Sampling theorem in macroscopic electrodynamics of crystal lattices

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Two ways may be used to describe the electromagnetic field-condensed media interaction. When one way is to get over a discrete structure of a medium by the averaging procedure, another way may be conceived as follows: to discretize fields on the basis of the discrete structure of a medium. When initial restrictions to the wave number spectrum take place, one can use the so-called sampling theorem for a medium modeled as a triple infinite periodic array of identical δ-functional scattering elements. Taking into account the Lorenz-Lorentz model one can develop a dynamical theory which considers strong field fluctuations in crystal lattices. [S1063-651X(98)08203-8]

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I. INTRODUCTION

Phenomenological macroscopic electrodynamics is based on microscopic equations for electromagnetic fields. Formal passage from microscopic equations to macroscopic description of condensed media is realized with an averaging atom or molecule positions. A similar procedure is used to describe artificial (composite) materials by effective parameters of continuous media [1,2].

To use macroscopic Maxwell's equations for the material continuum, the maximum scale of material nonhomogeneity has to be much less than distances of macroscopic field variations. For electromagnetic waves these distances correspond to the wavelength. Obviously, in any macroscopic problem there will be a natural scale of length and, therefore, we can use only those variables which have the Fourier-spectrum components up to some limiting cutoff wave number K (K may correspond, for example, to the inverse of spacing between particles). In other words, only those Fourier components with $k<K$ are relevant to the macroscopic problem. This question was discussed by Robinson [3]. In his book, Robinson makes a distinction between the so-called truncation (of the wave number spectrum) and the statistical-mechanical averaging over various sorts of ensembles. Usually $k\ll K$ and, therefore, these properties are not taken into account. When effects of material nonlocal relations are supposed to be considered, one can characterize a medium with constitutive parameters dependent on the wave vector. This is the so-called effect of spatial dispersion [4,5]. The notion of the material continuum is still taken into account in this case. Therefore, an analysis is made for small (compared to the inverse of spacing between particles) wave numbers.

Two ways may be used to describe the electromagnetic field-condensed media interaction. One way is to get over a discrete structure of a medium by the averaging procedure, while another way may be conceived as follows: to discretize fields on the basis of the discrete structure of a medium. Maxwell's electrodynamics is based on the space-time continuum. At the same time, the theory of information mostly deals with discrete elements. One of the fundamental results of the theory of information is expression of finite-spectrum functions by a series of samplings, or countings. These results are known as the theorem of samplings or countings, or as the Kotelnikov-Shenon theorem [6–8]. Because of the limiting cutoff wave number K, all variables in macroscopic electrodynamics are finite-spectrum functions. When initial restrictions to the wave number spectrum take place, one can use the sampling theorem for a medium modeled as a triple infinite periodic array of identical δ-functional scattering elements.

In this paper, we deliberately reject the spatial average of microscopic charges and will discretize the fields on the basis of the discrete structure of a medium. We will use the Lorenz-Lorentz theory which provides a solution that takes into account only the dipole term in the induced field. Since this theory considers only dipole interactions between particles, the results will be valid only for particles with small dimensions compared with their spacing. As it is a static field theory [1,2], the Lorenz-Lorentz theory may be extended to the dynamical regime, taking into account the dipole-dipole interaction in crystal lattices. Such an analysis was made in [5,9]. This method, however, is valid only for small (compared with the inverse of dimensions of a lattice cell) wave numbers. In our theory we do not consider the material continuum and therefore an analysis is not restricted by very small (because of the averaging procedure) wave numbers. The model makes it possible to take into account the retarded fields in dipole interactions, so we have the dynamical theory of crystal lattices.

This papers is devoted to dielectric crystal lattices. The proposed theory may be, however, successfully extended to complex media. In the following paper [10], we use our method for bianisotropic crystal lattices.

II. SPATIAL DISPERSION AND FIELD DISCRETIZATION

As a general description of a temporally causal and microscopically inhomogeneous medium, the integral-form constitutive relations have to be used. For dielectric media we have [4,5]

$$D_i(t,\vec{r})=\int_{-\infty}^{t}dt'\int d\vec{r}\,'\epsilon_{ij}(t,\vec{r},t',\vec{r}\,')E_j(t',\vec{r}\,'), \qquad (1)$$

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Here, only the causality principle (that the electric displacement $\vec{\mathcal{D}}$ at the time t is defined by the electric field $\vec{E}$ at the time $t'<t$) is taken into account.

