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Quasi-continuous model for a crystal with ionic and electronic polarization(*)

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A QUASI-CONTINUOUS model describing mechanical and electrical properties of crystals made up of deformable and polarizable ions has been constructed. In the first part of the paper, the notion of a three-dimensional crystal lattice of shell-model atoms is introduced and the Lagrangian of the crystal is expressed in terms of collective cell variables. Next, the equations of motion of the crystal are derived by means of quasi-continuum formalism. Finally, the interaction between the crystal and the external electric field, as well as the free motion of the crystal are analyzed.

Skonstruowano quasi-continualny model opisujący mechaniczne i elektryczne własności kryształów zbudowanych z deformowalnych i polaryzowalnych jonów. W pierwszej części pracy wprowadzono pojęcie trójwymiarowej sieci krystalicznej, złożonej z atomów opisywanych przez model powłokowy. Lagrangian kryształu wyrażono przez zmienne kolektywne komórek elementarnych. Następnie, przy użyciu formalizmu quasi-continuum, wyprowadzono równania ruchu kryształu. Na koniec przeanalizowano swobodny ruch kryształu, jak również jego oddziaływanie z zewnętrznym polem elektrycznym.

Построена квазиконтинуальная модель, описывающая механические и электрические свойства кристаллов, построенных из деформируемых и поляризуемых ионов. В первой части работы вводится понятие трехмерной кристаллической решетки, состоящей из атомов, описываемых с помощью оболочечной модели. Функция Лагранжа кристалла выражается через коллективные переменные элементарных ячеек. Затем, при использовании формализма квазиконтинуума выводятся уравнения движения кристалла. В заключение рассматривается как свободное движение кристалла, так и его взаимодействие с внешним электрическим полем.

1. Introduction

THE METHOD of quasi-continuum has been applied successfully to investigate the mechanical properties of crystal lattices [1, 2]. This method can also be employed in the analysis of the electro-elastic properties of crystals [3, 4].

The authors of the above papers start from the standard theory of crystal lattice, that is, they assume that the state of crystals is determined by displacements and velocities of their atoms. It is assumed further that the force acting on an arbitrary atom depends only upon its own displacement and the displacements of the other ions. From these assumptions it follows that also the local electric field and polarization are determined by displacements of the atoms of the crystal.

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In this paper a more adequate model of an ionic crystal is presented. In addition to the ionic polarization, electronic polarization is taken into account. It is assumed that the displacement and electronic polarization are the degrees of freedom of the ion. Such an approach makes possible a correct description of the interaction between the field of displacements of the atoms and their electronic polarization, as well as the interaction between the crystal and the electromagnetic field. In particular, the interaction of the dipole moments with the external electric field and the dispersion of electric susceptibility can be successfully investigated.

2. Lagrangian of the crystal

We consider a crystal as a system consisting of a set of particles (ions) of a fixed charge e_j and a fixed mass m_j at a position $\mathbf{x}(n,j)$. The index n has three integral components that name the unit cell and j is an index that labels the type of particle. The position vector of the j-th ion in the n-th unit cell (in the equilibrium configuration) can be represented in the form

$$\mathbf{x}(n,j) = \mathbf{x}(n)+\xi(j),$$

where $\mathbf{x}(n)$ determines the location of the mass centre of the cell and $\xi(j)$ — the location of ions in that cell with reference to the centre of mass. We shall use the coordinate system x^α ($\alpha = 1, 2, 3$) having translation vectors of the lattice $\mathbf{b}_\alpha$ as covariant basic vectors and $g_{\alpha\beta} = \mathbf{b}_\alpha \cdot \mathbf{b}_\beta$ as the covariant metric tensor. The corresponding contravariant basic vectors will be denoted by $\mathbf{b}^\alpha$. With these vectors we can form the contravariant metric tensor $g^{\alpha\beta} = \mathbf{b}^\alpha \cdot \mathbf{b}^\beta$. The time will be denoted by t.

