinate x along the crystal surface in the diffraction plane, we arrive at the Dyson equation in the mixed (q, z) representation:

$$\hat{G}^{coh}(q; z) = \hat{G}^{(E)}(q; z) + \sin^{-2}(2\vartheta) \times \int \hat{G}^{(E)}(q; z, z_2)\hat{\Pi}(q; z_2, z_1)\hat{G}^{coh}(q; z_1)\,dz_2\,dz_1, \tag{35}$$

where the Fourier components of $\hat{G}$ and $\hat{\Pi}$ are equal to

$$\hat{G}(q; z, z_1) = \int_{-\infty}^{\infty} \hat{G}(x; z, z_1)e^{-iqx}\,dx,$$
$$\hat{\Pi}(q; z, z_1) = \int_{-\infty}^{\infty} \hat{\Pi}(x; z, z_1)e^{-iqx}\,dx.$$

If, in addition, the polarization operator $\hat{\Pi}$ satisfies the condition

$$\hat{\Pi}(q; z, z_1)\begin{cases} =0 & \text{for } z<z_1 \\ \neq 0 & \text{for } z>z_1 \end{cases},$$

the general solution of (35) can be represented in the form of the Z-ordered exponential

$$\hat{G}^{coh}(q; z) = Z\exp\left\{\hat{\Gamma}\int_0^z dz_1\left[\hat{\Sigma}(q; z_1) + \int_{z_1}^z \frac{dz_2}{\sin(2\vartheta)}\hat{\Pi}(q; z_2, z_1)\right]\right\}\hat{G}^{coh}(q; 0). \tag{36}$$

Here we have introduced the notation

$$\hat{\Sigma}(q; z_1) = \begin{pmatrix} -iq\beta_0 & i\sigma_h E(z_1) \\ i\sigma_{-h}E(z_1) & -iq\beta_h \end{pmatrix}, \quad \hat{G}^{coh}(q; 0) = \sin(2\vartheta)\hat{\Gamma},$$
$$\hat{\Gamma} = \begin{pmatrix} \gamma_0^{-1} & 0 \\ 0 & \gamma_h^{-1} \end{pmatrix},$$

and the geometrical parameters are given by

$$\gamma_0 = \varkappa^{-1}(\mathbf{nk}_0), \quad \gamma_h = \varkappa^{-1}(\mathbf{nk}_h),$$
$$\beta_0 = [\cos(2\vartheta)\gamma_0 - \gamma_h]/\sin(2\vartheta), \quad \beta_h = -[\cos(2\vartheta)\gamma_h - \gamma_0]/\sin(2\vartheta).$$

In the derivation of (36) it has been taken into account that the static Debye-Waller factor E depends on the coordinate z (Ref. 13).

In the particular case of the τ-approximation (34) and one-dimensional uniform disorder, i.e., when $g_2(\mathbf{s}_1; \mathbf{s}_2) = g_2(z_1 - z_2)$ and $E = \text{const}$, the expression (36) describing the propagation of the coherent Green's function goes over into the asymptotic solution found in Ref. 20.

3. DIFFUSE SCATTERING

Following the general method for separating the coherent and diffuse scattering in statistical optics,[18] we introduce into the analysis the four-point correlator of the Green's functions (the mutual-coherence function)

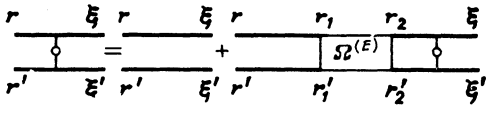
$$\hat{J}(\mathbf{r}, \mathbf{r}'; \boldsymbol{\xi}, \boldsymbol{\xi}') = \langle \hat{G}(\mathbf{r}; \boldsymbol{\xi}) \otimes \hat{G}^*(\mathbf{r}'; \boldsymbol{\xi}') \rangle. \tag{37}$$

The physical correlator $\hat{J}$ determines the angular distribution of the scattering intensity detected using a three-crystal x-ray spectrometer:[13]

$$\hat{I}(\mathbf{q}; \mathbf{q}_0) = \langle \hat{E}(\mathbf{q}) \otimes \hat{E}^*(\mathbf{q}) \rangle = \int \hat{J}(\boldsymbol{\eta}, \boldsymbol{\eta}'; \boldsymbol{\xi}, \boldsymbol{\xi}')\, e^{-i\mathbf{q}(\boldsymbol{\eta}-\boldsymbol{\eta}')} e^{i\mathbf{q}_0(\boldsymbol{\xi}-\boldsymbol{\xi}')}\, d^2\xi\, d^2\xi'\, d^2\eta\, d^2\eta' \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \tag{38}$$

where the integration is performed over the entrance surface ($d^2\xi$) and exit surface ($d^2\eta$) of the crystal, and the wave vectors $\mathbf{q}$ and $\mathbf{q}_0$ specify the directions of the scattered and incident radiation, respectively.

Representing (37) in the form of an infinite sum of two-row diagrams, corresponding to the direct product of the series (17), and performing cumulant averaging over the positions of the defects, we arrive at the diagrammatic equation[18]



(39a)

or, in explicit form (the Bethe-Salpeter equation),

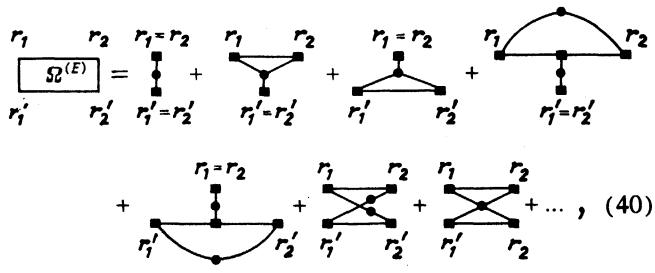
$$\hat{J}(\mathbf{r}, \mathbf{r}'; \boldsymbol{\xi}, \boldsymbol{\xi}') = \hat{J}^{coh}(\mathbf{r}, \mathbf{r}'; \boldsymbol{\xi}, \boldsymbol{\xi}') + \int d^3\mathbf{r}_1\, d^3\mathbf{r}_1'\, d^3\mathbf{r}_2\, d^3\mathbf{r}_2' \hat{J}^{coh}(\mathbf{r}, \mathbf{r}'; \mathbf{r}_1, \mathbf{r}_1') \times \hat{\Omega}^{(E)}(\mathbf{r}_1, \mathbf{r}_1'; \mathbf{r}_2, \mathbf{r}_2')\hat{J}(\mathbf{r}_2, \mathbf{r}_2'; \boldsymbol{\xi}, \boldsymbol{\xi}'), \tag{39b}$$

where

$$\hat{J}^{coh}(\mathbf{r}, \mathbf{r}'; \boldsymbol{\xi}, \boldsymbol{\xi}') = \hat{G}^{coh}(\mathbf{r}; \boldsymbol{\xi}) \otimes \hat{G}^{coh*}(\mathbf{r}'; \boldsymbol{\xi}'),$$

and the intensity operator $\hat{\Omega}$ is a sum of compact two-row

diagrams [compare with (21)]:



(40)

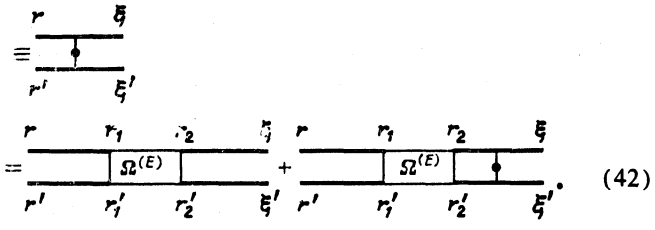
in which, if in a lower or an upper row in (40) there is only one vertex, a factor $\delta(\mathbf{r}_1' - \mathbf{r}_2')$ or $\delta(\mathbf{r}_1 - \mathbf{r}_2)$ corresponds to it.

We write the complete correlator $\hat{J}$ of the Green's functions in the form of the sum

$$J(\mathbf{r}, \mathbf{r}'; \boldsymbol{\xi}, \boldsymbol{\xi}') = J^{coh}(\mathbf{r}, \mathbf{r}'; \boldsymbol{\xi}, \boldsymbol{\xi}') + J^{dif}(\mathbf{r}, \mathbf{r}'; \boldsymbol{\xi}, \boldsymbol{\xi}'). \quad (41)$$

Substituting (41) into (39), for the diffusive part of the correlator we obtain the Bethe-Salpeter equation in the form

$J^{dif}(\mathbf{r}, \mathbf{r}'; \boldsymbol{\xi}, \boldsymbol{\xi}')$



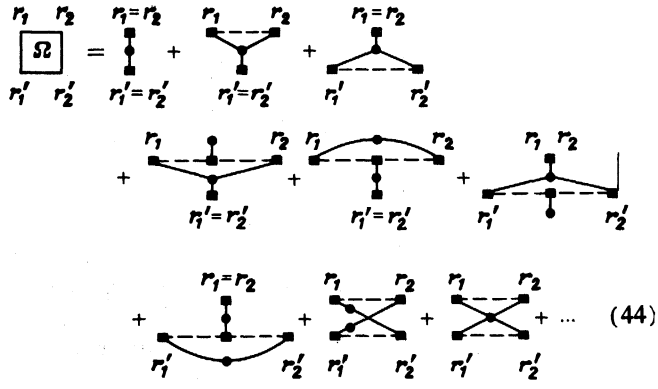
(42)

The first term in the right-hand side of (42) describes all possible mechanisms for the generation of diffuse waves as a result of the scattering of coherent waves by statistical inhomogeneities of the crystal lattice, and the second describes multiple diffuse scattering of diffuse waves, in which the propagation of the diffuse waves at the observation point $\mathbf{r}$, $\mathbf{r}'$ occurs in accordance with the coherent-wave propagation law specified by the correlator $\hat{J}^{coh}$.

Just as was done in the case of the polarization operator $\hat{\Pi}^{(E)}$ [see (23)], it can be proved that the following identity holds:

$$\hat{\Omega}(\mathbf{r}_1, \mathbf{r}_1'; \mathbf{r}_2, \mathbf{r}_2') \equiv \hat{\Omega}^{(E)}(\mathbf{r}_1, \mathbf{r}_1'; \mathbf{r}_2, \mathbf{r}_2')|_{E=0} = \hat{\Omega}^{(E)}(\mathbf{r}_1, \mathbf{r}_1'; \mathbf{r}_2, \mathbf{r}_2'), \quad (43)$$

where $\hat{\Omega}$ is the complete sum of all compact two-row diagrams



(44)

As was shown above, the condition $\lambda \ll \tau$ makes it possible to lower the dimensionality of the Dyson equation describing the coherent DXRS and to go over to the corresponding equations in the diffraction plane. This result can be generalized to the Bethe-Salpeter equation. A specific aspect of the proof in the latter case is that it is necessary to introduce the following restriction on the distances $|\mathbf{s} - \mathbf{s}'|$ and $|\boldsymbol{\xi} - \boldsymbol{\xi}'|$ between the observation points and the point sources:

$$\tau^2/\lambda \gg |\mathbf{s} - \mathbf{s}'| + |\boldsymbol{\xi} - \boldsymbol{\xi}'|, \quad (45)$$

and when this is fulfilled the three-dimensional Bethe-Salpeter equation (42) goes over into a two-dimensional equation of the form

$$J^{dif}(\mathbf{s}, \mathbf{s}'; \boldsymbol{\xi}, \boldsymbol{\xi}') = \int [J^{coh}(\mathbf{s}, \mathbf{s}'; \mathbf{s}_1, \mathbf{s}_1')\hat{\Omega}(\mathbf{s}_1, \mathbf{s}_1', \mathbf{s}_2, \mathbf{s}_2')J^{coh}(\mathbf{s}_2, \mathbf{s}_2'; \boldsymbol{\xi}, \boldsymbol{\xi}') + J^{coh}(\mathbf{s}, \mathbf{s}'; \mathbf{s}_1, \mathbf{s}_1')\hat{\Omega}(\mathbf{s}_1, \mathbf{s}_1'; \mathbf{s}_2, \mathbf{s}_2')J^{dif}(\mathbf{s}_2, \mathbf{s}_2'; \boldsymbol{\xi}, \boldsymbol{\xi}')] \times d^2\mathbf{s}_1\, d^2\mathbf{s}_1'\, d^2\mathbf{s}_2\, d^2\mathbf{s}_2'. \quad (46)$$