Usually integral relations (1) are considered for a case when the kernel ϵ_{ij} is dependable on differences $t-t'$ and $\vec{r}-\vec{r}\,'$. It means that a medium is supposed to be time invariant and spatially homogeneous. The Fourier-Laplace transformation gives for dielectric media

$$\tilde{\vec{\mathcal{D}}}(\omega,\vec{k})=\overleftrightarrow{\epsilon}(\omega,\vec{k})\cdot\tilde{\vec{E}}(\omega,\vec{k}), \tag{2}$$

where the tilde denotes the Fourier images. This relation is used to describe temporally and spatially dispersive continuous media [4,5]. Such relations are also useful to obtain the effective constitutive parameter $\overleftrightarrow{\epsilon}^{\mathrm{eff}}(\omega,\vec{k})$ for composite materials [11,12].

For a time-invariant and spatially homogeneous medium, the kernel $\epsilon_{ij}(t',\vec{r}\,')$ is the only characteristic of a dielectric medium. This function may be interpreted as a ''response'' of a medium to the field action described by the Dirac δ function. In the case of a magnetic medium, a system may be characterized by a similar response function. A local character of the response functions in magnetodielectric media shows that constitutive parameters of materials have to be obtained on the basis of solution of quasistatic problems.

It is supposed in crystal optics that in the integral Fourier transformation, the Fourier images with

$$k\ll k_L, \tag{3}$$

where $k_L=2\pi/L$, L is a characteristic length (a distance between atoms), are mainly essential [3–5]. The smallness of the parameter kL is a geometric criterion of homogenization of a medium into the material continuum. At the same time, spatial dispersion is also determined by the small parameter kL [4,5]. So, an obvious contradiction in initial assumptions of the theory takes place: we try to describe a certain effect in a continuous medium knowing that this effect is determined by the same small parameter as the parameter of homogenization in this medium. One can trace this ambiguous situation when effects of optical activity are analyzed. While the authors in [4,5] consider optical activity as a particular case of a general effect of spatial dispersion in dielectric media described by relations (1), (2), other researchers analyze optical activity (chirality) as an independent phenomenon with independently postulated constitutive relations [13–15]. This may play an essential role when effects of spatial dispersion in complex (bianisotropic) media are considered [16,17].

Another situation takes place when the scale of nonlocality l is essentially large in comparison with the characteristic length L but less in comparison with the wavelength, so the following relationships take place:

$$k\ll k_l\ll k_L, \tag{4}$$

where $k_l=2\pi/l$. Such nonlocal effects may take place in media with quasistatic (potential) wave propagation. To describe such media Barybin used the notion of active polarized media [18]. The potential wave propagation is due to the short-length interactions between adjacent polarization vectors (magnetostatic waves in ferromagnetics, elastodynamic quasielectrostatic waves in piezoelectrics) or due to the Coulomb interaction between the mobile charges (space-charge waves).

It is supposed that because of relationships (3) and (4) one can make the Taylor-series expansion of $\epsilon_{ij}(\omega,\vec{k})$ in powers of $\vec{k}$. Such an expansion is possible if the limit of the long-wavelength (quasistatic) approximation exists [4,5]:

$$\overleftrightarrow{\epsilon}(\omega,\vec{k})|_{|\vec{k}|\to 0}\to\overleftrightarrow{\epsilon}(\omega) \tag{5}$$

The linear response functions in the form of integral operator (1) have diverse applications, not only in the theory of continuous media. The same relationships also describe the linear systems for time and space signal processing [6–8]. Let us consider a spatially homogeneous dielectric medium as a linear system of space signal processing (supposing, of course, that the causality principle is taken into account). We have for relation (1)

$$\mathcal{D}_i(\vec{r})=L\left[\int d\vec{r}\,'\,\delta(\vec{r}-\vec{r}\,')E_j(\vec{r}\,')\right]$$
$$=\int d\vec{r}\,'L[\delta(\vec{r}-\vec{r}\,')]E_j(\vec{r}\,'), \tag{6}$$

where L is a linear operator describing the transformation of an input signal (E_j) into an output signal $(\mathcal{D}_i)$. In such a consideration,

$$\epsilon_{ij}(\vec{r}-\vec{r}\,')\equiv L[\delta(\vec{r}-\vec{r}\,')] \tag{7}$$

is the so-called apparatus function or impulse-response function [6,7].