The starting concept of the investigations is a shell model of an ionic crystal [5, 6]. In the shell model an ion is assumed to consist of an ion core of a mass m_j and a charge η_j and of a rigid shell of zero mass, but possessing a charge $\varkappa_j$. The centre of the core of the ion (n,j) can be displaced from its equilibrium position by an amount $\mathbf{w}(n,j,t)$. Moreover, the centre of the shell can be displaced with respect to its core. Let $\mathbf{v}(n,j,t)$ be the relative displacement of the shell and core of the ion (n,j). Then the dipole moment of this ion is

$$\mathbf{p}(n,j,t) = \varkappa_j \mathbf{v}(n,j,t).$$

We regard a crystal as a system described by the generalized coordinates $\mathbf{w}$ and $\mathbf{p}$. The Lagrangian for this system has the form [7]:

$$\begin{aligned}(2.1)\quad 2L = {} & g^{\alpha\beta}\sum_{n,j} m_j \dot{w}_\alpha(n,j,t)\dot{w}_\beta(n,j,t) - \sum_{\substack{n,n'\\ j,j'}} [w_\alpha(n,j,t)\Phi^{\alpha\beta}(n-n',j,j')w_\beta(n',j',t) \\ & + w_\alpha(n,j,t)\Phi_T^{\alpha\beta}(n-n',j,j')p_\beta(n',j',t) + p_\alpha(n,j,t)\Phi_S^{\alpha\beta}(n-n',j,j')p_\beta(n',j',t)] \\ & - \sum_{n,j}\left\{g^{\alpha\beta}\frac{1}{\alpha_j}p_\alpha(n,j,t)p_\beta(n,j,t) - 2[p_\alpha(n,j,t)+e_j w_\alpha(n,j,t)]E_L^\alpha(n,j,t)\right\}.\end{aligned}$$

Here $\Phi^{\alpha\beta}(n-n',j,j')$, $\Phi_T^{\alpha\beta}(n-n',j,j')$ and $\Phi_S^{\alpha\beta}(n-n',j,j')$ are force constants for core–core, core–dipole and dipole–dipole interactions, $E_L^\alpha(n,j,t)$ is the effective electric field acting on the ion (n,j), α_j is the polarizability of the j-th ion and $e_j = \eta_j + \varkappa_j$.

The Lagrangian (2.1) can be expressed in the equivalent form

$$2L = g^{\alpha\beta}\sum_n \int \varrho(\xi)\dot{w}_\alpha(n,\xi,t)\dot{w}_\beta(n,\xi,t)\,d\xi -$$

$$-\sum_{n,n'}\int\int [w_\alpha(n,\xi,t)\Phi^{\alpha\beta}(n-n',\xi,\xi')w_\beta(n',\xi',t)+w_\alpha(n,\xi,t)\Phi_T^{\alpha\beta}(n-n',\xi,\xi')$$

$$\times p_\beta(n',\xi',t)+p_\alpha(n,\xi,t)\Phi_S^{\alpha\beta}(n-n',\xi,\xi')p_\beta(n',\xi',t)]\,d\xi\,d\xi'$$

$$-\sum_n\Big\{\int g^{\alpha\beta}\varkappa(\xi)p_\alpha(n,\xi,t)p_\beta(n,\xi,t)\,d\xi - 2\int [\varepsilon(\xi)p_\alpha(n,\xi,t)$$

$$+\sigma(\xi)w_\alpha(n,\xi,t)]E_L^\alpha(n,\xi,t)\,d\xi\Big\}, \qquad d\xi = d\xi^1 d\xi^2 d\xi^3,$$

where

$$\varrho(\xi) = \sum_j m_j\,\delta(\xi-\xi_j), \qquad \varkappa(\xi) = \sum_j \frac{1}{\alpha_j}\,\delta(\xi-\xi_j),$$

$$\sigma(\xi) = \sum_j e_j\,\delta(\xi-\xi_j), \qquad \varepsilon(\xi) = \sum_j \delta(\xi-\xi_j),$$

$$\Phi^{\alpha\beta}(n-n',\xi,\xi') = \sum_{j,j'}\Phi^{\alpha\beta}(n-n',j,j')\delta(\xi-\xi_j)\delta(\xi'-\xi_{j'}),$$

$$\Phi_T^{\alpha\beta}(n-n',\xi,\xi') = \sum_{j,j'}\Phi_T^{\alpha\beta}(n-n',j,j')\delta(\xi-\xi_j)\delta(\xi'-\xi_{j'}),$$

$$\Phi_S^{\alpha\beta}(n-n',\xi,\xi') = \sum_{j,j'}\Phi_S^{\alpha\beta}(n-n',j,j')\delta(\xi-\xi_j)\delta(\xi'-\xi_{j'}).$$

Here $\xi_j = \xi(j)$, $\delta(\xi-\xi_j)$ is the Dirac delta function and integration is carried out throughout the unit cell.

It is assumed that the above form of the Lagrangian is also applicable to the case of continuous distribution of the mass, of electric charges, and of dipole moments.

