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Plane of Induced Dipoles in Self-Consistent Approach as a Unit of X-ray Scattering

by

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Scattering of the two harmonic EM plane waves by a plane of induced dipoles has been rigorously treated by means of the Hertz vector. It is shown that single plane solution may be used as a unit of X-ray scattering in the two-beam symmetrical Bragg case. This solution, given by a complex unimodular scattering matrix completely defines an interaction mode of the EM field with the single plane of dipoles for both states of polarization. The complex transmission coefficients derived determine step-like changes of phase and amplitude of both waves. In two particular vibrational states, when the two incident waves arrive at the dipole plane with the same or opposite phase, the actual phase shifts display a behavior predicted by the dynamic theory. However, as the relationship between two states is obtained in an exclusively analytical way, the customary geometrical arguments became redundant. It is shown that only a self-consistent solution, which includes cooperatives effects among scatterers, is able to conserve energy.

Key-words: Self-consistent approach; X-ray scattering.

I. INTRODUCTION

In a previous paper[1] (called paper I) we proposed a new method to evaluate the self-consistent interaction between a plane of induced dipoles and a single harmonic EM plane waves of the σ-polarization. The concept of self-consistency, introduced in the Ewald papers[2], was carried out by including in the total forcing field the field due to the induced dipoles of the scattering plane. This latter field outside that plane becomes two traveling waves outward the scattering plane, but inside that plane their mean and stationary value is summed with the field of the incident wave to form the total forcing field. The method efficiently calculates induced dipole vibrations in their proper self-consistent state by means of the Hertz vector formalism without approximations and with the transverse component of propagation included. The one and only assumption used, of dipoles vibrating without energy loss, was enough to guarantee that energy was conserved for the whole plane.

In the present paper we verify the new method within a more general scattering model involving two symmetrically incident harmonic plane-waves of independent elliptical polarization. The objective of this work is to show that the single plane solution may be used to handle all the X-ray scattering problems for the symmetrical Bragg case[3]. The crystal model is regarded as a stack of identical and equally spaced dipole planes of continuous and constant charge distribution. Diffraction on any set of such planes will involve then a second incident wave for all planes in the set except the last. One of these planes, filled up by the incident and transmitted EM waves on either side, which are in a self-consistent interacting mode with the plane dipoles, is regarded as a scattering unit.

The scattering unit concept is made possible by the bare results of the Hertz solution, verified now again for the two-wave model. These results are:

- the dipole fields are formed as a plane waves immediately after the take-off,
- they are propagating in the direction of the respective incident waves.

The last conclusion which excludes the presence of waves propagating in other directions than those defined by the incident waves also determines that the scattering by a stack of parallel dipole planes is an exclusively two beam case.

II. SCATTERING MODEL

In an orthonormal coordinate system, where the scattering plane is the plane defined by $x=0$, we calculate the outgoing dipole fields for a point $\vec{\mathbf{P}} = [x_P, y_P, z_P]$ outside that plane. We assume that the dipole plane is uniformly filled up by scattering electrons which behave as classical harmonic oscillators, vibrating without energy loss. The surface density of electrons distribution is described by σ_0. The two harmonic

EM plane wave A^{in} and B^{in} of an arbitrary elliptical polarization are symmetrically incident on the dipole plane at a general angle θ. The electrical parts of the waves are given by

$$\left.\begin{array}{l}\vec{\mathbf{E}}^{in}_{\mathrm{A}}(\vec{\mathbf{r}},t)=(\vec{\mathbf{A}}^{in}_{\pi}+\vec{\mathbf{A}}^{in}_{\sigma})\,\exp[\,i(\omega t-\vec{\mathbf{k}}^{in}_{\mathrm{A}}\cdot\vec{\mathbf{r}})\,]\\ \vec{\mathbf{E}}^{in}_{\mathrm{B}}(\vec{\mathbf{r}},t)=(\vec{\mathbf{B}}^{in}_{\pi}+\vec{\mathbf{B}}^{in}_{\sigma})\,\exp[\,i(\omega t-\vec{\mathbf{k}}^{in}_{\mathrm{B}}\cdot\vec{\mathbf{r}})\,]\end{array}\right\}\text{where}\left\{\begin{array}{l}\vec{\mathbf{k}}^{in}_{\mathrm{A}}=k\,[\;\;\sin\theta,\cos\theta,0]\\ \vec{\mathbf{k}}^{in}_{\mathrm{B}}=k\,[-\sin\theta,\cos\theta,0]\end{array}\right. \quad (1)$$

are wave vectors with magnitudes $k = 2\pi/\lambda$ of the incident waves A^{in} and B^{in}, respectively. The polarization vector components parallel to the plane of incidence are denoted by $\vec{\mathbf{A}}^{in}_{\pi}$ and $\vec{\mathbf{B}}^{in}_{\pi}$ while the components perpendicular to that plane, by $\vec{\mathbf{A}}^{in}_{\sigma}$ and $\vec{\mathbf{B}}^{in}_{\sigma}$. Each of these polarization vector components may be represented as a product of a complex amplitude which includes a phase and a respective versor indicating direction of vibration according to the following equations.

$$\begin{array}{l}\vec{\mathbf{A}}^{in}_{\pi}=\mathbf{A}^{in}_{\pi}\hat{\mathbf{e}}_{\mathrm{A}\pi},\;\;\mathbf{A}^{in}_{\pi}=|\,\mathbf{A}^{in}_{\pi}|\exp(i\alpha^{in}_{\pi}),\;\;\hat{\mathbf{e}}_{\mathrm{A}\pi}=[\cos\theta,-\sin\theta,0],\\ \vec{\mathbf{A}}^{in}_{\sigma}=\mathbf{A}^{in}_{\sigma}\hat{\mathbf{e}}_{\mathrm{A}\sigma},\;\;\mathbf{A}^{in}_{\sigma}=|\,\mathbf{A}^{in}_{\sigma}|\exp(i\alpha^{in}_{\sigma}),\;\;\hat{\mathbf{e}}_{\mathrm{A}\sigma}=[0,0,1],\\ \vec{\mathbf{B}}^{in}_{\pi}=\mathbf{B}^{in}_{\pi}\hat{\mathbf{e}}_{\mathrm{B}\pi},\;\;\mathbf{B}^{in}_{\pi}=|\,\mathbf{B}^{in}_{\pi}|\exp(i\beta^{in}_{\pi}),\;\;\hat{\mathbf{e}}_{\mathrm{B}\pi}=[\cos\theta,+\sin\theta,0],\\ \vec{\mathbf{B}}^{in}_{\sigma}=\mathbf{B}^{in}_{\pi}\hat{\mathbf{e}}_{\mathrm{B}\sigma},\;\;\mathbf{B}^{in}_{\sigma}=|\,\mathbf{B}^{in}_{\sigma}|\exp(i\beta^{in}_{\sigma}),\;\;\hat{\mathbf{e}}_{\mathrm{B}\sigma}=[0,0,1],\end{array} \quad (2)$$

where the initial phases of the two waves A^{in} and B^{in} in both states of polarization: (α^{in}_{π}, α^{in}_{σ}) and (β^{in}_{π}, β^{in}_{σ}), respectively, are included into complex values of all the amplitudes. These latter may be considered as vectors at complex plane and in this form will be used for graphical representations.

III. DIPOLE FIELDS

To find self-consistent dipole fields we follow the Hertz vector method applied in paper I. The solution presented there was obtained in two stages. At stage 1 the scattering was regarded as due to radiation from classical dipoles activated by an external field exclusively. The conclusion reached there was that the combined dipoles field take a plane wave form immediately with the two wave vectors identical to those of the incident field ($\vec{\mathbf{k}}^{di}_{\mathrm{A}} = \vec{\mathbf{k}}^{in}_{\mathrm{A}}$ and $\vec{\mathbf{k}}^{di}_{\mathrm{B}} = \vec{\mathbf{k}}^{in}_{\mathrm{B}}$). At stage 2 it was assumed that fields of neighboring radiating dipoles were also included by extending the dipole fields over the scattering plane itself. The assumption made was that the total forcing field includes a mean value of the self-consistent dipole fields. These traveling dipole fields were observed in two points separately for $\vec{\mathbf{P}}^{+} = [x_P > 0, y_P, z_P]$ and for one $\vec{\mathbf{P}}^{-} = [x_P < 0, y_P, z_P]$ on each side of the scattering plane. At the plane itself, however, they were counted as a part of the total forcing self-consistent field defined by its resultant polarization vector $\vec{\mathbf{F}}_{scf}(\vec{\mathbf{Q}}, t)$, ($\vec{\mathbf{Q}} = [0, y, z]$).