Together with mathematical problems of uniqueness and correctness of the solution of the integral equation (6), the question of interpolation arises: can one define (exactly or approximately) the input or output effects on the basis of discrete elements of the response [6]? In the theory of information these problems are analyzed in the scope of the sampling theorem [6]. In our case of an analysis of condensed media, an additional question arises: how does one correlate the polarization of every particle with sampling values of the electric field and define sampling values of the electric displacement?

Let the actual medium be modeled as a triple infinite periodic array of identical dipolar scattering elements in some homogeneous and isotropic host medium. Such a model, when the host medium is vacuum or dielectric, was used in a static field theory (the Lorenz-Lorentz theory) for natural dielectrics [1] or artificial dielectrics [2]. We will use this model to extend the Lorenz-Lorentz theory to the dynamical regime. The host medium we will characterize as a dielectric with permittivity ϵ (in a particular case, it may be vacuum with $\epsilon=\epsilon_0$) and the permeability μ_0. The wave number in the host medium $q(q^2=\omega^2\epsilon\mu_0)$ determines retardation in the dipole-dipole interaction between dipolar scattering elements.

Let in our model the spacing between elements be denoted by $\Delta x,\Delta y,\Delta z$. The elements are identified by the integer indices $m,n,l[-\infty<(m,n,l)<\infty]$. Every dipolar scatterer is considered as a δ source. Let us define the sampling values $f_s(\vec{r})$ of a continuous scalar function $f(\vec{r})$ in nodes of a lattice:

$$f_s(\vec{r}) = f(\vec{r}) \sum_{l=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \delta(x - m\Delta x)\,\delta(y - n\Delta y) \times \delta(z - l\Delta z) \equiv f(\vec{r})\, \frac{1}{\Delta V}\, \mathcal{C}\left(\frac{x}{\Delta x}\right) \mathcal{C}\left(\frac{y}{\Delta y}\right) \mathcal{C}\left(\frac{z}{\Delta z}\right) \quad (8)$$

where

$$\Delta V = \Delta x \Delta y \Delta z \quad (9)$$

is a volume of a cell. The $\mathcal{C}$ or comb functions are defined as sequences of δ-functions [7,8]. For example, $\mathcal{C}(x/\Delta x) = \Delta x \Sigma_{m=-\infty}^{\infty} \delta(x - m\Delta x)$.

We suppose that the function $f(\vec{r})$ is the function with finite $\vec{q}$ spectrum, where $\vec{q}$ is the wave vector in the host material. It means that the Fourier image $\tilde{f}(\vec{q})$ of the function f is equal to zero for $|q_x| > Q_x$, $|q_y| > Q_y$, $|q_z| > Q_z$, where Q_x, Q_y, Q_z are the limiting cutoff wave numbers. If spacings between nodes of a lattice are satisfied with the conditions

$$\Delta x \leqslant \frac{1}{2Q_x}, \quad \Delta y \leqslant \frac{1}{2Q_y}, \quad \Delta z \leqslant \frac{1}{2Q_z}, \quad (10)$$

one can obtain $\tilde{f}(\vec{q})$ on the basis of the Fourier image of $\tilde{f}_s(\vec{q})$ of the function $f_s(\vec{r})$ [6–8]:

$$\tilde{f}(\vec{q}) = \tilde{f}_s(\vec{q})\, \Delta V \sqcap\left(\frac{q_x}{2Q_x}\right) \sqcap\left(\frac{q_y}{2Q_y}\right) \sqcap\left(\frac{q_z}{2Q_z}\right) \quad (11)$$

where $\sqcap$ is the rectangle function and where for any i coordinate, we have

$$\sqcap\left(\frac{q_i}{2Q_i}\right) = \begin{cases} 1, & q_i \in [-Q_i, Q_i], \\ 0, & q_i \notin [-Q_i, Q_i]. \end{cases} \quad (12)$$

When the Fourier image $\tilde{f}(\vec{q})$ is known one can express the function $f(\vec{r})$ as follows [6–8]:

$$f(\vec{r}) = 8\Delta V Q_x Q_y Q_z \sum_{l=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} f(m\Delta x, n\Delta y, l\Delta z)\, \mathrm{sinc}(X_m)\, \mathrm{sinc}(Y_n)\, \mathrm{sinc}(Z_l), \quad (13)$$

where the sinc function is defined as $\mathrm{sinc}x = \sin x / x$ and where

$$\mathrm{sinc}(X_m) = \frac{\sin[2\pi Q_x(x - m\Delta x)]}{2\pi Q_x(x - m\Delta x)}, \quad (14)$$

$$\mathrm{sinc}(Y_n) = \frac{\sin[2\pi Q_y(y - n\Delta y)]}{2\pi Q_y(y - n\Delta y)}, \quad (15)$$

$$\mathrm{sinc}(Z_l) = \frac{\sin[2\pi Q_z(z - l\Delta z)]}{2\pi Q_z(z - l\Delta z)}. \quad (16)$$