Instead of individual displacements of each particle in a cell, it is convenient to introduce collective cell variables following Kunin's method [8]. Let us first define the tensors characterizing the mass distribution in the unit cell.

$$\varrho^{\hat{s}} \overset{\text{df}}{=} \int \varrho(\xi)\,\xi^{\lambda_1}\ldots\xi^{\lambda_s}d\xi, \qquad s = 0, 1, \ldots.$$

Here $\hat{s}$ is the multi-index $\lambda_1, \ldots, \lambda_s$. Next, we define the matrices

$$I^{\hat{s}\hat{s}'} \overset{\text{df}}{=} \varrho^{\hat{2}\hat{s}}\delta^{ss'}, \qquad I^{-1}_{\hat{s}\hat{s}'} \overset{\text{df}}{=} \varrho^{-1}_{\hat{2}\hat{s}}\,\delta_{ss'},$$

where $\varrho^{-1}_{\hat{2}\hat{s}}$ is the inverse of $\varrho^{\hat{2}\hat{s}}$ and $\delta^{ss'}$ is the Kronecker delta. Finally, using Schmidt orthogonalization procedure we construct the polynomial basic system $e^{\hat{s}}(\xi)$ and a conjugate system of basic functions $e^{\hat{s}}_{\hat{s}}(\xi)$, which satisfy the relations

$$\int \varrho(\xi)e^{\hat{s}}(\xi)e^{\hat{s}'}(\xi)\,d\xi = I^{\hat{s}\hat{s}'},$$

$$\int e^{\hat{s}}_{\hat{s}}(\xi)e^{\hat{s}'}(\xi)\,d\xi = \delta^{\hat{s}'}_{\hat{s}}.$$

It is important to note that for a finite number of particles in a unit cell our basic system is also finite-dimensional. We can now decompose the functions $w_\alpha, p_\alpha, E_L^\alpha, \Phi^{\alpha\beta}, \Phi_T^{\alpha\beta}, \Phi_S^{\alpha\beta}$ into the following sums:

$$w_\alpha(n,\xi,t) = w_{r\alpha}^{\wedge}(n,t)\hat{e^r}(\xi), \quad p_\alpha(n,\xi,t) = p_{r\alpha}^{\wedge}(n,t)\hat{e^r}(\xi),$$
$$E_L^\alpha(n,\xi,t) = \hat{E_L^{r\alpha}}(n,t)e_r^{\wedge}(\xi),$$
$$\Phi^{\alpha\beta}(n-n',\xi,\xi') = \hat{\Phi^{r\alpha s\beta}}(n-n')e_r^{\wedge}(\xi)e_s^{\wedge}(\xi'),$$
$$\Phi_T^{\alpha\beta}(n-n',\xi,\xi') = \hat{\Phi_T^{r\alpha s\beta}}(n-n')e_r^{\wedge}(\xi)e_s^{\wedge}(\xi'),$$
$$\Phi_S^{\alpha\beta}(n-n',\xi,\xi') = \hat{\Phi_S^{r\alpha s\beta}}(n-n')e_r^{\wedge}(\xi)e_s^{\wedge}(\xi'),$$

where

$$w_{r\alpha}^{\wedge}(n,t) = \int w_\alpha(n,\xi,t)e_r^{\wedge}(\xi)d\xi, \quad \hat{E_L^{r\alpha}}(n,t) = \int E_L^\alpha(n,\xi,t)\hat{e^r}(\xi)d\xi,$$
$$p_{r\alpha}^{\wedge}(n,t) = \int p_\alpha(n,\xi,t)e_r^{\wedge}(\xi)d\xi,$$
$$\hat{\Phi^{r\alpha s\beta}}(n-n') = \int \Phi^{\alpha\beta}(n-n',\xi,\xi')\hat{e^r}(\xi)\hat{e^s}(\xi')d\xi d\xi',$$
$$\hat{\Phi_T^{r\alpha s\beta}}(n-n') = \int \Phi_T^{\alpha\beta}(n'-n',\xi,\xi')\hat{e^r}(\xi)\hat{e^s}(\xi')d\xi d\xi',$$
$$\hat{\Phi_S^{r\alpha s\beta}}(n-n') = \int \Phi_S^{\alpha\beta}(n-n',\xi,\xi')\hat{e^r}(\xi)\hat{e^s}(\xi')d\xi d\xi'.$$