In the physically interesting case of small τ ($\pi\tau/\Lambda \ll 1$), an estimate of the diagrams with n vertices in the upper row and n' vertices in the lower row in the series (44) for the intensity operator $\hat{\Omega}$ leads to the following expressions:

$$_{(1,1)}\hat{\Omega}(\mathbf{s}, \mathbf{s}'; \mathbf{s}_1, \mathbf{s}_1') \equiv \hat{\Omega}_\tau(\mathbf{s}, \mathbf{s}')\delta(\mathbf{s} - \mathbf{s}_1)\delta(\mathbf{s}' - \mathbf{s}_1') = \langle \hat{P}^{(0)}(\mathbf{s}) \otimes \hat{P}^{(0)}(\mathbf{s}') \rangle_0 = \begin{pmatrix} 0 & 0 & 0 & |\sigma_{-\mathbf{h}}|^2 g_2(\mathbf{s}, \mathbf{s}') \\ 0 & 0 & \sigma_{\mathbf{h}}^* \sigma_{-\mathbf{h}} g_2^+(\mathbf{s}, \mathbf{s}') & 0 \\ 0 & \sigma_{\mathbf{h}} \sigma_{-\mathbf{h}}^* g_2^+(\mathbf{s}, \mathbf{s}') & 0 & 0 \\ |\sigma_{\mathbf{h}}|^2 g_2(\mathbf{s}, \mathbf{s}') & 0 & 0 & 0 \end{pmatrix}, \quad (47)$$

$$|_{(2,1)}\hat{\Omega}(\mathbf{s}, \mathbf{s}'; \mathbf{s}_1, \mathbf{s}_1')| \sim (\pi/\Lambda)|\hat{\Pi}_\tau(\mathbf{s}; \mathbf{s}_1)|g_2(\mathbf{s}, \mathbf{s}')\delta(\mathbf{s}' - \mathbf{s}_1'),$$
$$|_{(1,2)}\hat{\Omega}(\mathbf{s}, \mathbf{s}'; \mathbf{s}_1, \mathbf{s}_1')| \sim (\pi/\Lambda)|\hat{\Pi}_\tau(\mathbf{s}'; \mathbf{s}_1')|g_2(\mathbf{s}, \mathbf{s}')\delta(\mathbf{s} - \mathbf{s}_1),$$
$$|_{(3,1)}\hat{\Omega}(\mathbf{s}, \mathbf{s}'; \mathbf{s}_1, \mathbf{s}_1')| \sim (\pi/\Lambda)^4 g_2(\mathbf{s}, \mathbf{s}_1)\delta(\mathbf{s}' - \mathbf{s}_1'),$$
$$|_{(1,3)}\hat{\Omega}(\mathbf{s}, \mathbf{s}'; \mathbf{s}_1, \mathbf{s}_1')| \sim (\pi/\Lambda)^4 g_2(\mathbf{s}', \mathbf{s}_1')\delta(\mathbf{s} - \mathbf{s}_1),$$
$$|_{(n,1)}\hat{\Omega}(\mathbf{s}, \mathbf{s}'; \mathbf{s}_1, \mathbf{s}_1')| \sim (\pi\tau/\Lambda)^{n-3}|_{(3,1)}\hat{\Omega}(\mathbf{s}, \mathbf{s}'; \mathbf{s}_1, \mathbf{s}_1')| \quad (n > 3),$$
$$|_{(1,n')}\hat{\Omega}(\mathbf{s}, \mathbf{s}'; \mathbf{s}_1, \mathbf{s}_1')| \sim (\pi\tau/\Lambda)^{n'-3}|_{(1,3)}\hat{\Omega}(\mathbf{s}, \mathbf{s}'; \mathbf{s}_1, \mathbf{s}_1')| \quad (n' > 3),$$
$$|_{(2,3)}\hat{\Omega}(\mathbf{s}, \mathbf{s}'; \mathbf{s}_1, \mathbf{s}_1')| \sim (\pi/\Lambda)^3|\hat{\Pi}_\tau(\mathbf{s}; \mathbf{s}_1)|g_2(\mathbf{s}', \mathbf{s}_1')g_2(\mathbf{s}, \mathbf{s}'),$$
$$|_{(3,2)}\hat{\Omega}(\mathbf{s}, \mathbf{s}'; \mathbf{s}_1, \mathbf{s}_1')| \sim (\pi/\Lambda)^3|\hat{\Pi}_\tau(\mathbf{s}'; \mathbf{s}_1')|g_2(\mathbf{s}, \mathbf{s}_1)g_2(\mathbf{s}, \mathbf{s}'),$$
$$|_{(n,2)}\hat{\Omega}(\mathbf{s}, \mathbf{s}'; \mathbf{s}_1, \mathbf{s}_1')| \sim (\pi\tau/\Lambda)^{n-3}|_{(3,2)}\hat{\Omega}(\mathbf{s}, \mathbf{s}'; \mathbf{s}_1, \mathbf{s}_1')| \quad (n > 3),$$
$$|_{(2,n')}\hat{\Omega}(\mathbf{s}, \mathbf{s}'; \mathbf{s}_1, \mathbf{s}_1')| \sim (\pi\tau/\Lambda)^{n'-3}|_{(2,3)}\hat{\Omega}(\mathbf{s}, \mathbf{s}'; \mathbf{s}_1, \mathbf{s}_1')| \quad (n' > 3),$$
$$|_{(3,3)}\hat{\Omega}(\mathbf{s}, \mathbf{s}'; \mathbf{s}_1, \mathbf{s}_1')| \sim (\pi/\Lambda)^6 g_2(\mathbf{s}', \mathbf{s}_1')g_2(\mathbf{s}, \mathbf{s}_1)g_2(\mathbf{s}, \mathbf{s}'),$$
$$|_{(n,n')}\hat{\Omega}(\mathbf{s}, \mathbf{s}'; \mathbf{s}_1, \mathbf{s}_1')| \sim (\pi\tau/\Lambda)^{n+n'-6}|_{(3,3)}\hat{\Omega}| \quad (n, n' > 3). \quad (48)$$

In (47) we have introduced the correlation function

$$g_2^+(\mathbf{s},\ \mathbf{s}') = \langle e^{ih(u(\mathbf{s})+u(\mathbf{s}'))}\rangle_c. \tag{49}$$

The Bethe-Salpeter equation (46) and Eqs. (47) and (48) are the starting points for the construction of the τ-approximation of the theory of the formation and propagation of diffuse waves in crystals with random distributions of defects. We note that if for the calculation of the intensity operator $\hat{\Omega}$ we confine ourselves just to the expression (47), Eq. (46) goes over into the Bethe-Salpeter equation obtained earlier in Ref. 15.

4. THE τ-APPROXIMATION OF THE THEORY OF DXRS IN HOMOGENEOUSLY DISORDERED CRYSTALS

As follows from (33), in the τ-approximation the boundary-value problem of the propagation of coherent waves in a disordered crystal lattice reduces to solving the Dyson equation (35) with the expression (34) for the polarization operator $\hat{\Pi}_\tau$, which, in the $(q; z)$ representation, has the form

$$\hat{\Pi}_\tau(q; z, z_1) = \hat{\Pi}_\tau(q; z-z_1)$$
$$= -\sin(2\vartheta)\tau^2 \begin{pmatrix} |\gamma_h|^{-1} g_2\left(\frac{z-z_1}{\gamma_h}\right)\exp\left[-iq\frac{\beta_h}{\gamma_h}(z-z_1)\right] \\ \times\theta(\varepsilon(z-z_1)) \quad 0 \\ 0 \quad \gamma_0^{-1} g_2\left(\frac{z-z_1}{\gamma_0}\right) \\ \times\exp\left[-iq\frac{\beta_0}{\gamma_0}(z-z_1)\right]\theta(z-z_1) \end{pmatrix} \tag{50}$$

Here $\varepsilon = 1$ in the case of Laue-diffraction geometry ($\gamma_h > 0$), and $\varepsilon = -1$ in the case of Bragg geometry ($\gamma_h < 0$). In the derivation of (50) it has been assumed that the two-point correlator $g_2(\mathbf{s})$ is an isotropic function, i.e., $g_2(\mathbf{s}) = g_2(|\mathbf{s}|)$.