For a medium modeled as a triple infinite periodic array, components of continuous fields may be represented as sampling values on the basis of the procedure shown above for an arbitrary scalar function f. One can correlate polarization of every particle with sampling values of the effective fields and define samplings of the electric displacement and magnetic flux density. The sampling theorem enables us to reconstruct the full Fourier spectrum of the electromagnetic field. So, we have field discretization based on the discrete structure of a medium.

III. FIELD SAMPLINGS IN DIELECTRIC CRYSTAL LATTICES

Let $\vec{E}^{(0)}$ be the electric field in the homogeneous isotropic host medium (vacuum, in a particular case) with the permittivity ϵ. This field is considered as the external field applied to a condensed medium quasistatically modeled as a triple periodic array of electric dipoles. Let $\vec{E}^{(p)}$ be the dipole field produced by all the particles in the infinite array. The average value of the total field in the medium (which, in fact, appears in macroscopic Maxwell equations) is defined as a sum of two fields:

$$\vec{E}_a^{(t)} = \vec{E}^{(0)} + \vec{E}_a^{(p)}, \quad (17)$$

The averaged dipole field $\vec{E}_a^{(p)}$ is dependable on the wave vector $\vec{q}$. For a particle that is symmetrical about the coordinate planes passing through the center of the particle, the quasistatic averaged dipole field

$$E_a^{(p)}(\vec{q})|_{q\to 0} = 0. \quad (18)$$

This is correct because of the symmetry of the three-dimensional array [2].

For the i component of the total field, the field samplings are defined as

$$E_{s_i}^{(t)}(\vec{r}) = \sum_{l=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} E_{a_i}^{(t)}(m\Delta x, n\Delta y, l\Delta z) \times \delta(x - m\Delta x)\,\delta(y - n\Delta y)\,\delta(z - l\Delta z). \quad (19)$$

For the fields $E_i^{(0)}$ and $E_{a_i}^{(p)}$ we have similar expressions denoted, respectively, by $E_{s_i}^{(0)}$ and $E_{s_i}^{(p)}$. Because of the linearity of relationships, one has

$$E_{s_i}^{(t)} = E_{s_i}^{(0)} + E_{s_i}^{(p)}. \quad (20)$$

The microscopic dipole moment density $\vec{p}_{\rm mic}$ is expressed as sequences of δ functions [19] and, therefore, is represented as a series of samplings. For the i component we have

$$(\vec{p}_{\rm mic})_i = \sum_{l=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} p_i(m\Delta x, n\Delta y, l\Delta z) \times \delta(x-m\Delta x)\,\delta(y-n\Delta y)\,\delta(z-l\Delta z) \equiv p_{s_i}, \tag{21}$$

where $\vec{p}(m\Delta x, n\Delta y, l\Delta z)$ is the dipole moment of the particle characterized by the numbers m,n,l.

Now we define the sampling vector $\vec{\mathcal{D}}_s$ with the i component as

$$\mathcal{D}_{s_i} = \epsilon E_{s_i}^{(t)} + P_{s_i}, \tag{22}$$

where

$$P_{s_i} = \frac{p_{s_i}}{\Delta V}. \tag{23}$$

Taking Eq. (20) into account, one obtains

$$\mathcal{D}_{s_i} = \epsilon[E_{s_i}^{(0)} + E_{s_i}^{(p)}] + P_{s_i}. \tag{24}$$

The induced dipole moment of every particle is proportional to the electric field. We have for sampling functions

$$p_{s_i} = \epsilon \alpha_{ij}(E_{s_j}^{(0)} + E_{s_j}^{(i)}), \tag{25}$$

where α_{ij} is the tensor of polarizability and $\vec{E}_s^{(i)}$ is the sampling vector of the interaction field, i.e., the field acting to the particle at the origin due to all the neighboring particles [1,2]. The interaction field is proportional to the induced dipole moment of the particle and may be expressed as

$$E_{s_j}^{(i)} = C_{jk} p_{s_k}, \tag{26}$$

where C_{jk} is the interaction tensor dependable on the wave vector $\vec{q}$. In the next section, the interaction tensor $\overleftrightarrow{C}(\vec{q})$ will be evaluated. One can solve a system of two vector equations, Eqs. (25) and (26), and represent the result in the general form

$$P_{s_i} = \frac{1}{\Delta V} g_{ij} E_{s_j}^{(0)}. \tag{27}$$

Here Eq. (23) is taken into account. The tensor g_{ij} in Eq. (27) is dependent on the wave vector $\vec{q}$.