To simplify matters, we start calculations at a point related to stage 2 of paper I. We will derive the dipole fields at the two observation points $\vec{\mathbf{P}}^+$ and $\vec{\mathbf{P}}^-$, presupposing presence of these fields in the total forcing field. In other words we look for proper solutions of the dipole fields in only one step. The infinitesimal dipole moment at the point $\vec{\mathbf{Q}}$ is given by

$$d\vec{\mathbf{M}}(\vec{\mathbf{Q}},t) = (e^2\sigma_0/mc^2k^2)\exp[\,i(\omega t - ky\cos\theta\,)\,]\,dydz\,\vec{\mathbf{F}}_{scf}, \tag{3}$$

where $\vec{\mathbf{F}}_{scf}$, a total or resultant polarization vector, is the sum of all the polarization vectors involved:

$$\vec{\mathbf{F}}_{scf} = \vec{\mathbf{A}}^{in} + \vec{\mathbf{B}}^{in} + 1/2 < \vec{\mathbf{A}}^{di} + \vec{\mathbf{B}}^{di} > \tag{4}$$

and where $\vec{\mathbf{A}}^{di}$ and $\vec{\mathbf{B}}^{di}$ are the solution polarization vectors of the dipole fields. The last term in the sum indicates a mean value of the expected discontinuity in the resultant dipole fields at the plane of dipoles, in a treatment analogous to that of the standard Fourier Transform theory[4]. The $x-$, $y-$ and $z-$vector components of the polarization vectors are given by

$$\begin{aligned}\vec{\mathbf{A}}^{di} &= \vec{\mathbf{A}}^{di}_x + \vec{\mathbf{A}}^{di}_y + \vec{\mathbf{A}}^{di}_z,\\ \vec{\mathbf{B}}^{di} &= \vec{\mathbf{B}}^{di}_x + \vec{\mathbf{B}}^{di}_y + \vec{\mathbf{B}}^{di}_z.\end{aligned} \tag{5}$$

No assumption is made concerning polarization of these fields. As before, each of these polarization vector components may be represented as a product of an amplitude and a respective versor indicating direction of vibration.

$$\begin{aligned}&\vec{\mathbf{A}}^{di}_x = \mathbf{A}^{di}_x\hat{\mathbf{x}},\ \ \mathbf{A}^{di}_x = |\,\mathbf{A}^{di}_x|\exp(i\alpha^{di}_x), \quad \vec{\mathbf{B}}^{di}_x = \mathbf{B}^{di}_x\hat{\mathbf{x}},\ \ \mathbf{B}^{di}_x = |\,\mathbf{B}^{di}_x|\exp(i\beta^{di}_x),\\ &\vec{\mathbf{A}}^{di}_y = \mathbf{A}^{di}_y\hat{\mathbf{y}},\ \ \mathbf{A}^{di}_y = |\,\mathbf{A}^{di}_y|\exp(i\alpha^{di}_y), \quad \vec{\mathbf{B}}^{di}_y = \mathbf{B}^{di}_y\hat{\mathbf{y}},\ \ \mathbf{B}^{di}_y = |\,\mathbf{B}^{di}_y|\exp(i\beta^{di}_y),\\ &\vec{\mathbf{A}}^{di}_z = \mathbf{A}^{di}_z\hat{\mathbf{z}},\ \ \mathbf{A}^{di}_z = |\,\mathbf{A}^{di}_z|\exp(i\alpha^{di}_z), \quad \vec{\mathbf{B}}^{di}_z = \mathbf{B}^{di}_z\hat{\mathbf{z}},\ \ \mathbf{B}^{di}_z = |\,\mathbf{B}^{di}_z|\exp(i\beta^{di}_z).\end{aligned} \tag{6}$$

It will be convenient to express the polarization vectors of the two incident waves $\vec{\mathbf{A}}^{in}$ and $\vec{\mathbf{B}}^{in}$ also in terms of their $x-$, $y-$ and $z-$vector components for which the above set of equations may be opportunely used by a simple substitution of the superscript *di* by the superscript *in*.

We will calculate the resultant Hertz vector at the observation point $\vec{\mathbf{P}}$, due to the whole plane of dipole oscillation which is defined by

$$\vec{\mathbf{Z}}(\vec{\mathbf{P}},t) = -r_e k^{-2}\sigma_0\exp(i\omega t)\iint_{-\infty}^{+\infty} R^{-1}\exp[\,ik(R + y\cos\theta\,)\,]\,dydz\,\vec{\mathbf{F}}_{scf}, \tag{7}$$

where r_e is the classical electron radius and $\vec{\mathbf{R}} = \vec{\mathbf{P}} - \vec{\mathbf{Q}}$. Throughout this paper we use CGS units. We refer for actual calculations of the resultant Hertz vector to paper I. Here, we give the final result,

$$\vec{\mathbf{Z}}(\vec{\mathbf{P}},t) = ik^{-2}f_p \exp\{\, i[\omega t - k(\,|x_P|\sin\theta + y_P\cos\theta\,)]\,\}\,\vec{\mathbf{F}}_{scf},$$
$$\text{where} \qquad f_p = r_e\sigma_0\lambda/\sin\theta \tag{8}$$

is defined as the *plane scattering factor.* The respective resultant electric vector is obtained from the first of the known relations

$$\vec{\mathbf{E}}(\vec{\mathbf{P}},t) = \vec{\nabla}(\vec{\nabla}\cdot\vec{\mathbf{Z}}) - c^{-2}\ddot{\vec{\mathbf{Z}}},$$
$$\vec{\mathbf{B}}(\vec{\mathbf{P}},t) = \quad c^{-1}\vec{\nabla}\times\dot{\vec{\mathbf{Z}}} \tag{9}$$

which used at the observation point below the scattering plane $\vec{\mathbf{P}}^+$ gives the following expression

$$\vec{\mathbf{E}}(\,\vec{\mathbf{P}}^+,t) = (\mathbf{A}_x^{di}\hat{\mathbf{x}} + \mathbf{A}_y^{di}\hat{\mathbf{y}} + \mathbf{A}_z^{di}\hat{\mathbf{z}})\exp[\,i(\omega t - kx_P\sin\theta - ky_P\cos\theta\,)\,],$$
$$\mathbf{A}_x^{di} = \; if_p\,[\,\mathbf{A}_\pi^{in} + \mathbf{B}_\pi^{in}\cos 2\theta + 1/2 < (\mathbf{A}_x^{di} + \mathbf{B}_x^{di})\cos\theta - (\mathbf{A}_y^{di} + \mathbf{B}_y^{di})\sin\theta >]\cos\theta,$$
$$\mathbf{A}_y^{di} = -if_p\,[\,\mathbf{A}_\pi^{in} + \mathbf{B}_\pi^{in}\cos 2\theta + 1/2 < (\mathbf{A}_y^{di} + \mathbf{B}_y^{di})\cos\theta - (\mathbf{A}_y^{di} + \mathbf{B}_y^{di})\sin\theta >]\sin\theta,$$
$$\mathbf{A}_z^{di} = \; if_p\,[\,\mathbf{A}_\sigma^{in} + \mathbf{B}_\sigma^{in}] + 1/2 < \mathbf{A}_z^{di} + \mathbf{B}_z^{di} >] \tag{10}$$

and a similar one for the observation point above the scattering plane $\vec{\mathbf{P}}^-$