Applying to (35) a Laplace transformation in the coordinate z, from the Dyson equation we obtain the following expression for the Laplace transform $\hat{G}^{coh}(q,\ p)$:

$$\hat{G}^{coh}(q,p) = D^{-1}\begin{bmatrix} \gamma_h p+i\beta_h q+\sigma^2 g_2(\gamma_0 p+i\beta_0 q) & i\sigma_{-h}E \\ i\sigma_h E & \gamma_0 p+i\beta_0 q+\sigma^2 g_2(\gamma_h p+i\beta_h q)\end{bmatrix}$$
$$\times\left\{\begin{bmatrix}\gamma_0 & 0\\ 0 & \gamma_h\end{bmatrix}\hat{G}^{coh}(q, z=0) - \frac{\varepsilon-1}{2}\begin{bmatrix} G_{00}^{coh}(q,z=0) & G_{0h}^{coh}(q,z=0)\\ 0 & 0\end{bmatrix}\right\}$$
$$\times\sigma^2\int_0^\infty e^{-pz}dz\left\{|\gamma_h|^{-1}\int_{-\infty}^{-z}\exp\left[-\left(p+i\frac{\beta_h}{\gamma_h}q\right)z_1\right]g_2(z_1/\gamma_h)\,dz_1\right\}. \tag{51}$$

Here $g_2(p)$ is the Laplace transform of the two-point correlation function; D is the characteristic denominator, and has the form

$$D = [\gamma_h p+i\beta_h q+\sigma^2 g_2(\gamma_0 p+i\beta_0 q)]$$
$$\times[\gamma_0 p+i\beta_0 q+\sigma^2 g_2(\gamma_h p+i\beta_h q)]+\sigma^2 E^2; \tag{52}$$

in addition, for $\varepsilon = 1$,

$$\hat{G}^{coh}(q, z=0) = \sin(2\vartheta)\begin{bmatrix}\gamma_0^{-1} & 0\\ 0 & \gamma_h^{-1}\end{bmatrix},$$

while for $\varepsilon = -1$,

$$\hat{G}^{coh}(q, z=0) = \sin(2\vartheta)\begin{bmatrix}\gamma_0^{-1} & 0\\ G_{h0}^{coh}(q,z=0) & G_{hh}^{coh}(q,z=0)\end{bmatrix},$$

where the components $G_{h0}^{coh}(q,\ z=0)$ and $G_{hh}^{coh}(q,\ z=0)$ are determined with allowance for the boundary conditions $G_{h0}^{coh}(q,\ z=0) = G_{hh}^{coh}(q,\ z=t) = 0$.

It can be seen from (51) that, at least to within $(\pi\tau/\Lambda)^2 \ll 1$, the second term in the curly brackets in the right-hand side can be neglected, and the solution of the problem of coherent DXRS finally takes the form

$$\hat{G}^{coh}(q,p) = D^{-1}\begin{bmatrix} \gamma_h p+i\beta_h q+\sigma^2 g_2(\gamma_0 p+i\beta_0 q) & i\sigma_{-h}E \\ i\sigma_h E & \gamma_0 p+i\beta_0 q+\sigma^2 g_2(\gamma_h p+i\beta_h q)\end{bmatrix}$$
$$\times\begin{bmatrix}\gamma_0 & 0\\ 0 & \gamma_h\end{bmatrix}\hat{G}^{coh}(q, z=0). \tag{53}$$

Without loss of generality, we shall consider a disorder model with correlation function

$$g_2(\mathbf{s}) = (1-E^2)e^{-|\mathbf{s}|/\tau}.$$

In this case the dispersion law of the coherent waves propagating in the crystal has the form

$$\left[\left(\tilde{p}+i\tilde{q}+\frac{1}{\tau\gamma_0}\right)\left(\tilde{p}-i\tilde{q}+\frac{1}{\tau\gamma_h}\right) + (1-E^2)\frac{\sigma^2}{\gamma_0\gamma_h}\right]\left[\tilde{p}^2+\tilde{q}^2+\frac{\sigma^2}{\gamma_0\gamma_h}\right]$$
$$= (1-E^2)\frac{\sigma^2}{\gamma_0\gamma_h}\left[E^2\frac{\sigma^2}{\gamma_0\gamma_h}+\frac{1}{(\tau\gamma_0)(\tau\gamma_h)}\right]. \tag{54}$$

In writing (54) we have used the symmetrized variables

$$\tilde{p} = p+i\left[\frac{\beta_0}{\gamma_0}+\frac{\beta_h}{\gamma_h}\right]q, \qquad \tilde{q} = \left[\frac{\beta_0}{\gamma_0}-\frac{\beta_h}{\gamma_h}\right]q.$$

It follows from the form of the dispersion equation (54) that the dispersion surface $p = p(q)$ has four branches, of which two correspond to Bloch waves attenuating over distances of the order of the correlation length τ, while the other two are analogs of the dispersion surface of the perfect crystal (or of the crystal with averaged electric susceptibility) but with dispersion laws differing from the latter and having the following asymptotic forms: In the region $|\tilde{q}|\tau \ll 1$,

$$\tilde{p}_{1,2} = -\frac{(1-E^2)\sigma^2\tau}{2\gamma_0\gamma_h}[\gamma_h+\gamma_0+2i\tilde{q}\tau[\gamma_h^2-\gamma_0^2]]$$
$$\pm\left\{\left[i\tilde{q}+\frac{(1-E^2)\sigma^2\tau}{2\gamma_0\gamma_h}[\gamma_h-\gamma_0+2i\tilde{q}\tau[\gamma_h^2+\gamma_0^2]]\right]^2 - \frac{E^2\sigma^2}{\gamma_0\gamma_h}\left[1+\frac{(1-E^2)\sigma^2\tau^2}{\gamma_0\gamma_h}[\gamma_h^2+\gamma_0^2]\right]\right\}^{1/2}$$
$$+\frac{(1-E^2)\sigma^2\tau^3}{\gamma_0\gamma_h}\left\{\left[4\tilde{q}^2-(1-2E^2)\frac{\sigma^2}{\gamma_0\gamma_h}\right][\gamma_h^3+\gamma_0^3]\right.$$
$$\left.\mp\left[4\tilde{q}^2+(1+2E^2)\frac{\sigma^2}{\gamma_0\gamma_h}\right][\gamma_h^3-\gamma_0^3]\frac{\tilde{q}}{[\tilde{q}^2+E^2\sigma^2/(\gamma_0\gamma_h)]^{1/2}}\right\}, \tag{55}$$