Now let us define the field $E_{s_i}^{(p)}$ in Eq. (24). The dipole field produced by all the particles $\vec{E}^{(p)}$ is equal to the sum of the interaction field $\vec{E}^{(i)}$ and the dipole field produced by the particle located at the origin $\vec{E}^{(1)}$. Because of the dipole field structure [1], the sampling function $E_{s_i}^{(1)}$ is modeled by two types of comb-functions which are distinguished in signs. Since particles have dimensions very small compared with their spacing, these positive and negative comb functions are displaced from each other on negligible small distances (compared with spacing between particles). As a result, one has $E_{s_i}^{(1)} = 0$. So, one can write that $E_{s_i}^{(p)}$ is equal to $E_{s_i}^{(i)}$. However, we have to keep only the radiated (curl) part of $\vec{E}_s^{(i)}$ and therefore, we have

$$E_{s_i}^{(p)} = \Delta V[C_{ij}(\vec{q}) - C_{ij}(0)]P_{s_j}, \tag{28}$$

where $C_{ij}(0)$ is the interaction tensor at the quasistatic limit. At the quasistatic limit ($q \to 0$) the field samplings $\vec{E}_s^{(p)}$ are equal to zero.

Taking Eqs. (27) and (28) into account we can represent Eq. (24) as

$$\mathcal{D}_{s_i} = \epsilon E_{s_i}^{(0)} + \epsilon[C_{ij}(\vec{q}) - C_{ij}(0)](g_{jk}E_{s_k}^{(0)}) + \frac{1}{\Delta V} g_{ij} E_{s_j}^{(0)}. \tag{29}$$

This expression may be written in the form

$$\mathcal{D}_{s_i}(\vec{r}) = \chi_{ij}(\vec{q}) E_{s_j}^{(0)}(\vec{r}). \tag{30}$$

Here $\vec{q}$ is considered as a parameter.

When the sampling function $\vec{\mathcal{D}}_s(\vec{r})$ is known, one can reconstruct the Fourier spectrum of the displacement vector $\tilde{\vec{\mathcal{D}}}(\vec{q})$. On the basis of Eq. (11), we have

$$\tilde{\mathcal{D}}_i(\vec{q}) = \chi_{ij}(\vec{q}) \tilde{E}_{s_j}^{(0)}(\vec{q}) \Delta V \Pi\left(\frac{q_x}{2Q_x}\right) \Pi\left(\frac{q_y}{2Q_y}\right) \Pi\left(\frac{q_z}{2Q_z}\right) \equiv \tilde{\mathcal{D}}_{s_i}(\vec{q}) \Delta V \Pi\left(\frac{q_x}{2Q_x}\right) \Pi\left(\frac{q_y}{2Q_y}\right) \Pi\left(\frac{q_z}{2Q_z}\right). \tag{31}$$

This expression may be written as

$$\tilde{\vec{\mathcal{D}}}(\vec{q}) = \overleftrightarrow{\chi}(\vec{q}) \tilde{\vec{E}}^{(0)}(\vec{q}), \tag{32}$$

where $\tilde{\vec{E}}^{(0)}(\vec{q})$ is the Fourier image of the field $\vec{E}^{(0)}(\vec{r})$.

Expression (32) may be considered as an analog of formula (2) used in [4,5] for spatially dispersive continuous media. In our case, however, the wave vector $\vec{q}$ and the electric field $\vec{E}^{(0)}$ do not correspond to the wave vector and the electric field in the actual medium, but correspond to the wave vector and the electric field in the host medium (vacuum, in a particular case). At the same time, our derivation shows that tensor $\overleftrightarrow{\chi}$ has to be considered as the effective parameter of the actual medium. The reader should not be confused by this point. As we have pointed out above, in our model of dipolar scattering elements in the host medium, the wave number q determines retardation in the dipole-dipole interaction. Therefore, in the proposed dynamical theory of crystal lattices, all effective-medium quantities, which describe the actual medium, are dependent on the wave number in the host medium. The static-field theory of crystal lattices shows that because of symmetry of the three-dimensional array, the average value of the total field is equal to the field in the host medium [2]. Our dynamical theory also shows that sampling functions could be expressed by the sampling of the electric field in the host medium [see expression (29)]. Thus, the physical meaning of expression (32) becomes clear.