$$\vec{\mathbf{E}}(\,\vec{\mathbf{P}}^-,t) = (\mathbf{B}_x^{di}\hat{\mathbf{x}} + \mathbf{B}_y^{di}\hat{\mathbf{y}} + \mathbf{B}_z^{di}\hat{\mathbf{z}})\exp[\,i(\omega t + kx_P\sin\theta - ky_P\cos\theta\,)\,],$$
$$\mathbf{B}_x^{di} = \; if_p\,[\,\mathbf{B}_\pi^{in} + \mathbf{A}_\pi^{in}\cos 2\theta + 1/2 < (\mathbf{B}_x^{di} + \mathbf{A}_x^{di})\cos\theta - (\mathbf{B}_y^{di} + \mathbf{A}_y^{di})\sin\theta >]\cos\theta,$$
$$\mathbf{B}_y^{di} = \; if_p\,[\,\mathbf{B}_\pi^{in} + \mathbf{A}_\pi^{in}\cos 2\theta + 1/2 < (\mathbf{B}_y^{di} + \mathbf{A}_y^{di})\cos\theta - (\mathbf{B}_y^{di} + \mathbf{A}_y^{di})\sin\theta >]\sin\theta,$$
$$\mathbf{B}_z^{di} = \; if_p\,[\,\mathbf{B}_\sigma^{in} + \mathbf{A}_\sigma^{in}] + 1/2 < \mathbf{B}_z^{di} + \mathbf{A}_z^{di} >]. \tag{11}$$

In both expressions the solutions fall into two groups, one of which contains only the components parallel to the plane of incidence (indices x, y and π) while the other contains only those perpendicular to that plane (indices z and σ). These two kinds of vibrations are, therefore, independent of one another.

In the first group we observe that terms which appear in the brackets $[\cdots]$ in (10) and (11) are equal in both expressions and multiplied by the factors such as $\cos\theta$ and $\pm\sin\theta$. The only conclusion to be drawn from this fact is that they represent the amplitudes $\mathbf{A}_\pi^{di}$ and $\mathbf{B}_\pi^{di}$ of the π-components of the respective polarization vectors $\vec{\mathbf{A}}_\pi^{di}$ and $\vec{\mathbf{B}}_\pi^{di}$.

In the second group, the amplitudes $\mathbf{A}_z^{di}$ and $\mathbf{B}_z^{di}$, respectively identical with $\mathbf{A}_\sigma^{di}$ and $\mathbf{B}_\sigma^{di}$, represent the amplitudes of the σ-components of the respective polarization vectors $\vec{\mathbf{A}}_\sigma^{di}$ and $\vec{\mathbf{B}}_\sigma^{di}$.

Between $x-, y-$ and z-components of the polarization vectors on one side and π- and σ-components on the other we have the same relations as between the respective components of the polarization vectors defined for the two incident waves. We obtain the following set of equation

$$\begin{aligned} \mathbf{A}_x^{di} &= \mathbf{A}_\pi^{di}\cos\theta, & \mathbf{B}_x^{di} &= \mathbf{B}_\pi^{di}\cos\theta, \\ \mathbf{A}_y^{di} &= \mathbf{A}_\pi^{di}\sin\theta, & \mathbf{B}_y^{di} &= \mathbf{B}_\pi^{di}\sin\theta, \\ \mathbf{A}_z^{di} &= \mathbf{A}_\sigma^{di}, & \mathbf{B}_z^{di} &= \mathbf{B}_\sigma^{di}. \end{aligned} \tag{12}$$

in which the superscripts di substitute their equivalents in in an analogous set of equations (not given) for the incident waves.

As no restrictions are placed on the observation points, we can make them variable, equaling both to $\vec{\mathbf{r}}$ and the expressions (10) and (11) assume a simpler form with

$$\vec{\mathbf{E}}_{\mathrm{A}}^{di}(\vec{\mathbf{r}},t) = (\mathbf{A}_\pi^{di}\hat{\mathbf{e}}_{\mathrm{A}\pi} + \mathbf{A}_\sigma^{di}\hat{\mathbf{e}}_{\mathrm{A}\sigma})\exp[i(\omega t - kx\sin\theta - ky\cos\theta)] \quad \text{for } x > 0,$$
$$\begin{aligned} \text{where} \quad \mathbf{A}_\pi^{di} &= if_p[\mathbf{A}_\pi^{in} + \mathbf{B}_\pi^{in}\cos 2\theta + 1/2 < \mathbf{A}_\pi^{di} + \mathbf{B}_\pi^{di}\cos 2\theta >], \\ \mathbf{A}_\sigma^{di} &= if_p[\mathbf{A}_\sigma^{in} + \mathbf{B}_\sigma^{in} + 1/2 < \mathbf{A}_\sigma^{di} + \mathbf{B}_\sigma^{di} >] \quad \text{and} \end{aligned} \tag{13}$$

$$\mathbf{E}_{\mathrm{B}}^{di}(\vec{\mathbf{r}},t) = (\mathbf{B}_\pi^{di}\hat{\mathbf{e}}_{\mathrm{B}\pi} + \mathbf{B}_\sigma^{di}\hat{\mathbf{e}}_{\mathrm{B}\sigma})\exp[i(\omega t + kx\sin\theta - ky\cos\theta)] \quad \text{for } x < 0,$$
$$\begin{aligned} \text{where} \quad \mathbf{B}_\pi^{di} &= if_p[\mathbf{B}_\pi^{in} + \mathbf{A}_\pi^{in}\cos 2\theta + 1/2 < \mathbf{B}_\pi^{di} + \mathbf{A}_\pi^{di}\cos 2\theta >], \\ \mathbf{B}_\sigma^{di} &= if_p[\mathbf{B}_\sigma^{in} + \mathbf{A}_\sigma^{in} + 1/2 < \mathbf{B}_\sigma^{di} + \mathbf{A}_\sigma^{di} >]. \end{aligned} \tag{14}$$

Since $\vec{\mathbf{k}}_{\mathrm{A}} \cdot \vec{\mathbf{A}}_\pi^{di} = \vec{\mathbf{k}}_{\mathrm{A}} \cdot \vec{\mathbf{A}}_\sigma^{di} = \vec{\mathbf{k}}_{\mathrm{B}} \cdot \vec{\mathbf{A}}_\pi^{di} = \vec{\mathbf{k}}_{\mathrm{B}} \cdot \vec{\mathbf{A}}_\sigma^{di} = 0$ the combined dipole fields assume the form of two traveling plane waves defining harmonic electric vibrations of transverse type.

$$\left.\begin{aligned} \vec{\mathbf{E}}_{\mathrm{A}}^{di}(\vec{\mathbf{r}},t) &= (\vec{\mathbf{A}}_\pi^{di} + \vec{\mathbf{A}}_\sigma^{di})\exp[i(\omega t - \vec{\mathbf{k}}_{\mathrm{A}}^{di}\cdot\vec{\mathbf{r}})] \\ \vec{\mathbf{E}}_{\mathrm{B}}^{di}(\vec{\mathbf{r}},t) &= (\vec{\mathbf{B}}_\pi^{di} + \vec{\mathbf{B}}_\sigma^{di})\exp[i(\omega t - \vec{\mathbf{k}}_{\mathrm{B}}^{di}\cdot\vec{\mathbf{r}})] \end{aligned}\right\} \text{where} \left\{\begin{aligned} \vec{\mathbf{k}}_{\mathrm{A}}^{di} &= k[\ \sin\theta, \cos\theta, 0] \\ \vec{\mathbf{k}}_{\mathrm{B}}^{di} &= k[-\sin\theta, \cos\theta, 0] \end{aligned}\right. \tag{15}$$

The first expression represents now the dipole wave A^{di}, for $x > 0$, traveling in the direction of the incident wave A^{in}. Likewise, the second expression defines the dipole wave B^{di}, for $x < 0$, leaving symmetrically the scattering plane in the direction of the incident wave B^{in}.

Following paper I, we can repeat parallel calculations for magnetic vectors to obtain analogous results, that the magnetic vibrations are also transverse. Thus, the conclusion that two dipole waves are truly electromagnetic traveling plane waves results from the Hertz vector formalism. In order to calculate the actual values of the

$x-, y-$, and z-components of the dipole fields we have to resort again to the Ewald self-consistency principle.