Substituting the above expansions in the Lagrangian (2.2), we obtain

$$(2.3)\quad 2L = \sum_n [\dot{w}_{r\alpha}^{\wedge}(n,t)\hat{I^{r\alpha s\beta}}\dot{w}_{s\beta}^{\wedge}(n,t) - p_{r\alpha}^{\wedge}(n,t)\hat{J^{r\alpha s\beta}}p_{s\beta}^{\wedge}(n,t)$$
$$+2p_{r\alpha}^{\wedge}(n,t)\hat{P_s^r}E_L^{\hat{s\alpha}}(n,t) + 2w_{r\alpha}^{\wedge}(n,t)\hat{R_s^r}E_L^{\hat{s\alpha}}(n,t)]$$
$$-\sum_{n,n'}[w_{r\alpha}^{\wedge}(n,t)\hat{\Phi^{r\alpha s\beta}}(n-n')w_{s\beta}^{\wedge}(n',t) + w_{r\alpha}^{\wedge}(n,t)\hat{\Phi_T^{r\alpha s\beta}}(n-n')p_{s\beta}^{\wedge}(n',t)$$
$$+p_{r\alpha}^{\wedge}(n,t)\hat{\Phi_S^{r\alpha s\beta}}(n-n')p_{s\beta}^{\wedge}(n',t)],$$

where the matrices $\hat{I^{r\alpha s\beta}}, \hat{J^{r\alpha s\beta}}, \hat{R_s^r}, \hat{P_s^r}$ are given by

$$\hat{I^{r\alpha s\beta}} = g^{\alpha\beta}\hat{I^{rs}},$$
$$\hat{J^{r\alpha s\beta}} = g^{\alpha\beta}\int \varkappa(\xi)\hat{e^r}(\xi)\hat{e^s}(\xi)d\xi,$$
$$\hat{P_s^r} = \int \varepsilon(\xi)\hat{e^r}(\xi)e_s^{\wedge}(\xi)d\xi,$$
$$\hat{R_s^r} = \int \sigma(\xi)\hat{e^r}(\xi)e_s^{\wedge}(\xi)d\xi.$$

Thus we have expressed the Lagrangian of the crystal in terms of collective cell variables.

3. Equations of motion

Assuming that $w_{r\alpha}^{\wedge}$ and $p_{rx}^{\wedge}$ are generalized coordinates of the system, we can write Lagrange's equations of motion in the form

(3.1)

$$\hat{I^{r\alpha s\beta}}\ddot{w}_{s\beta}^{\wedge}(n,t) - \hat{R_s^r}E_L^{\hat{s\alpha}}(n,t) + \sum_{n'}[\hat{\Phi^{r\alpha s\beta}}(n-n')w_{s\beta}^{\wedge}(n',t) + \frac{1}{2}\hat{\Phi_T^{r\alpha s\beta}}(n-n')p_{s\beta}^{\wedge}(n',t)] = 0,$$

$$\hat{J^{r\alpha s\beta}}p_{s\beta}^{\wedge}(n,t) - \hat{P_s^r}E_L^{\hat{s\alpha}}(n,t) + \sum_{n'}[\hat{\Phi_S^{r\alpha s\beta}}(n-n')p_{s\beta}^{\wedge}(n',t) + \frac{1}{2}\hat{\Phi_T^{s\beta r\alpha}}(n'-n)w_{s\beta}^{\wedge}(n',t)] = 0.$$

The above equations describe a discrete system. In order to obtain the corresponding continuum theory we construct, following [8], the model of quasi-continuum.

Let $N'(B)$ be the linear space of scalar or tensor functions $u(n)$, defined on the set of discrete points n, such that $|u(n)| \leqslant C|n|^p$ when $|n| \to \infty$. The space $N'(B)$ can also be interpreted as the space of linear functionals on the space $N(B)$ of test functions. The space $N(B)$ consists of functions $\varphi(n)$ which tend to zero at infinity more rapidly than any power of n. By definition, the value of the functional $u(n)$ on the test function $\varphi(n)$ is

$$(u, \varphi) \stackrel{\text{df}}{=} v \sum_n \overline{u(n)}\varphi(n),$$

where v is the volume of the unit cell and $\overline{u(n)}$ denotes the complex conjugate to $u(n)$.

Next, we define the space $K'(B)$ of distributions $u(\mathbf{k})$, $\mathbf{k} = k_\alpha \mathbf{b}^\alpha$, on the space $K(B)$. The space $K(B)$ consists of infinitely differentiable functions of compact support localized in the first Brillouin zone $B = \{-\pi \leqslant k_\alpha \leqslant \pi\}$. Let us denote by $X(B)$ and $X'(B)$ the Fourier transforms of the spaces $K(B)$ and $K'(B)$. It can be demonstrated that the functions $u(\mathbf{x}) \in X'(B)$ are regular distributions represented by entire analytic functions.