When we consider $\overleftrightarrow{\chi}(\vec{q})$ as the Fourier image of a certain original function $\overleftrightarrow{\chi}(\vec{r})$, the following convolution-form expression takes place:

$$\mathcal{D}_i(\vec{r})=\int d\vec{r}\,'\chi_{ij}(\vec{r}-\vec{r}\,')E_j^{(0)}(\vec{r}\,'). \qquad (33)$$

This is an analog of Eq. (1) for spatially homogeneous media when the causality principle is taken into account.

IV. EVALUATION OF THE INTERACTION TENSOR

We have introduced tensor $\overleftrightarrow{\chi}(\vec{q})$ on the basis of the formal procedure supposing that interaction tensor $\overleftrightarrow{C}(\vec{q})$ is known. Therefore the question of how one evaluates the interaction tensor arises.

The interaction tensor is given from the summation of the electric fields due to the array of dipoles:

$$C_{jk}(\vec{q})p_k=\sum_{l=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty}{}' E_j(m,n,l), \qquad (34)$$

where the prime indicates the omission of the term with $m=n=l=0$.

Electric field $\vec{E}(m,n,l)$ we define as the electric dipole field [1]

$$\vec{E}(m,n,l)=\frac{1}{4\pi\epsilon}\left\{[3\vec{u}(\vec{u}\cdot\vec{p})-\vec{p}]\left(\frac{1}{r_{mnl}^3}-\frac{i2\pi q}{r_{mnl}^2}\right)-[\vec{u}(\vec{u}\cdot\vec{p})-\vec{p}]\,\frac{4\pi^2q^2}{r_{mnl}}\right\}\exp(i2\pi q r_{mnl}), \qquad (35)$$

where r_{mnl} is the distance from the particle at the origin to the particle characterized by numbers m,n,l; $\vec{u}$ is the unit vector directed along the radius vector $\vec{r}_{mnl}$. Substitution of Eq. (35) into Eq. (34) gives $C_{ij}(\vec{q})$ when summations over m,n,l for a three-dimensional array of unit dipoles are made.

At the quasistatic limit, one obtains the interaction tensor on the basis of summations for the quasistatic term $(q\rightarrow 0)$ in Eq. (35). These summations over m,n,l give, for example, for the y component of the field,

$$E(m,n,l)_y|_{q\rightarrow 0}=\frac{1}{4\pi\epsilon}\sum_{l=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty}{}'\frac{[3\vec{u}(\vec{u}\cdot\vec{p})-\vec{p}]_y}{r_{mnl}^3}$$
$$=\sum_{l=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty}{}'\frac{3[(m\Delta x)(n\Delta y)p_x+(n\Delta y)^2p_y+(n\Delta y)(l\Delta z)p_z]-[(m\Delta x)^2+(n\Delta y)^2+(l\Delta z)^2]p_y}{[(m\Delta x)^2+(n\Delta y)^2+(l\Delta z)^2]^{5/2}}. \qquad (36)$$

Since the indices in Eq. (36) run equally over positive and negative values, the cross terms involving $(m\Delta x)(n\Delta y)p_x$ and $(h\Delta y)(l\Delta z)p_z$ vanish. One can rewrite Eq. (36) as

$$E(m,n,l)_y|_{q\rightarrow 0}=\frac{1}{4\pi\epsilon}\sum_{l=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty}{}'\frac{2(n\Delta y)^2-(m\Delta x)^2-(l\Delta z)^2}{[(m\Delta x)^2+(n\Delta y)^2+(l\Delta z)^2]^{5/2}}\,p_y. \qquad (37)$$

This shows, in result, that the interaction constant $\overleftrightarrow{C}(0)$ is a diagonal tensor:

$$E(m,n,l)_j|_{q\rightarrow 0}=C_{jj}(0)p_j. \qquad (38)$$

The series (37) has been summed, using the Poisson summation formula. One can also use an alternative approach based on the method of images [2].