while for $|\tilde{q}|\tau \gtrsim 1$,

$$\tilde{p}_{1,2}=\pm i\Big[\tilde{q}^2+\frac{\sigma^2}{\gamma_0\gamma_h}\Big]^{1/2}-\frac{(1-E^2)\sigma^2}{8\gamma_0\gamma_h\tilde{q}^2\tau}\Big\{\Big(\frac{1}{\gamma_0}+\frac{1}{\gamma_h}\Big)\pm\Big(\frac{1}{\gamma_0}-\frac{1}{\gamma_h}\Big)\frac{\tilde{q}}{[\tilde{q}^2+\sigma^2/(\gamma_0\gamma_h)]^{1/2}}\Big\}. \quad (56)$$

Physically, these differences are due to incoherent scattering by the disordered crystal lattice, leading to bending and broadening of the "dispersion law." It is interesting that this phenomenon has a direct analogy with the changes of the electron spectrum in disordered metals near a Brillouin-zone boundary.[21]

The figure shows the form of the dispersion branches 1 and 2 in the space Re $(\tilde{p}(\tilde{q}))$, Im $(\tilde{p}(\tilde{q}))$, $\tilde{q}$ in the symmetric Laue-diffraction geometry. It can be seen that for $|\tilde{q}|\tau<1$ the two branches of Im $(\tilde{p}(\tilde{q}))$ coincide (to within terms $\sim(1-E^2)\mathrm{Im}\,(\sigma)\pi\tau/\Lambda$) with the corresponding branches for the crystal with the averaged electric susceptibility, but have the additional broadening

$$\mathrm{Re}(\tilde{p}(\tilde{q}))=-(1-E^2)\mathrm{Re}(\sigma^2)\tau/\gamma_0.$$

In the opposite limit $|\tilde{q}|\tau>1$ they go over asymptotically into the branches of the dispersion surface for the perfect crystal.

Thus, applying the theory of residues to calculate the Laplace integral, with exponential accuracy we find for the coherent Green's function in the mixed (q,z) representation [see (53)]

$$\hat{G}^{coh}(q,z)=\sum_{i=1,2}\frac{\partial\ln(D(p))}{\partial p}\Big|_{p=p_i}\hat{G}^{coh}(q,p_i)\exp(p_iz). \quad (57)$$

The explicit form of the function $\hat{G}^{coh}$ in coordinate space is determined by applying the inverse Fourier transformation to (57). Using (55) for the approximate roots p_i of the characteristic equation, after direct calculations we obtain for $\hat{G}^{coh}$ in the region of influence $s_0, s_h>0$, except in the immediate vicinity of the characteristics $s_0, s_h=0$, the following expression:

$$\hat{G}^{coh}(s_0,s_h)=\begin{bmatrix}-E\sigma(s_0/s_h)^{1/2}J_1(S) & i\sigma_{-h}EJ_0(S)\\ i\sigma_hEJ_0(S) & -E\sigma(s_h/s_0)^{1/2}J_1(S)\end{bmatrix}\times\exp[-(1-E^2)\sigma^2\tau(s_0+s_h)]. \quad (58)$$

Here $J_0(S)$ and $J_1(S)$ are Bessel functions of real argument, and the function S is equal to

$$S(s_0,s_h)=\sigma E[(s_0+(1-E^2)\sigma^2\tau^2s_h)(s_h+(1-E^2)\sigma^2\tau^2s_0)]^{1/2}. \quad (59)$$

The region of applicability of (58) and (59), related to the discarding of the last term in the right-hand side of (55), is determined by the condition

$$(1-E^2)E^2(\pi^2\tau t/\Lambda^2)^2\ll1. \quad (60)$$

It is interesting that the expression (58) goes over into the corresponding expression for the matrix of the coherent Green's functions obtained by Kato[11] if in (58) and (59) we may neglect the τ^2 terms, which is equivalent to the more stringent [as compared with (60)] condition

$$2E(1-E^2)(\pi^2\tau t/\Lambda^2)^{3/2}\ll1. \quad (61)$$

The corresponding expressions for the coherent Green's functions near the characteristics $s_0, s_h=0$ have the following form [see (56)]:

1) In the region $s_h\ll\tau/(1-E^2)$, $s_0\gg(1-E^2)\tau(\pi\tau/\Lambda)^2$,

$$\hat{G}^{coh}(s_0,s_h)=\begin{bmatrix}\theta(s_0)\delta(s_h)-\sigma(s_0/s_h)^{1/2}J_1(2\sigma(s_0s_h)^{1/2}) & i\sigma_{-h}EJ_0(2\sigma(s_0s_h)^{1/2})\\ i\sigma_hEJ_0(2\sigma(s_0s_h)^{1/2}) & -\sigma E^2(s_h/s_0)^{1/2}J_1(2\sigma(s_0s_h)^{1/2})\end{bmatrix}, \quad (62)$$

2) in the region $s_0\ll\tau/(1-E^2)$, $s_h\gg(1-E^2)\tau(\pi\tau/\Lambda)^2$,

$$\hat{G}^{coh}(s_0,s_h)=\begin{bmatrix}-\sigma E^2(s_0/s_h)^{1/2}J_1(2\sigma(s_0s_h)^{1/2}) & i\sigma_{-h}EJ_0(2\sigma(s_0s_h)^{1/2})\\ i\sigma_hEJ_0(2\sigma(s_0s_h)^{1/2}) & \theta(s_h)\delta(s_0)-\sigma(s_h/s_0)^{1/2}J_1(2\sigma(s_0s_h)^{1/2})\end{bmatrix}. \quad (63)$$

On the characteristics the expressions (62) and (63) satisfy conditions for $\hat{G}^{coh}$ that correspond to averaging of the exact boundary relations (8) for the Green's functions $\hat{G}$.