IV. SELF-CONSISTENT SOLUTION

The idea of self-consistency is being carried out by including in the total forcing field the mean and stationary value of the two traveling dipole waves extrapolated on the plane of the scattering dipoles. Within that plane are valid expressions:

$$\vec{\mathbf{E}}^{for}_{con}(\vec{\mathbf{Q}},t) = \vec{\mathbf{E}}^{in}_{\mathbf{A}}(\vec{\mathbf{Q}},t) + \vec{\mathbf{E}}^{in}_{\mathbf{B}}(\vec{\mathbf{Q}},t),$$
$$\vec{\mathbf{E}}^{for}_{scf}(\vec{\mathbf{Q}},t) = \vec{\mathbf{E}}^{for}_{con}(\vec{\mathbf{Q}},t) + 1/2 < \vec{\mathbf{E}}^{di}_{\mathbf{A}}(\vec{\mathbf{Q}},t) + \vec{\mathbf{E}}^{di}_{\mathbf{B}}(\vec{\mathbf{Q}},t) > \tag{16}$$

the first of which represents the forcing field calculated in a conventional way (subscript *con*) and the second one stands for the self-consistent forcing field which includes also a contribution of the dipole fields (subscript *scf*). We can make the same observation, as in paper I, that the self-consistent dipole fields are related to the self-consistent forcing field in exactly the same way as their conventional equivalents are related to the conventional forcing field. This relationship between the respective dipole fields is determined by the same ratio of amplitudes and by the same phase shifts, as it is shown by the two following expressions the first of which represents a self-consistent way of calculation and the second a conventional one

$$i f_p \vec{\mathbf{E}}^{for}_{scf}(\vec{\mathbf{Q}},t) = \vec{\mathbf{E}}^{di}_{A,scf}(\vec{\mathbf{Q}},t) = \vec{\mathbf{E}}^{di}_{B,scf}(\vec{\mathbf{Q}},t), \tag{17}$$
$$i f_p \vec{\mathbf{E}}^{for}_{con}(\vec{\mathbf{Q}},t) = \vec{\mathbf{E}}^{di}_{A,con}(\vec{\mathbf{Q}},t) = \vec{\mathbf{E}}^{di}_{B,con}(\vec{\mathbf{Q}},t). \tag{18}$$

Since the second of the above relations is valid for every point within the dipole plane and for every moment of scattering, defined by variables $\vec{\mathbf{Q}}$ and t respectively, we look for a solution which refers to the amplitudes of the polarization vectors exclusively. This solution can be conveniently separated into its $x-, y-$ and z-components. By taking into account expressions (10), (11) and (12) we obtain the following relations:

$$1/2 < \mathbf{A}^{di}_x + \mathbf{B}^{di}_x > = i f_p [\mathbf{A}^{in}_x + \mathbf{B}^{in}_x + 1/2 < \mathbf{A}^{di}_x + \mathbf{B}^{di}_x >] \cos^2\theta,$$
$$1/2 < \mathbf{A}^{di}_y + \mathbf{B}^{di}_y > = i f_p [\mathbf{A}^{in}_y + \mathbf{B}^{in}_y + 1/2 < \mathbf{A}^{di}_y + \mathbf{B}^{di}_y >] \sin^2\theta,$$
$$1/2 < \mathbf{A}^{di}_z + \mathbf{B}^{di}_z > = i f_p [\mathbf{A}^{in}_z + \mathbf{B}^{in}_z + 1/2 < \mathbf{A}^{di}_z + \mathbf{B}^{di}_x >] \tag{19}$$

from which the above components of the polarization vectors are found by help of coefficients $\mathbf{f}_x, \mathbf{f}_y$ and $\mathbf{f}_z$, defined by:

$$\mathbf{f}_x = i \sin\varepsilon_x \exp(i\varepsilon_x), \quad \varepsilon_x = \arctan(f_p \cos^2\theta),$$
$$\mathbf{f}_y = i \sin\varepsilon_y \exp(i\varepsilon_y), \quad \varepsilon_y = \arctan(f_p \sin^2\theta),$$
$$\mathbf{f}_z = i \sin\varepsilon_z \exp(i\varepsilon_z), \quad \varepsilon_z = \arctan(f_p). \tag{20}$$

The self-consistency relationship between the amplitudes of the incident and dipole fields is illustrated by Fig.1 on which a similarity in behavior of the conventional and self-consistent fields, represented by the two expressions (17,18), is geometrically illustrated for only z-components of the fields.

Finally, the expression for the mean and stationary value of the electric part of the self-consistent dipole field generated within the scattering plane is given by

$$\begin{aligned}
&1/2 < \vec{\mathbf{E}}^{di}_{\mathrm{A}}(\vec{\mathbf{Q}},t) + \vec{\mathbf{E}}^{di}_{\mathrm{B}}(\vec{\mathbf{Q}},t) > = \\
&1/2\,[(\mathbf{A}^{di}_x + \mathbf{B}^{di}_x)\,\hat{\mathbf{x}} + (\mathbf{A}^{di}_y + \mathbf{B}^{di}_y)\,\hat{\mathbf{y}} + (\mathbf{A}^{di}_z + \mathbf{B}^{di}_z)\,\hat{\mathbf{z}}]\exp[\,i(\omega t - ky\cos\theta)\,] \\
&\text{with}\;\; \mathbf{A}^{di}_x = \mathbf{B}^{di}_x = \mathbf{f}_x(\mathbf{A}^{in}_x + \mathbf{B}^{in}_x), \\
&\qquad \mathbf{A}^{di}_y = \mathbf{B}^{di}_y = \mathbf{f}_y(\mathbf{A}^{in}_y + \mathbf{B}^{in}_y), \\
&\qquad \mathbf{A}^{di}_z = \mathbf{B}^{di}_z = \mathbf{f}_z(\mathbf{A}^{in}_z + \mathbf{B}^{in}_z).
\end{aligned} \tag{21}$$

The factors $\mathbf{f}_x, \mathbf{f}_y$ and $\mathbf{f}_z$ may be looked upon as components of a new self-consistent plane factor defined as an operator valid at the complex plane

$$\widehat{\mathbf{f}}_p = [\mathbf{f}_x, \mathbf{f}_y, \mathbf{f}_z]. \tag{22}$$

Since the expression (21) can be also ratified for the magnetic part of the self-consistent dipole field generated within the scattering plane, the operator $\widehat{\mathbf{f}}_p$ transforms the stationary incident EM field into its respective stationary dipole equivalent. The stationary dipole EM field gives rise to the two traveling dipole waves A^{di} and B^{di}. The amplitudes of the σ-components, $\mathbf{A}^{di}_\sigma$ and $\mathbf{B}^{di}_\sigma$, of the polarization vectors of the latter are already known while the amplitudes of the π-components, $\mathbf{A}^{di}_\pi$ and $\mathbf{B}^{di}_\pi$, of these polarization vectors may be obtained from the expressions (12), (13) and (14) as

$$\begin{aligned}
\mathbf{A}^{di}_\pi &= \mathbf{f}_x(\mathbf{A}^{in}_\pi + \mathbf{B}^{in}_\pi) + \mathbf{f}_y(\mathbf{A}^{in}_\pi - \mathbf{B}^{in}_\pi), \\
\mathbf{B}^{di}_\pi &= \mathbf{f}_x(\mathbf{A}^{in}_\pi + \mathbf{B}^{in}_\pi) - \mathbf{f}_y(\mathbf{A}^{in}_\pi - \mathbf{B}^{in}_\pi).
\end{aligned} \tag{23}$$

The solutions obtained for the dipole fields represent four EM waves which are formed immediately and are leaving symmetrically the dipole plane at the same angle, equal to the incidence angle θ.