We can now introduce isomorphism between the spaces $N'(B) \leftrightarrow X'(B) \leftrightarrow K'(B)$ given by the following relations:

$$\begin{aligned} u(\mathbf{x}) &= v \sum_n u(n)\, \delta_B(\mathbf{x}-\mathbf{x}(n)), \\ u(\mathbf{k}) &= \int u(\mathbf{x}) e^{i\mathbf{k}\cdot\mathbf{x}} dx = vB(\mathbf{k}) \sum_n u(n) e^{i\mathbf{x}(n)\cdot\mathbf{k}}, \qquad dx = dx^1 dx^2 dx^3, \end{aligned} \tag{3.2}$$

where $B(\mathbf{k})$ is the characteristic function of B, and $\delta_B(\mathbf{x})$ is its inverse Fourier transform:

$$\delta_B(\mathbf{x}) \stackrel{\text{df}}{=} \frac{1}{(2\pi)^3} \int B(\mathbf{k}) e^{-i\mathbf{x}\cdot\mathbf{k}} dk = \frac{1}{\pi^3 v} \prod_{\alpha=1}^{3} \frac{\sin \pi(\mathbf{x}\cdot\mathbf{b}^\alpha)}{(\mathbf{x}\cdot\mathbf{b}^\alpha)}, \qquad dk = dk_1\, dk_2\, dk_3.$$

If $\Phi(n)$ is a sufficiently rapidly decreasing function for $|n| \to \infty$, then, in the established isomorphism, the following relations are valid:

$$v \sum_{n'} \Phi(n-n')u(n') \leftrightarrow \int \Phi(\mathbf{x}-\mathbf{x}')u(\mathbf{x}')\, dx' \leftrightarrow \Phi(\mathbf{k})u(\mathbf{k}). \tag{3.3}$$

It is easy to show that $u(\mathbf{x})$ defined by Eq. $(3.2)_1$ is the interpolating function for $u(n)$, i.e. $u(\mathbf{x}) = u(n)$ for $\mathbf{x} = \mathbf{x}(n)$. Thus a discrete system described by the functions $u(n)$ can also be described by the functions of the continuous argument $u(\mathbf{x})$ or $u(\mathbf{k})$. Usually the functions describing a system depend also on time t. In this case it is sometimes convenient to use instead of $u(n, t)$, $u(\mathbf{x}, t)$ and $u(\mathbf{k}, t)$ their Fourier transforms with respect to time, i.e. $u(n, \omega)$, $u(\mathbf{x}, \omega)$ and $u(\mathbf{k}, \omega)$. These Fourier transforms are given by the formula

$$u(\omega) = \int u(t) e^{-i\omega t} dt.$$

Equations (3.1) can be interpreted as equations of motion of quasi-continuum in the (n, t) representation. According to the method presented above, these equations can also

be formulated in the $(\mathbf{k}, \omega)$ representation. Using the relations (3.3) and performing the Fourier transformation with respect to t, we obtain from Eq. (3.1)

$$
\begin{aligned}
&-\omega^2 I^{\hat{r}\alpha\hat{s}\beta} w_{\hat{s}\beta}(\mathbf{k},\omega) - R^{\hat{r}}_{\hat{s}} E^{\hat{s}\alpha}_{L}(\mathbf{k},\omega) + \Phi^{\hat{r}\alpha\hat{s}\beta}(\mathbf{k}) w_{\hat{s}\beta}(\mathbf{k},\omega) + \frac{1}{2}\Phi^{\hat{r}\alpha\hat{s}\beta}_{T}(\mathbf{k}) p_{\hat{s}\beta}(\mathbf{k},\omega) = 0, \\
&J^{\hat{r}\alpha\hat{s}\beta} p_{\hat{s}\beta}(\mathbf{k},\omega) - P^{\hat{r}}_{\hat{s}} E^{\hat{s}\alpha}_{L}(\mathbf{k},\omega) + \Phi^{\hat{r}\alpha\hat{s}\beta}_{S}(\mathbf{k}) p_{\hat{s}\beta}(\mathbf{k},\omega) + \frac{1}{2}\overline{\Phi^{\hat{s}\beta\hat{r}\alpha}_{T}(\mathbf{k})} w_{\hat{s}\beta}(\mathbf{k},\omega) = 0,
\end{aligned}
\tag{3.4}
$$

where, in accordance with Eq. $(3.2)_2$,

$$
\Phi^{\hat{r}\alpha\hat{s}\beta}(\mathbf{k}) = \frac{1}{v}\sum_{n} \Phi^{\hat{r}\alpha\hat{s}\beta}(n) e^{i\mathbf{x}(n)\cdot\mathbf{k}},
$$