We make here the following remark. The expressions (58), (62), and (63) obtained above in different regions of influence of $\hat{G}^{coh}$ do not depend on the concrete form of the two-point correlation function g_2. It is not difficult to show that they keep the same form if in their derivation we use for

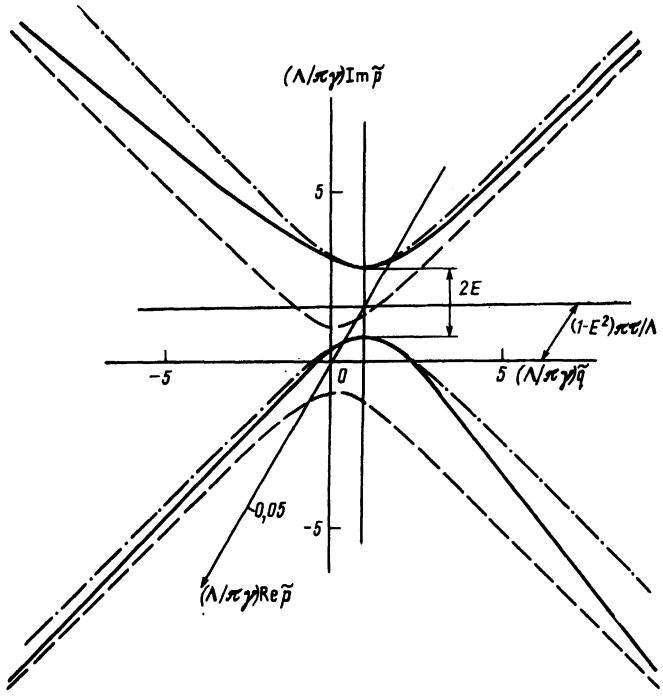


FIG. 1. Distortion Im $\tilde{p}$ and broadening (absorption) Re $\tilde{p}$ of the dispersion law $\tilde{p}(\tilde{q})$ for a disordered crystal in the region of values of $\tilde{q}$ in which, in the perfect crystal (the dashed curve) and in the crystal with the averaged electric susceptibility (the dashed-dotted curve), hyperbolic dependences Im $\tilde{p}(\tilde{q})$, shifted relative to each other by an amount equal to the additional absorption Re $\tilde{p}_0=-(1-E^2)\pi^2\tau/\gamma\Lambda^2$, would hold. The quantities Re $\tilde{p}$, Im $\tilde{p}$, and $\tilde{q}$ are measured in units of $\pi/\Lambda\gamma$. In the calculation we have taken the values $E=0.9$, $\pi\tau/\Lambda=0.1$, and $\gamma_0=\gamma_n=\gamma$. The scale along the Re $\tilde{p}$ axis is magnified by a factor of 100.

the arbitrary function $g_2(p)$ the appropriate expansions in a Taylor series in powers of $p\tau$ or $(p\tau)^{-1}$ and confine ourselves to the first significant terms.

We proceed now to the analysis in the τ-approximation of the Bethe-Salpeter equations (42) describing the formation and propagation of the diffuse waves. To this end we introduce the new coordinates

$$\rho={}^1/_2(s+s'),\quad \eta={}^1/_2(\xi+\xi'),$$
$$\Delta=s-s',\quad \delta=\xi-\xi',$$

in which the Bethe-Salpeter equation for the diffuse part of the correlator of the Green's functions in the τ-approximation has the following form [see (41) and (42)]:

$$\begin{aligned}&\hat{J}^{dif}(\rho;\Delta;\eta;\delta)\\&=\int d^2\rho_1 d^2\Delta_1[\hat{J}^{coh}(\rho;\Delta;\rho_1;\Delta_1)\hat{\Omega}_\tau(\Delta_1)\hat{J}^{coh}(\rho_1;\Delta_1;\eta;\delta)\\&\quad+\hat{J}^{coh}(\rho;\Delta;\rho_1;\Delta_1)\hat{\Omega}_\tau(\Delta_1)\hat{J}^{dif}(\rho_1;\Delta_1;\eta;\delta)].\end{aligned}\tag{64}$$

Using the symmetry of Eq. (64) with respect to the processes of diffuse and coherent scattering ($\hat{J}^{dif}\rightleftarrows\hat{J}^{coh}$), we can represent Eq. (64) identically as follows:

$$\begin{aligned}&\hat{J}^{dif}(\rho,\Delta;\eta,\delta)\\&=\int d^2\rho_1\,d^2\Delta_1[\hat{J}^{coh}(\rho,\Delta;\rho_1,\Delta_1)\hat{\Omega}_\tau(\Delta_1)\hat{J}^{coh}(\rho_1,\Delta_1;\eta,\delta)]\\&\quad+\int d^2\rho_1\,d^2\Delta_1\,d^2\rho_2\,d^2\Delta_2[\hat{J}^{coh}(\rho,\Delta;\rho_1,\Delta_1)\hat{\Omega}_\tau(\Delta_1)\\&\quad\times\hat{J}^{coh}(\rho_1,\Delta_1;\rho_2,\Delta_2)\\&\quad\times\hat{\Omega}_\tau(\Delta_2)\hat{J}^{coh}(\rho_2,\Delta_2;\eta,\delta)\\&\quad+\hat{J}^{coh}(\rho,\Delta;\rho_1,\Delta_1)\hat{\Omega}_\tau(\Delta_1)\hat{J}^{dif}(\rho_1,\Delta_1;\rho_2,\Delta_2)\\&\quad\times\hat{\Omega}_\tau(\Delta_2)\hat{J}^{coh}(\rho_2,\Delta_2;\eta,\delta)].\end{aligned}\tag{65}$$

Assuming that $\hat{J}^{dif}(\rho,\Delta;\eta,\delta)$ changes in the variables Δ and δ over distances greater in order of magnitude than τ, which enables us to set $\Delta_1\approx\Delta_2\approx0$ in (65), we arrive as a result at the equation

$$\begin{aligned}&\hat{J}^{dif}(\rho,\Delta;\eta,\delta)\\&=\int d^2\rho_1\,d^2\Delta_1[\hat{J}^{coh}(\rho,\Delta;\rho_1,\Delta_1)\hat{\Omega}_\tau(\Delta_1)\hat{J}^{coh}(\rho_1,\Delta_1;\eta,\delta)]\\&\quad+\int d^2\rho_1\,d^2\Delta_1\,d^2\rho_2\,d^2\Delta_2[\hat{J}^{coh}(\rho,\Delta;\rho_1,\Delta_1)\hat{\Omega}_\tau(\Delta_1)\\&\quad\times\hat{J}^{coh}(\rho_1,\Delta_1;\rho_2,\Delta_2)\hat{\Omega}_\tau(\Delta_2)\\&\quad\times\hat{J}^{coh}(\rho_2,\Delta_2;\eta,\delta)+\hat{J}^{coh}(\rho,\Delta;\rho_1,\Delta_1)\hat{\Omega}_\tau(\Delta_1)\\&\quad\times\hat{I}^{dif}(\rho_1;\rho_2)\hat{\Omega}_\tau(\Delta_2)\hat{J}^{coh}(\rho_2,\Delta_2;\eta,\delta)],\end{aligned}\tag{66}$$

where in the right-hand side we have introduced the matrix of the diffuse-scattering intensities

$$\hat{I}^{dif}(\rho;\eta)=\hat{J}^{dif}(\rho,0;\eta,0).\tag{67}$$

The physical meaning of going from (64) to (66) is that in the τ-approximation the diffuse part $\hat{J}^{dif}$ of the correlator is expressed in terms of the diffuse-scattering intensities and the problem reduces to solving the Bethe-Salpeter equation (64) for $\hat{I}^{dif}$:

$$\begin{aligned}\hat{I}^{dif}(s;\xi)=\int d^2s_1\,d^2\Delta_1[&\hat{J}^{coh}(s,0;s_1,\Delta_1)\hat{\Omega}_\tau(\Delta_1)\hat{J}^{coh}(s_1,\Delta_1;s_2,0)\\&+\hat{J}^{coh}(s,0;s_1,\Delta_1)\hat{\Omega}_\tau(\Delta_1)\hat{I}^{dif}(s_1;\xi)],\end{aligned}\tag{68}$$

which is none other than the transport equation for the matrix of the diffuse-scattering intensities, written in integral form.