The first pair of dipole waves, A^{di}_π and A^{di}_σ, is traveling in the direction of the incident waves, A^{in}_π and A^{in}_σ. The second pair of dipoles waves, B^{di}_π and B^{di}_σ, is traveling in the direction of the incident waves, B^{in}_π and B^{in}_σ. The dipole fields do not exist independently. When added to the incident waves the four transmitted waves A^{tr}_π, A^{tr}_σ, B^{tr}_π and B^{tr}_σ are generated according to

$$\left.\begin{aligned}
\vec{\mathbf{E}}^{tr}_{\mathrm{A}}(\vec{\mathbf{r}},t) &= (\vec{\mathbf{A}}^{tr}_\pi + \vec{\mathbf{A}}^{tr}_\sigma)\exp[\,i(\omega t - \vec{\mathbf{k}}^{tr}_{\mathrm{A}}\cdot\vec{\mathbf{r}})\,] \\
\vec{\mathbf{E}}^{tr}_{\mathrm{B}}(\vec{\mathbf{r}},t) &= (\vec{\mathbf{B}}^{tr}_\pi + \vec{\mathbf{B}}^{tr}_\sigma)\exp[\,i(\omega t - \vec{\mathbf{k}}^{tr}_{\mathrm{B}}\cdot\vec{\mathbf{r}})\,]
\end{aligned}\right\}\text{where}\left\{\begin{aligned}
\vec{\mathbf{k}}^{tr}_{\mathrm{A}} &= \vec{\mathbf{k}}^{in}_{\mathrm{A}} = \vec{\mathbf{k}}^{di}_{\mathrm{A}} \\
\vec{\mathbf{k}}^{tr}_{\mathrm{B}} &= \vec{\mathbf{k}}^{tr}_{\mathrm{B}} = \vec{\mathbf{k}}^{tr}_{\mathrm{B}}
\end{aligned}\right. \tag{24}$$

represent the two wave vectors. The corresponding four polarization vectors are

$$\vec{\mathbf{A}}_{\pi}^{tr} = (\mathbf{A}_{\pi}^{in} + \mathbf{A}_{\pi}^{di})\,\hat{\mathbf{e}}_{\mathrm{A}\pi}, \quad \vec{\mathbf{A}}_{\sigma}^{tr} = (\mathbf{A}_{\sigma}^{in} + \mathbf{A}_{\sigma}^{di})\,\hat{\mathbf{e}}_{\mathrm{A}\sigma},$$
$$\vec{\mathbf{B}}_{\pi}^{tr} = (\mathbf{B}_{\pi}^{in} + \mathbf{B}_{\pi}^{di})\,\hat{\mathbf{e}}_{\mathrm{B}\pi}, \quad \vec{\mathbf{B}}_{\sigma}^{tr} = (\mathbf{B}_{\sigma}^{in} + \mathbf{B}_{\sigma}^{di})\,\hat{\mathbf{e}}_{\mathrm{B}\sigma}. \tag{25}$$

The self-consistent solution admits no waves that could leave the scattering plane at an angle different from that defined by the incident one. As a consequence, the scattering by a plane of dipoles is exclusively a two-beam case. The results obtained here also shown that scattering by a dipole plane of two beams with arbitrary polarization can be decomposed into the two independent vibrations: perpendicular (index σ) and parallel (index π) to the plane of incidence. Accordingly, while general considerations with regard to the scattering model itself are the same, numerical results will differ. The angle θ becomes identically equal to 0 in all the corresponding expressions for the σ-polarization with one exception of the expression for f_p.

V. SCATTERING UNIT

We define the *scattering unit* as a dipole plane with its empty space environment, filled up by incident and transmitted EM field, self-consistently interacting with the dipoles of the plane. Scattering parameters for a set of parallel planes can be derived from corresponding ones, proper for a single plane. The importance of the unit may be estimated by considering it a *building brick* of the exact vectorial-wave solution from which more complex ones may be obtained by a synthesis process. The continuity of all the wave and polarization vectors of the electromagnetic field propagating between the adjoining units is a key to new complex solutions.

The origin of the scattering unit is due to the Ewald principle of self-consistency[2] which is now applied, however, to a plane of electrons rather than to a single one.

It will now be convenient to give some attention to the two different kinds of stationary electromagnetic fields which appear in connection with the introduced unit. The fields propagating inwards and outwards the scattering plane we will termed now the *mesofield*. We differentiate this field, calling the two incident waves jointly the *incident mesofield* while the two transmitted waves will be called together the *transmitted mesofield*. At the boundary planes of adjoining units the mesofield should be continuous with respect to all the wave and polarization vectors. At these planes, which may be chosen arbitrarily, the transmitted waves from an upper dipole plane become the incident waves for a lower one and vice versa.

The fields generated within a dipole plane due to the combined dipole radiation we will term the *epifield*. The epifield in the first place depends on the factor and in succession on the incident mesofield. For the case of σ-polarization the epifield is a function of the incident mesofield as a whole, while this dependence for π-polarization involves the actual composition of this incident field, such as it was shown in equations (20). It is be noted that up to now a self-consistent contribution to the epifield has been consequently denoted by '$1/2 < \cdots >$'.

The scattering unit function can be represented by means of a matrix which transforms a complex vector of the two incident amplitudes $[\mathbf{A}^{in}, \mathbf{B}^{in}]$ into a complex vector of the transmitted amplitudes $[\mathbf{A}^{tr}, \mathbf{B}^{tr}]$. This matrix will be defined in two versions for the π- and σ-polarization states and shown only for the former state.

$$\begin{bmatrix} \mathbf{A}^{tr} \\ \mathbf{B}^{tr} \end{bmatrix} = \begin{bmatrix} \mathbf{f}_t & \mathbf{f}_r \\ \mathbf{f}_r & \mathbf{f}_t \end{bmatrix} \cdot \begin{bmatrix} \mathbf{A}^{in} \\ \mathbf{B}^{in} \end{bmatrix}, \tag{26}$$

where the two matrix elements $\mathbf{f}_t$ and $\mathbf{f}_r$ called the *transmission* and *reflection coefficients*, respectively, are given by

$$\left.\begin{aligned} \mathbf{f}_t &= \mathbf{f}_x + \mathbf{f}_y + 1 = \cos\varepsilon_\theta \exp(i\,\varepsilon_\pi), \\ \mathbf{f}_r &= \mathbf{f}_x - \mathbf{f}_y \quad\;\; = i\sin\varepsilon_\theta \exp(i\,\varepsilon_\pi), \end{aligned}\right\}\text{where}\left\{\begin{aligned} \varepsilon_\pi &= \varepsilon_x + \varepsilon_y, \\ \varepsilon_\theta &= \varepsilon_x - \varepsilon_y. \end{aligned}\right. \tag{27}$$

The just introduced angles ε_π and ε_θ are exclusively defined for the π-polarization state. For the σ-polarization state the two above angles are equal and will be denominated by $\varepsilon_\sigma = \varepsilon_\theta = \varepsilon_x = \varepsilon_z$, while $\varepsilon_y = 0$.

All angles indicated by the letter ε applied in due context of the formalism allow the energy of the scattering system to be conserved. Such angles were conceived by Ewald[5] which predicted that both reflected and forward scattered waves should lag in phase by an angle slightly greater than $\pi/2$ behind the incident wave to produce a diminution in the transmitted amplitude and thus allowing for energy transfer into the reflected beam. In the present treatment, generalized for the two incident waves, no assumption of very small values of the respective phase lags, usually made in the all actual X-ray diffraction theories, is necessary to satisfy conservation of energy.

Taking into account that the dipole vibrations of both states of polarization are independent, the formulas from now on will be shown only for the π-polarization state. The corresponding ones for the σ-polarization state are readily obtained through substitution of the two angles ε_π and ε_θ by the unique angle ε_σ as shown before and the two versors $\hat{\mathbf{e}}_{A\pi}$ and $\hat{\mathbf{e}}_{B\pi}$ by the unique versor $\hat{\mathbf{e}}_\sigma$. The relationship between the amplitudes of two EM waves and the factors just introduced and angles for both states of polarization is illustrated in Fig. 1 and Fig. 2.