$$
\Phi^{\hat{r}\alpha\hat{s}\beta}_{T}(\mathbf{k}) = \frac{1}{v}\sum_{n} \Phi^{\hat{r}\alpha\hat{s}\beta}_{T}(n) e^{i\mathbf{x}(n)\cdot\mathbf{k}},
$$

$$
\Phi^{\hat{r}\alpha\hat{s}\beta}_{S}(\mathbf{k}) = \frac{1}{v}\sum_{n} \Phi^{\hat{r}\alpha\hat{s}\beta}_{S}(n) e^{i\mathbf{x}(n)\cdot\mathbf{k}}.
$$

Equations (3.4) are equations of motion of quasi-continuum in the $(\mathbf{k}, \omega)$ representation.

4. Crystal in external electric field

Equations (3.4) can be used for investigating the interaction of the crystal with the external electric field. We shall now present an approximated description of this interaction.

In the Lagrangian (2.1) $E^{\alpha}_{L}(n, j, t)$ is the local electric field, i.e. the field which acts on the particle (n, j). We assume that this field is equal to the sum of the external electric field $E^{\alpha}_{\mathrm{ext}}(n, j, t)$ and the field $E^{\alpha}_{\mathrm{cr}}(n, j, t)$ due to the dipole moments localized in the crystal. Thus,

$$
E^{\alpha}_{L}(n, j, t) = E^{\alpha}_{\mathrm{ext}}(n, j, t) + E^{\alpha}_{\mathrm{cr}}(n, j, t). \tag{4.1}
$$

In the crystal at every point (n, j) is situated the dipole moment $e_j w_{\alpha}(n, j, t)$ due to the displacement of the ion, and the dipole moment $p_{\alpha}(n, j, t)$ due to the electronic polarization of the ion. So the total dipole moment $d_{\alpha}(n, j, t)$ localized in the point (n, j) is

$$
d_{\alpha}(n, j, t) = e_j w_{\alpha}(n, j, t) + p_{\alpha}(n, j, t).
$$

If we confine ourselves to the quasi-static approximation, we can express the Fourier transform of the electric field arising from this distribution of the dipole moments by the formula

$$
E^{\alpha}_{\mathrm{cr}}(\mathbf{k}, j, \omega) = -\sum_{j'} F^{\alpha\beta}(j, j', \mathbf{k})[e_{j'} w_{\beta}(\mathbf{k}, j', \omega) + p_{\beta}(\mathbf{k}, j', \omega)]. \tag{4.2}
$$

The function $F^{\alpha\beta}$ is well-known in the theory of crystal lattices [7]. It has the form

$$
F^{\alpha\beta}(j, j', \mathbf{k}) = \frac{4\pi k^{\alpha} k^{\beta}}{v|\mathbf{k}|^2} - Q^{\alpha\beta}(j, j', \mathbf{k}),
$$

where

$$(4.3)\qquad Q^{\alpha\beta}(j,j',\mathbf{k}) = -\frac{4\pi k^\alpha k^\beta}{v|\mathbf{k}|^2}\left[\exp\left(-\frac{|\mathbf{k}|^2}{4P}\right)-1\right]$$
$$-\frac{4\pi}{v}\sum_{\mathbf{h}\neq 0}\frac{(2\pi h^\alpha+k^\alpha)(2\pi h^\beta+k^\beta)}{|2\pi\mathbf{h}+\mathbf{k}|^2}\exp\left(-\frac{|2\pi\mathbf{h}+\mathbf{k}|^2}{4P}\right)e^{i2\pi\mathbf{h}\cdot(\xi(j)-\xi(j'))}$$
$$+P^{3/2}\sum_{l'}H^{\alpha\beta}\left(\sqrt{P}\,|\mathbf{x}(l,j)-\mathbf{x}(l',j')|\right)e^{-i\mathbf{k}\cdot(\mathbf{x}(l,j)-\mathbf{x}(l',j'))},$$

h_α – integers and $h^\alpha = g^{\alpha\beta}h_\beta$.