The matrix integral equation (68) makes it possible to obtain transport equations in differential form for the diffuse-scattering intensities of the transmitted wave ($I_{00}^{dif}\equiv I_{00,00}^{dif}$) and diffracted wave ($I_{hh}^{dif}\equiv I_{h0,h0}^{dif}$).

In fact, differentiating (68) for $I_{00,00}^{dif}$ and $I_{h0,h0}^{dif}$ with respect to the variable s_0 and s_h, respectively, and taking into account the equality [see (12) and (30)]

$$\hat{L}_s^{(E)}\hat{G}^{coh}(s;\xi)-\int\hat{\Pi}_\tau(s;s_1)\hat{G}^{coh}(s_1;\xi)\,d^2s_1=\delta(s-\xi)\hat{I},$$

after direct calculations, to terms of order $(\pi\tau/\Lambda)<1$ inclusive, we obtain

$$\begin{aligned}&\frac{\partial I_{00}^{dif}}{\partial s_0}-i[\sigma_{-h}EI_{h0}^{dif}-\sigma_{-h}^{*}EI_{0h}^{dif}]\\&\quad+2\,\mathrm{Re}(\sigma^2)\int_0^{s_h}g_2(0,s_h')I_{00}^{dif}(s_0,s_h-s_h')\,ds_h'\\&\quad-2|\sigma_{-h}|^2\int_0^{s_0}g_2(s_0',0)I_{hh}^{dif}(s_0-s_0',s_h)\,ds_0'\\&=2\,\mathrm{Re}\left\{|\sigma_{-h}|^2\int_0^{s_0}g_2(s_0',0)G_{h0}^{coh}(s_0-s_0',s_h)\,ds_0'\,G_{h0}^{coh*}(s_0,s_h)\right\},\end{aligned}\tag{69}$$

$$\begin{aligned}&\frac{\partial I_{hh}^{dif}}{\partial s_h}-i[\sigma_hEI_{0h}^{dif}-\sigma_h^{*}EI_{0h}^{dif}]\\&\quad+2\,\mathrm{Re}(\sigma^2)\int_0^{s_0}g_2(s_0',0)I_{hh}^{dif}(s_0-s_0',s_h)\,ds_0'\\&\quad-2|\sigma_h|^2\int_0^{s_h}g_2(0,s_h')I_{00}^{dif}(s_0,s_h-s_h')\,ds_h'\\&=2\,\mathrm{Re}\left\{|\sigma_h|^2\int_0^{s_h}g_2(0,s_h')G_{00}^{coh}(s_0,s_h-s_h')\,ds_h'\,G_{00}^{coh*}(s_0,s_h)\right\}.\end{aligned}$$

In the derivation of (69) we have confined ourselves to treating the case of Laue-diffraction geometry with the radiation source on the crystal surface at the point $s_0=s_h=0$.

A system of equations of the type (69) was first obtained by Kato[11] in first order of perturbation theory in the fluctuations of the amplitude of the wave field in the crystal, in the microscopic Takagi-Taupin equations (6). Here, inasmuch as Eqs. (69) are not a closed system, i.e., they contain "nondiagonal" averages $I_{0h}^{dif}\equiv I_{00,h0}^{dif}$ and $I_{h0}^{dif}\equiv I_{h0,00}^{dif}$, in the framework of the theory of Ref. 11 the question of the relation of these components to the diagonal components I_{00}^{dif} and I_{hh}^{dif} remained unsolved. From general considerations, Kato postulated the relation

$$i[\sigma_{-h}EI_{h0}^{dif}-\sigma_{-h}^{*}EI_{0h}^{dif}]=2E^2\Gamma[|\sigma_{-h}|^2I_{hh}^{dif}-\mathrm{Re}(\sigma^2)I_{00}^{dif}],\tag{70}$$

where the length Γ was taken to be equal to $(\pi E/\Lambda)^{-1}$.

Using the matrix transport equation (68), which is a closed system of integral equations, and assuming that the components of the matrix of the diffuse-scattering intensities vary slowly over distances of the order of the correlation length τ, one can show that the relation (70) takes the form

$$i[\sigma_{-h}EI_{h0}^{dif}-\sigma_{-h}{}^{*}EI_{0h}^{dif}]=2E^{2}\Gamma[|\sigma_{-h}|^{2}I_{hh}^{dif}-\mathrm{Re}(\sigma^{2})I_{00}^{dif}]$$
$$+2|\sigma_{h}|^{2}\int_{0}^{s_0}ds_0'\int_{0}^{s_0}ds_0''\,\mathrm{Im}\{G_{0h}^{coh}(s_0-s_0',s_h)\sigma_{-h}{}^{*}EG_{hh}^{coh*}$$
$$\times(s_0-s_0'',s_h)g_2(s_0'-s_0'',0)\},\qquad(71)$$

and (of no less importance from the point of view of the construction of a general theory of diffuse scattering in disordered media) the following estimate is found to be valid for the length Γ:

$$\Gamma\sim(1-E^{2})|\pi/\Lambda|E^{-1}\tau^{2}\ll\Lambda/\pi E.\qquad(72)$$

As a result, from (69) with (71) and (72) taken into account, we arrive at the following closed system of differential equations describing the propagation of diffuse waves in disordered crystals when the correlation length $\tau\ll\Lambda/\pi$:

$$\frac{\partial I_{00}^{dif}}{\partial s_0}+2\,\mathrm{Re}(\sigma^{2})\int_{0}^{s_h}g_2(0,s_h')I_{00}^{dif}(s_0,s_h-s_h')\,ds_h'$$
$$-2|\sigma_{-h}|^{2}\int_{0}^{s_0}g_2(s_0',0)I_{hh}^{dif}(s_0-s_0',s_h)\,ds_0'$$
$$=2\,\mathrm{Re}\left\{|\sigma_{-h}|^{2}\int_{0}^{s_0}g_2(s_0',0)G_{h0}^{coh}(s_0-s_0',s_h)\,ds_0'\,G_{h0}^{coh*}(s_0,s_h)\right\}$$
$$+2|\sigma_{h}|^{2}\int_{0}^{s_0}ds_0'\int_{0}^{s_0}ds_0''\,\mathrm{Im}\{G_{0h}^{coh}(s_0-s_0',s_h)\sigma_{-h}{}^{*}EG_{hh}^{coh*}$$
$$\times(s_0-s_0'',s_h)g_2(s_0'-s_0'',0)\},$$
$$\frac{\partial I_{hh}^{dif}}{\partial s_0}+2\,\mathrm{Re}(\sigma^{2})\int_{0}^{s_0}g_2(s_0',0)I_{hh}^{dif}(s_0-s_0',s_h)\,ds_0'$$
$$-2|\sigma_{h}|^{2}\int_{0}^{s_h}g_2(0,s_h')I_{00}^{dif}(s_0,s_h-s_h')\,ds_h'$$
$$=2\,\mathrm{Re}\left\{|\sigma_{h}|^{2}\int_{0}^{s_h}g_2(0,s_h')G_{00}^{coh}(s_0,s_h-s_h')\,ds_h'\,G_{00}^{coh*}(s_0,s_h)\right\}$$
$$+2|\sigma_{h}|^{2}\int_{0}^{s_0}ds_0'\int_{0}^{s_0}ds_0''\,\mathrm{Im}\{\sigma_{h}EG_{0h}^{coh}(s_0-s_0',s_h)G_{hh}^{coh*}$$
$$\times(s_0-s_0'',s_h)g_2(s_0'-s_0'',0)\}.\qquad(73)$$

It can be seen from (73) that the characteristic mean free paths of the coherent and diffuse waves coincide and are given by a quantity

$$l\sim(\Lambda\tau/\pi E\Gamma)\approx(1-E^{2})^{-1}(\Lambda/\pi)^{2}\tau^{-1}\qquad(74)$$

equal, as follows from general physical considerations, to the absorption length associated with the extra absorption of the coherent waves on account of their transformation into diffuse waves [see (58)].

We note that, when compared with the equations of the theory of Ref. 11, Eqs. (72) now contain new terms, corresponding to processes of coherent propagation of the diffuse waves that are formed on the characteristic $s_h=0$.

In the limiting case $\tau\to0$ (the so-called case of kinematic scattering of diffuse waves), Eqs. (73) are simplified to the equations

$$\partial I_{00}^{dif}/\partial s_0=0,$$
$$\partial I_{hh}^{dif}/\partial s_h=(1-E^{2})|\sigma_{h}|^{2}\delta(s_h),$$

the solution of which for the diffuse-scattering intensities takes a simple form in the whole region of influence:

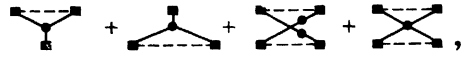
$$I_{00}^{dif}=0,\quad I_{hh}^{dif}=(1-E^{2})|\sigma_{h}|^{2}.\qquad(75)$$

It is not difficult to show that (75) is an exact solution of the Bethe-Salpeter equation (42) for $\tau\to0$.

It is interesting that, as follows from the differential transport equations (73), the boundary conditions on the characteristics s_0, $s_h=0$ for the diffuse-scattering intensities:

$$I_{00}^{dif}(0,s_h)=0,$$
$$I_{hh}^{dif}(0,s_h)=(1-E^{2})|\sigma_{h}|^{2},$$
$$I_{00}^{dif}(s_0,0)=2(1+E^{2})|\sigma|^{4}\int_{0}^{s_0}(s_0-s_{0,1})g_2(s_{0,1},0)\,ds_{0,1},\qquad(76)$$
$$I_{hh}^{dif}(s_0,0)=(1-E^{2})|\sigma_{h}|^{2},$$

coincide [except for the relation for $I_{00}^{dif}(s_0,0)$] with the exact boundary conditions stemming from the conditions (8) for the Green's functions G_0 and G_h on the boundaries of the region of their influence. The difference of the boundary condition for I_{00}^{dif} in (76) from the exact boundary condition $I_{00}^{dif}(s_0,0)=0$ is due to the τ-approximation ($\hat{\Omega}\to\Omega_\tau$). Analysis shows that this contradiction is removed if in the derivation of the first equation (73), in the transport equation (68), for the intensity operator $\hat{\Omega}$ we take into account the corrections

$\Delta\hat{\Omega}_\tau$ =  , (77)

which are important in the τ-neighborhood of the characteristic $s_h=0$.

With the intention of applying the theory developed to the method of three-crystal x-ray spectrometry, we apply a two-sided Fourier transformation to (66). As a result we obtain [cf. (38)]

$$\hat{I}^{dif}(q;q_0)$$
$$=\frac{1}{\gamma_0^{2}}\int dz_1\int dz_1'\int dz_2\int dz_2'\,[\hat{G}^{coh}(q;z,z_1)\otimes\hat{G}^{coh}(q;z,z_1')]$$
$$\times\Big\{\int dx_1\int dx_1'\,[\hat{\Omega}_\tau(x_1-x_1';z_1,z_1')$$
$$\times\exp[-i(q-q_0)(x_1-x_1')]]$$
$$\times\delta(z_1-z_2)\,\delta(z_1'-z_2')+\frac{1}{\gamma_0^{2}}\int dx_1\int dx_1'\int dx_2\int dx_2'$$
$$\times[\hat{\Omega}_\tau(x_1-x_1';z_1,z_1')$$
$$\times(\hat{G}^{coh}(x_1-x_2;z_1,z_2)\otimes\hat{G}^{coh}(x_1'-x_2';z_1',z_2'))$$
$$\times\hat{\Omega}_\tau(x_2-x_2';z_2,z_2')+\hat{\Omega}_\tau(x_1-x_1';z_1,z_1')\hat{I}^{dif}$$
$$\times\left(\frac{x+x_1'-x_2-x_2'}{2};\frac{z_1+z_1'}{2},\frac{z_2+z_2'}{2}\right)$$
$$\times\hat{\Omega}_\tau(x_2-x_2';z_2,z_2')$$
$$\times\exp\left[-i(q(x_1-x_1')-q_0(x_2-x_2')\right]\Big\}[\hat{G}^{coh}(q_0;z_2,0)$$
$$\otimes\hat{G}^{coh*}(q_0;z_2';0)]\begin{pmatrix}1\\0\\0\\0\end{pmatrix}.\qquad(78)$$

Thus, Eqs. (73) and the relation (78) completely deter

mine the angular distribution of the diffuse-scattering intensity $\hat{I}^{dif}(q, q_0)$ in the τ-approximation of the theory of DXRS from crystals with randomly distributed microdefects.

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