The polarization vectors of the transmitted mesofield can be easily obtained by means of the introduced matrix (26) as

$$\begin{aligned} \vec{\mathbf{A}}_\pi^{tr} &= \vec{\mathbf{A}}_\pi^{in} + \vec{\mathbf{A}}_\pi^{di} = [\,\mathbf{A}_\pi^{in}\cos\varepsilon_\theta + \mathbf{B}_\pi^{in}\, i\sin\varepsilon_\theta]\exp(\,i\varepsilon_\pi)\,\hat{\mathbf{e}}_{A\pi}, \\ \vec{\mathbf{B}}_\pi^{tr} &= \vec{\mathbf{B}}_\pi^{in} + \vec{\mathbf{B}}_\pi^{di} = [\,\mathbf{B}_\pi^{in}\cos\varepsilon_\theta + \mathbf{A}_\pi^{in}\, i\sin\varepsilon_\theta]\exp(\,i\varepsilon_\pi)\,\hat{\mathbf{e}}_{B\pi}. \end{aligned} \tag{28}$$

Summarizing, the results obtained indicate that the plane of induced dipoles acts as a plane wave transformer by changing in a steplike way the amplitude and phase of all waves of π- and σ-polarization. This function of the dipole plane as a stationary solution for the two pairs of interacting waves enables us to look upon it as a unit of scattering.

In a paper to follow we will show how the unit introduced can be used to analyze scattering pattern obtained from a set of parallel dipole planes, representing the crystal, where any of its planes can be considered as a scattering unit. Here, we shall derive all necessary parameters for scattering from only a single unit.

Formally we define the scattering unit as a plane of induced dipoles with its neighborhood of empty space filled up by the propagating field termed mesofield. The scattering unit function is a stationary solution involving changes of amplitude and phase for the two pairs of interacting waves with π- and σ-polarization states. This function can be most adequately expressed by a set of complex factors, each of them representing a ratio of two amplitudes for a chosen pair of waves. These ratios can be defined in versions corresponding to both polarization states. Physically, most significant is the amplitudes ratio of the incident wave B^{in} to the incident wave A^{in}. This factor unequivocally defines the composition of the incident mesofield. Its value is constant throughout the entire scattering plane and for the π-polarization is defined as

$$\mathcal{F}_\pi = \mathbf{B}_\pi^{in}/\mathbf{A}_\pi^{in} = f_\pi \exp(i\varphi_\pi) \quad \text{with} \;\; f_\pi = |\mathcal{F}_\pi|, \quad \varphi_\pi = \beta_\pi^{in} - \alpha_\pi^{in}. \tag{29}$$

The important pair of ratios which relate amplitudes of the transmitted waves with those of the incident ones is given by:

$$\begin{aligned} \mathcal{A}_\pi &= \mathbf{A}_\pi^{tr}/\mathbf{A}_\pi^{in} = a_\pi \exp(i\alpha_\pi) \quad \text{with} \;\; a_\pi = |\mathcal{A}_\pi|, \quad \alpha_\pi = \alpha_\pi^{tr} - \alpha_\pi^{in}, \\ \mathcal{B}_\pi &= \mathbf{B}_\pi^{tr}/\mathbf{B}_\pi^{in} = b_\pi \exp(i\beta_\pi) \quad \text{with} \;\; b_\pi = |\mathcal{B}_\pi|, \quad \beta_\pi = \beta_\pi^{tr} - \beta_\pi^{in}. \end{aligned} \tag{30}$$

The two last factors can be expressed in a form more suitable for applications by means of the two introduced angles ε_θ and ε_π. The new version of the above factors reads now, after carrying out some simple calculations,

$$\begin{aligned} \mathcal{A}_\pi &= [\cos\varepsilon_\theta + \mathcal{F}_\pi^{+1} i \sin\varepsilon_\theta] \exp(i\varepsilon_\pi) = a_\pi \exp[i(\varepsilon_{\alpha\pi} + \varepsilon_\pi)], \\ \mathcal{B}_\pi &= [\cos\varepsilon_\theta + \mathcal{F}_\pi^{-1} i \sin\varepsilon_\theta] \exp(i\varepsilon_\pi) = b_\pi \exp[i(\varepsilon_{\beta\pi} + \varepsilon_\pi)]. \end{aligned} \tag{31}$$

While the total phase shifts due to the contribution of the scattering dipoles for the two transmitted waves A^{tr} and B^{tr} are respectively defined as α_π and β_π by (30) it may be an opportune moment to separate the previously obtained constant part ε_π from the variable parts. This is done by introducing the following pair of new variables, $\varepsilon_{\alpha\pi}$ and $\varepsilon_{\beta\pi}$, given by two equations valid for the π-polarization state:

$$\varepsilon_{\alpha\pi} = \alpha_\pi - \varepsilon_\pi = \arcsin[(f_\pi/a_\pi)^{+1}\sin\varepsilon_\theta\cos\varphi_\pi],$$
$$\varepsilon_{\beta\pi} = \beta_\pi - \varepsilon_\pi = \arcsin[(f_\pi/b_\pi)^{-1}\sin\varepsilon_\theta\cos\varphi_\pi]. \tag{32}$$

The steplike changes in amplitude for both waves are defined by their absolute ratios a_π and b_π. These latter are easily derived from eqs.(58, 59)

$$a_\pi = [\cos^2\varepsilon_\theta + f_\pi^{+1}\sin(2\varepsilon_\theta)\sin\varphi_\pi + f_\pi^{+2}\sin^2\varepsilon_\theta]^{1/2},$$
$$b_\pi = [\cos^2\varepsilon_\theta - f_\pi^{-1}\sin(2\varepsilon_\theta)\sin\varphi_\pi + f_\pi^{-2}\sin^2\varepsilon_\theta]^{1/2}. \tag{33}$$

Similarly to the transmission factors just introduced we define in addition two other factors, conveniently called *reflection factors*. These latter are defined by the amplitudes ratios of the transmitted waves to those of the incident ones but now both propagating in space on the same side of the dipole plane. According to the equations valid for π-state of polarization and for $x < 0$ and for $x > 0$ we have

$$\mathcal{R}_\pi = \mathbf{B}_\pi^{tr}/\mathbf{A}_\pi^{in} = r_\pi\exp(i\rho_\pi) = [\mathcal{F}_\pi^{+1}\cos\varepsilon_\theta + i\sin\varepsilon_\theta]\exp(i\varepsilon_\pi),$$
$$\mathcal{S}_\pi = \mathbf{A}_\pi^{tr}/\mathbf{B}_\pi^{in} = s_\pi\exp(i\sigma_\pi) = [\mathcal{F}_\pi^{-1}\cos\varepsilon_\theta + i\sin\varepsilon_\theta]\exp(i\varepsilon_\pi) \tag{34}$$

where as before r_π and s_π are the absolute amplitudes ratios while ρ_π and σ_π are the relative phase shifts of the respective pairs of waves.

VI. SELF-CONSISTENCY AND CONSERVATION OF ENERGY

In paper I it was shown, for the single EM wave interacting with a plane of dipoles in the σ-polarization state, that the energy is conserved only when the Ewald principle of self-consistency has been respected. We will extend the above proof to a more general case of two such waves with an arbitrary elliptical polarization. We will also verify the validity of a reverse allegation, which should be ratified for two states of polarization, that satisfaction of the conservation of energy principle implies a self-consistent mode of the interaction of the two waves with the plane of dipoles. A required proof by help of the absolute amplitude ratios a_π and b_π given by (36) for the π-polarization and supplemented by a corresponding pair a_π and b_π for the σ-polarization is a trivial one. We obtain the two following equalities:

$$a_\pi^2 + f_\pi^2 b_\pi^2 = 1 + f_\pi^2$$
$$a_\sigma^2 + f_\sigma^2 b_\sigma^2 = 1 + f_\sigma^2 \tag{35}$$

from where we have for both polarization states

$$|\mathbf{A}_\pi^{tr}|^2 + |\mathbf{B}_\pi^{tr}|^2 = |\mathbf{A}_\pi^{in}|^2 + |\mathbf{B}_\pi^{in}|^2,$$
$$|\mathbf{A}_\sigma^{tr}|^2 + |\mathbf{B}_\sigma^{tr}|^2 = |\mathbf{A}_\sigma^{in}|^2 + |\mathbf{B}_\sigma^{in}|^2. \tag{36}$$