Here we have used the following notation:

$$H(x) \stackrel{\mathrm{df}}{=} \frac{2}{\sqrt{\pi}}\frac{1}{x}\int_x^\infty \exp(-s^2)\,ds,$$

$$H_{\alpha\beta}(|\mathbf{x}|) = \frac{\partial^2}{\partial x^\alpha \partial x^\beta}H(|\mathbf{x}|),$$

$$H^{\alpha\beta} = g^{\alpha\gamma}g^{\beta\delta}H_{\gamma\delta}.$$

The parameter P can be chosen so as to make both sums in Eq. (4.3) rapidly convergent. It should be emphasized that the function $Q^{\alpha\beta}(j,j',\mathbf{k})$ is independent of P. This problem has been investigated in detail in the work [7]. For the case $j=j'$ the function $H_{\alpha\beta}(|\mathbf{x}|)$ must be replaced by

$$H^0_{\alpha\beta}(|\mathbf{x}|) = -\frac{\partial^2}{\partial x^\alpha \partial x^\beta}H^0(|\mathbf{x}|),$$

$$H^0(x) = -\frac{2}{\sqrt{\pi}}\frac{1}{x}\int_0^x \exp(-s^2)\,ds.$$

From Eqs. (4.1) and (4.2) we obtain finally the Fourier transform of the local electric field

$$E^\alpha_L(\mathbf{k},j,\omega) = E^\alpha_{\mathrm{ext}}(\mathbf{k},j,\omega) - \sum_{j'}F^{\alpha\beta}(j,j',\mathbf{k})[e_j, w_\beta(\mathbf{k},j',\omega)+p_\beta(\mathbf{k},j',\omega)],$$

where $E^\alpha_{\mathrm{ext}}(\mathbf{k},j,\omega)$ is the Fourier transform of $E^\alpha_{\mathrm{ext}}(n,j,t)$.

Now we pass from the quantities describing the electric field in the discrete points (n,j) to the collective cell quantities. It can be done as in Sect. 2. After simple calculations we obtain

$$E^{\hat{s}\alpha}_L(\mathbf{k},\omega) = E^{\hat{s}\alpha}_{\mathrm{ext}}(\mathbf{k},\omega) - F^{\hat{s}\alpha\hat{m}\beta}(\mathbf{k})[w_{i\beta}(\mathbf{k},\omega)R^{\hat{i}}_{\hat{m}}+p_{\hat{m}\beta}(\mathbf{k},\omega)],$$

where

$$E^{\hat{s}\alpha}_{\mathrm{ext}}(\mathbf{k},\omega) = \int E^\alpha_{\mathrm{ext}}(\mathbf{k},\xi,\omega)e^{\hat{s}}(\xi)\,d\xi,$$

$$F^{\hat{s}\alpha\hat{r}\beta}(\mathbf{k}) = \int F^{\alpha\beta}(\xi,\xi',\mathbf{k})e^{\hat{s}}(\xi)e^{\hat{r}}(\xi')\,d\xi\,d\xi'.$$

After substitution of $E_L^{\hat{s}\alpha}(\mathbf{k}, \omega)$ in Eqs. (3.4) we obtain finally the following equations of motion:

$$
\begin{aligned}
&-\omega^2 I^{\hat{r}\alpha\hat{s}\beta} w_{\hat{s}\beta}(\mathbf{k}, \omega) - R_{\hat{s}}^{\hat{r}}\left[E_{\mathrm{ext}}^{\hat{s}\alpha}(\mathbf{k}, \omega) - F^{\hat{s}\alpha\hat{m}\beta}(\mathbf{k})\left(R_{\hat{m}}^{\hat{i}} w_{\hat{i}\beta}(\mathbf{k}, \omega) + p_{\hat{m}\beta}(\mathbf{k}, \omega)\right)\right] \\
&\qquad + \Phi^{\hat{r}\alpha\hat{s}\beta}(\mathbf{k}) w_{\hat{s}\beta}(\mathbf{k}, \omega) + \frac{1}{2}\Phi_T^{\hat{r}\alpha\hat{s}\beta}(\mathbf{k}) p_{\hat{s}\beta}(\mathbf{k}, \omega) = 0, \qquad (4.4) \\
&J^{\hat{r}\alpha\hat{s}\beta} p_{\hat{s}\beta}(\mathbf{k}, \omega) - P_{\hat{s}}^{\hat{r}}\left[E_{\mathrm{ext}}^{\hat{s}\alpha}(\mathbf{k}, \omega) - F^{\hat{s}\alpha\hat{m}\beta}(\mathbf{k})\left(R_{\hat{m}}^{\hat{i}} w_{\hat{i}\beta}(\mathbf{k}, \omega) + p_{\hat{m}\beta}(\mathbf{k}, \omega)\right)\right] \\
&\qquad + \Phi_S^{\hat{r}\alpha\hat{s}\beta}(\mathbf{k}) p_{\hat{s}\beta}(\mathbf{k}, \omega) + \frac{1}{2}\overline{\Phi_T^{\hat{s}\beta\hat{r}\alpha}(\mathbf{k})} w_{\hat{s}\beta}(\mathbf{k}, \omega) = 0.
\end{aligned}
$$