Now we will analyze the general expression for $\overleftrightarrow{C}(\vec{q})(q\neq 0)$ based on Eqs. (34) and (35). Let the limiting cutoff wave numbers be defined as

$$Q_x=\frac{1}{2\Delta x},\quad Q_y=\frac{1}{2\Delta y},\quad Q_z=\frac{1}{2\Delta z}. \qquad (39)$$

In our model of small particles in comparison with their spacing $qr\simeq\vec{q}\cdot\vec{r}$. We have, for example, for the y component of the field

$$E(m,n,l)_y=\frac{1}{4\pi\epsilon}\sum_{l=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty}{}' \left\{\frac{3(m/2Q_x)(n/2Q_y)p_x+(n^2/Q_y^2)p_y+3(n/2Q_y)(l/2Q_z)p_z-(m^2/4Q_x^2+l^2/4Q_x^2)p_y}{(m^2/4Q_x^2+n^2/4Q_y^2+l^2/4Q_z^2)^{5/2}}\right.$$
$$\times\left[1-i2\pi\left(m\,\frac{q_x}{2Q_x}+n\,\frac{q_y}{2Q_y}+l\,\frac{q_z}{2Q_z}\right)\right]-\pi^2\,\frac{(m/Q_x)(n/Q_y)p_x+(n/Q_y)(l/Q_z)p_z-(m^2/Q_x^2+l^2/Q_x^2)p_y}{(m^2/4Q_x^2+n^2/4Q_y^2+l^2/4Q_z^2)^{5/2}}$$
$$\left.\times\left(m\,\frac{q_x}{2Q_x}+n\,\frac{q_y}{2Q_y}+l\,\frac{q_z}{2Q_z}\right)^2\right\}\exp\left[i2\pi\left(m\,\frac{q_x}{2Q_x}+n\,\frac{q_y}{2Q_y}+l\,\frac{q_z}{2Q_z}\right)\right]. \tag{40}$$

In these sums, the cross terms involving $(m/Q_x)(n/Q_y)p_x$ and $(n/Q_y)(l/Q_z)p_z$ vanish and one obtains the diagonal tensor $\overleftrightarrow{C}(\vec{q})$:

$$E(m,n,l)_j=C_{jj}(\vec{q})p_j\,. \tag{41}$$

For given quantities Q_x,Q_y,Q_z the interaction tensor $C_{jj}(\vec{q})$ may be represented in the form

$$C_{jj}(\vec{q})=\sum_{l=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty}{}' F_{jj}(q_x,q_y,q_z,m,n,l)\exp\left[i2\pi\left(m\,\frac{q_x}{2Q_x}+n\,\frac{q_y}{2Q_y}+l\,\frac{q_z}{2Q_z}\right)\right]. \tag{42}$$

It is necessary to note that in our consideration $C_{jj}(\vec{q})$ is the finite-spectrum function. This means that Eq. (42) gives $C_{jj}(\vec{q})$ only for $|q_x|\leqslant Q_x$, $|q_y|\leqslant Q_y$, $|q_z|\leqslant Q_z$. For other values of q we have $C_{jj}(\vec{q})=0$.

Because of the finite-spectrum functions, one can express

$$\sum_{l=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty}{}' F_{jj}\,\exp\left[i2\pi\left(m\,\frac{q_x}{2Q_x}+n\,\frac{q_y}{2Q_y}+l\,\frac{q_z}{2Q_z}\right)\right]$$
$$=\Pi\left(\frac{q_x}{2Q_x}\right)\Pi\left(\frac{q_y}{2Q_y}\right)\Pi\left(\frac{q_z}{2Q_z}\right)\sum_{l=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty}{}' F_{jj}\exp\left[i2\pi\left(m\,\frac{q_x}{2Q_x}+n\,\frac{q_y}{2Q_y}+l\,\frac{q_z}{2Q_z}\right)\right]. \tag{43}$$

This relation makes it possible to rewrite Eq. (42) as

$$C_{jj}(\vec{q})=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}G_{jj}(x,y,z)\exp[2\pi i(q_xx+q_yy+q_zz)]dxdydx, \tag{44}$$

where

$$G_{jj}(x,y,z)=8Q_xQ_yQ_z\sum_{l=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty}{}' F_{jj}\,\frac{\sin(2\pi Q_xx-\pi m)}{2\pi Q_xx-\pi m}\,\frac{\sin(2\pi Q_yy-\pi n)}{2\pi Q_yy-\pi n}\,\frac{\sin(2\pi Q_zz-\pi l)}{2\pi Q_zz-\pi l}. \tag{45}$$

When wave numbers q_x,q_y,q_z are considered as parameters in the expression for the function F_{jj}, one can see that $C_{jj}(\vec{q})$ is the Fourier image of the function $G_{jj}(\vec{r})$ taking into account that F_{jj} is equal to zero for $m=n=l=0$.