By adding the left and right sides of the latter equations we note that the energy of all interacting waves is invariant in the act of scattering. The above equations, separately analyzed, show that energy is also independently conserved for σ- and π-polarization components. The same is equally true for x-, y- and z-rectangular components of radiation as shown by other easy-to-prove equations

$$\begin{aligned} |\mathbf{A}_x^{tr}|^2+|\mathbf{B}_x^{tr}|^2 &= |\mathbf{A}_x^{in}|^2+|\mathbf{B}_x^{in}|^2, \\ |\mathbf{A}_y^{tr}|^2+|\mathbf{B}_y^{tr}|^2 &= |\mathbf{A}_y^{in}|^2+|\mathbf{B}_y^{in}|^2, \\ |\mathbf{A}_z^{tr}|^2+|\mathbf{B}_z^{tr}|^2 &= |\mathbf{A}_z^{in}|^2+|\mathbf{B}_z^{in}|^2. \end{aligned} \qquad (37)$$

The situation through which self-consistency is bound to produce conservation of energy can be geometrically justified on Fig.2 by means of the appropriate Argand diagram. Only the z-component will be shown out of the three pertinent ones which, of course, is also identical with the σ-component of the same polarization vector. We assume that the incident mesofield $\mathbf{M}_z^{in}$ formed by the z-components of the two incident traveling waves A^{in} and B^{in} and observed within the plane of dipoles has a unitary absolute value with the initial phase equal to zero. We note that the fact that an end-point of the amplitude vector $\mathbf{A}_z^{in}$ is also the beginning point of the amplitude vector $\mathbf{B}_z^{in}$, uniquely describes a content of the incident mesofield and will be termed a *complex tie point* of the z-field components and denoted $\mathbf{T}^{in}$. We note also that its definition could equally be carried out by means of another pair of amplitude vectors $\mathbf{A}_z^{tr}$ and $\mathbf{B}_z^{tr}$ of the two transmitted traveling waves A^{tr} and B^{tr} which jointly form a *transmitted mesofield* $\mathbf{M}_z^{tr}$. This last field may obtained from the incident mesofield from:

$$\mathbf{M}_z^{tr} = \mathbf{A}_z^{tr}+\mathbf{B}_z^{tr} = (\mathbf{A}_z^{in}+\mathbf{B}_z^{in})\exp(i2\varepsilon_z) = \mathbf{M}_z^{in}\exp(i2\varepsilon_z) \qquad (38)$$

which represents just another evidence of conservation of energy in the present model of scattering. The rotation angle ε_z depends on the actual epifield formed within the dipole plane. The introduced complex tie point uniquely defines the scattering unit function. Its utility comes from the fact that the amplitude of any wave out of four interacting ones can be found if amplitudes of two others are known, as shown by the Argand diagram in Fig. 2.

The presented pattern of the self-consistent mode of scattering is interesting from still another point of view. If the time is reversed the transmitted waves become the incident waves and vice versa but the general pattern of scattering remains unaltered. Since the analysis for the other x- and y-components of the EM field is essentially the same we consider the proof concluded.

In order to check the reverse allegation, proposed before, we will proceed in another direction. Under an assumption that the energy is conserved we will prove that the self-consistency principle is valid. We begin from bare results of the Hertz solution which, we remind, are:

- the dipole waves are formed immediately after the take-off,
- they are propagating in direction of the respective incident waves.

We repeat the assumption of self-consistency made in the first part that the field formed by the dipole radiation and included into the two transmitted waves appears as a part of the total forcing in a form of standing field represented by the mean value of these fields and called 'epifield' as before. We will obtain complex coefficients which transform the x-, y- and z-components of the incident mesofield into corresponding components of the epifield.

From the last of equations (21) we obtain two equations

$$\begin{aligned} \mathbf{A}_z^{tr} &= \mathbf{A}_z^{in} + \mathbf{A}_z^{di} = \mathbf{A}_z^{in} + \mathbf{f}_z(\mathbf{A}_z^{in} + \mathbf{B}_z^{in}), \\ \mathbf{B}_z^{tr} &= \mathbf{B}_z^{in} + \mathbf{B}_z^{di} = \mathbf{B}_z^{in} + \mathbf{f}_z(\mathbf{A}_z^{in} + \mathbf{B}_z^{in}) \end{aligned} \tag{39}$$

where $\mathbf{f}_z$ is considered now an unknown complex coefficient. From here we get:

$$|\mathbf{A}_z^{tr}|^2 + |\mathbf{B}_z^{tr}|^2 = |\mathbf{A}_z^{in}|^2 + |\mathbf{B}_z^{in}|^2 + |\mathbf{A}_z^{in} + \mathbf{B}_z^{in}|^2(\mathbf{f}_z + \mathbf{f}_z^* + 2\mathbf{f}_z\mathbf{f}_z^*). \tag{40}$$

If energy is to be conserved the term in parenthesis should be equal identically to zero together with two other similar ones formed by the coefficients f_x and f_y for respective x- and y-components of radiation. The general solutions are

$$\begin{aligned} \mathbf{f}_x + \mathbf{f}_x^* + 2\mathbf{f}_x\mathbf{f}_x^* \equiv 0 &\Rightarrow \mathbf{f}_x = i f_{px}/(1 - i f_{px}), \\ \mathbf{f}_y + \mathbf{f}_y^* + 2\mathbf{f}_y\mathbf{f}_y^* \equiv 0 &\Rightarrow \mathbf{f}_y = i f_{py}/(1 - i f_{py}), \\ \mathbf{f}_z + \mathbf{f}_z^* + 2\mathbf{f}_z\mathbf{f}_z^* \equiv 0 &\Rightarrow \mathbf{f}_z = i f_{pz}/(1 - i f_{pz}). \end{aligned} \tag{41}$$

Due to the loss of phase information the above set of equations (41) is the maximal result to be obtained from the energy conservation equation. Taking into account the transversal character of the incident mesofield and the assumed orientation of the scattering dipole plane in relation to the coordinate origin it is possible to show that $f_{px} = f_p \cos^2\theta$, $f_{py} = f_p \sin^2\theta$, and $f_{pz} = f_p$ which confirm the earlier result (20).

We have just proved that the energy is conserved only when the Ewald self-consistency principle has been respected. As the opposite assertion, with some necessary additional information, is equally true, then the equivalence of these two principles which has been first demonstrated in paper I for the single electromagnetic wave interacting with a plane of dipoles in the σ-polarization is now being extended for a more general case of the two such waves with an arbitrary elliptical polarization.

The conclusion reached is that the Ewald self-consistency may be considered a general principle valid for the EM scattering. In consequence, energy conservation may be used to verify if the calculations for more complex scattering models made in a self-consistent mode (without considering absorption) are correct. We have shown that if self-consistency is taken into account the energy conservation is, *per se*, satisfied. The opposite allegation, on the other hand, is only partially true, because of the simple reason, well known in crystallography, of the *phase problem.* Scalar formulation of energy conservation does not involve enough information to be reworked into a vectorial self-consistent mode of scattering. For just that reason the above relation can be qualified as semi-equivalent and the Ewald self-consistency principle as a more general one in, at least, the classical EM scattering.

VII. CONCLUSIONS

As we mentioned in the preceding section, the full analysis of results obtained and comparison with presently used forms of the dynamical X-ray diffraction theories can only be made after application of the introduced scattering unit for two more complex models:

- a set composed of equal and equidistant parallel planes of dipoles which, as representing the most simple model of a crystal, should result in the modified Bragg equation,
- a set of parallel dipole planes with a different dipole density and with irregular spacing should enable one to define the self-consistent structure factor.

Joining the two above models we will have a representative model of a crystal in a two-beam model of the self-consistent scattering. The importance of the unit of scattering introduced in these applications is based on the fact that it represents a 'brick' of the exact solution from which all more complicated solutions may be obtained by way of synthesis. A key to new solutions is the continuity of mesofields between the adjoining units. The microscopic solution rigorously obtained for a single dipole plane can be generalized into more complex models in which a self-consistent structure factor will be obtained in a non-primitive unit of scattering.

VIII. ACKNOWLEDGMENTS

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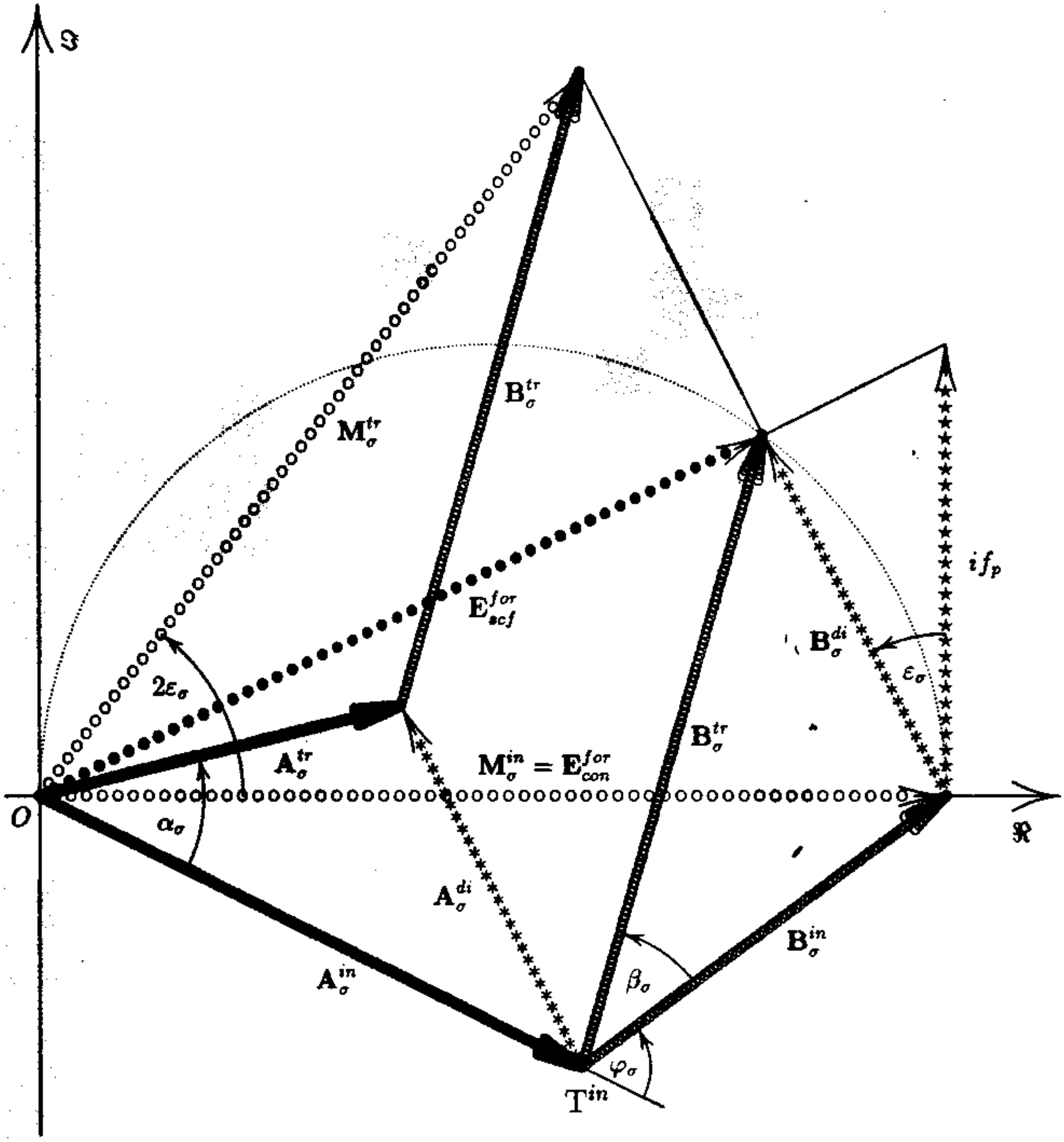

Fig. 1

FIG. 1. Argand diagram of the complex amplitude vectors for σ polarization state, equivalent also for the complex amplitude vectors represented in the x-, y- and z-rectangular components.

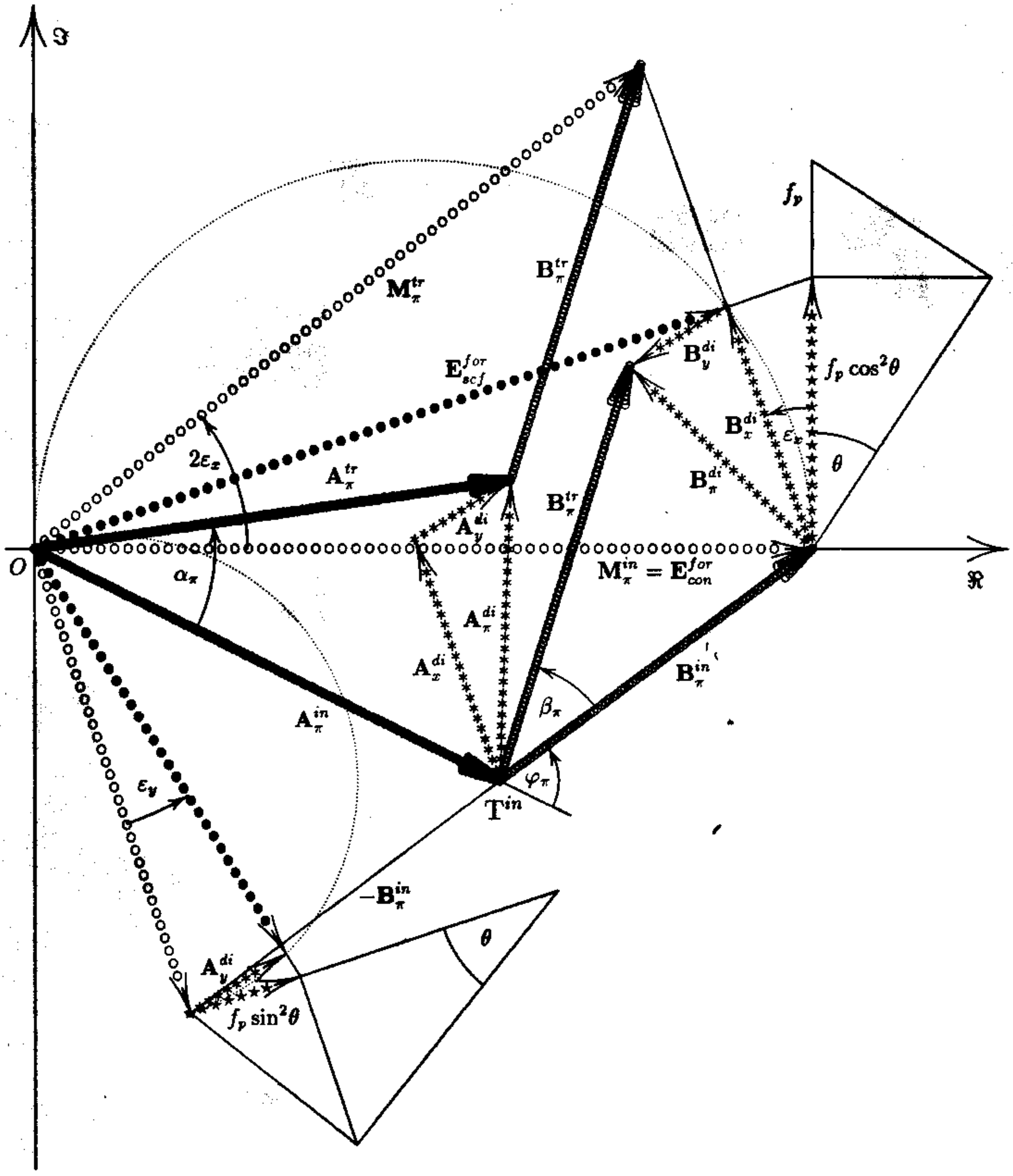

Fig. 2

FIG. 2. Argand diagram of the complex amplitude vectors for π polarization state.

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