V. CONCLUDING REMARKS

The actual Coulomb field in the crystal lattice is different from the macroscopic field. In their dynamical theory of crystal lattices, Born and Huang used Ewald's method for providing a way of separating the macroscopic field from the actual Coulomb field [9]. It was supposed that due to the dipole-dipole interaction, the lattice could be imagined as a polarized continuum with small perturbation of dielectric polarization.

Based on the Lorenz-Lorentz theory (which provides a solution that takes into account only the dipole term in the induced field), one can develop a dynamical theory which considered strong field fluctuations in crystal lattices. One of the ways to realize the dynamical theory of crystal lattices is to reject the spatial average of microscopic charges and discretize the fields on the basis of the discrete structure of a medium. This method is based on the use of the so-called sampling theorem.

In this paper we have shown how the sampling theorem may be applied to the dynamical theory of crystal lattices. Our method becomes very important when the wave length in a medium is comparable with the spacing between particles. In such a case the known methods of an analysis of spatially dispersive media based on the concept of a material continuum has obvious contradictions in the initial assumption.

Any numerical examples to illustrate the usefulness of our method are beyond the scope of this paper. Nevertheless, it is important to point out some aspects concerning the effectiveness of the necessary computations. In our analysis we supposed that the fields are described by finite-spectrum functions. Let us assume additionally that the fields are also restricted in space by intervals $|x|\leqslant x_{\max}$, $|y|\leqslant y_{\max}$, $|z|\leqslant z_{\max}$. When $x_{\max}Q_x, y_{\max}Q_y, z_{\max}Q_z \gg 1$, one can use the discrete Fourier transform to calculate $\overleftrightarrow{C}(\vec{q})$. The fast Fourier transform is an efficient method for computing the discrete Fourier transform [20].

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[1] J. D. Jackson, *Classical Electrodynamics* (Wiley, New York, 1975).
[2] R. E. Collin, *Field Theory of Guided Waves* (IEEE, New York, 1991).
[3] F. N. Robinson, *Macroscopic Electromagnetism* (Pergamon, Oxford, 1973).
[4] L. D. Landau and E. M. Lipshitz, *Electrodynamics of Continuous Media*, 2nd ed. (Pergamon, Oxford, 1984).
[5] V. M. Agranovich and V. L. Ginzburg, *Crystal Optics with Spatial Dispersion and Excitons*, 2nd ed. (Springer-Verlag, New York, 1984).
[6] Ja. I. Khurgin and V. P. Jakovlev, *Finite Functions in Physics and Engineering* (Nauka, Moscow, 1971) (in Russian).
[7] J. Max, *Methodes et Techniques de Traitement du Signal et Applications aux Mesures Physiques* (Masson, Paris, 1981).
[8] R. J. Collier, C. B. Burckhard, and L. H. Lin, *Optical Holography* (Academic, New York, 1971).
[9] M. Born and K. Huang, *Dynamic Theory of Crystal Lattices* (Clarendon, Oxford, 1954).
[10] E. O. Kamenetskii, following paper. Phys. Rev. E **57** 3563 (1998).
[11] L. Tsang and J. A. Kong, Radio Sci. **16**, 303 (1981).
[12] M. Barthelemy, H. Orland, and G. Zerah, Phys. Rev. E **52**, 1123 (1995).
[13] E. U. Condon, Rev. Mod. Phys. **9**, 432 (1937).
[14] I. V. Lindell, A. H. Sihvola, S. A. Tretyakov, and A. J. Viitanen, *Electromagnetics in Chiral and Bi-Isotropic Media* (Artech House, Boston, 1993).
[15] A. Lakhtakia, *Beltrami Fields in Chiral Media* (World Scientific, Singapore, 1994).
[16] E. O. Kamenetskii, Phys. Rev. E **54**, 4359 (1996).
[17] S. A. Tretyakov (private communication).
[18] A. A. Barybin, J. Appl. Phys. **46**, 1707 (1975).
[19] G. Russakoff, Am. J. Phys. **38**, 1188 (1970).
[20] W. T. Cochran, J. W. Cooley, D. L. Favin, H. D. Helms, R. A. Kaenel, W. W. Lang, G. C. Maling, Jr., D. E. Nelson, C. M. Rader, and P. D. Welch, Proc. IEEE **55**, 1664 (1967).