This is the system of equations describing the interaction of the ionic crystal with the external electric field in $(\mathbf{k}, \omega)$ representation. Naturally, we can also pass to other representations. For instance, the equations of motion in the $(\mathbf{x}, t)$ representation are

$$
\begin{aligned}
&I^{\hat{r}\alpha\hat{s}\beta} \ddot{w}_{\hat{s}\beta}(\mathbf{x}, t) - R_{\hat{s}}^{\hat{r}}\left\{E_{\mathrm{ext}}^{\hat{s}\alpha}(\mathbf{x}, t) - \int F^{\hat{s}\alpha\hat{m}\beta}(\mathbf{x}-\mathbf{x}')\left[R_{\hat{m}}^{\hat{i}} w_{\hat{i}\beta}(\mathbf{x}', t) + p_{\hat{m}\beta}(\mathbf{x}', t)\right] d\mathbf{x}'\right\} \\
&\qquad + \int \Phi^{\hat{r}\alpha\hat{s}\beta}(\mathbf{x}-\mathbf{x}') w_{\hat{s}\beta}(\mathbf{x}', t)\, d\mathbf{x}' + \frac{1}{2}\int \Phi_T^{\hat{r}\alpha\hat{s}\beta}(\mathbf{x}-\mathbf{x}') p_{\hat{s}\beta}(\mathbf{x}', t)\, d\mathbf{x}' = 0, \qquad (4.5) \\
&J^{\hat{r}\alpha\hat{s}\beta} p_{\hat{s}\beta}(\mathbf{x}, t) - P_{\hat{s}}^{\hat{r}}\left\{E_{\mathrm{ext}}^{\hat{s}\alpha}(\mathbf{x}, t) - \int F^{\hat{s}\alpha\hat{m}\beta}(\mathbf{x}-\mathbf{x}')\left[R_{\hat{m}}^{\hat{i}} w_{\hat{i}\beta}(\mathbf{x}', t) + p_{\hat{m}\beta}(\mathbf{x}', t)\right] d\mathbf{x}'\right\} \\
&\qquad + \int \Phi_S^{\hat{r}\alpha\hat{s}\beta}(\mathbf{x}-\mathbf{x}') p_{\hat{s}\beta}(\mathbf{x}', t)\, d\mathbf{x}' + \frac{1}{2}\int \Phi_T^{\hat{s}\beta\hat{r}\alpha}(\mathbf{x}'-\mathbf{x}) w_{\hat{s}\beta}(\mathbf{x}', t)\, d\mathbf{x}' = 0,
\end{aligned}
$$

where $E_{\mathrm{ext}}^{\hat{s}\alpha}(\mathbf{x}, t)$, $F^{\hat{s}\alpha\hat{m}\beta}(\mathbf{x}-\mathbf{x}')$, $\Phi^{\hat{r}\alpha\hat{s}\beta}(\mathbf{x}-\mathbf{x}')$, $\Phi_T^{\hat{r}\alpha\hat{s}\beta}(\mathbf{x}-\mathbf{x}')$ and $\Phi_S^{\hat{r}\alpha\hat{s}\beta}(\mathbf{x}-\mathbf{x}')$ are corresponding inverse Fourier transforms of the functions $E_{\mathrm{ext}}^{\hat{s}\alpha}(\mathbf{k}, \omega)$, $F^{\hat{s}\alpha\hat{m}\beta}(\mathbf{k})$, $\Phi^{\hat{r}\alpha\hat{s}\beta}(\mathbf{k})$, $\Phi_T^{\hat{r}\alpha\hat{s}\beta}(\mathbf{k})$ and $\Phi_S^{\hat{r}\alpha\hat{s}\beta}(\mathbf{k})$.

In the case of free motion of the crystal one must set $E_{\mathrm{ext}}^{\hat{s}\alpha}(\mathbf{x}, t) = 0$ in Eqs. (4.4) and (4.5).

5. Final remarks

The method presented in Sect. 4 is based on the assumption that the ions interact with the unretarded Coulomb forces. It can be shown that the use of the unretarded Coulomb interactions is equivalent to neglecting the transverse electromagnetic field.

In our opinion, by using Eqs. (3.4) one can build up a more exact theory. One can start with the Lorentz equations where distributions of the charges and currents are expressed in terms of $\mathbf{w}$ and $\mathbf{p}$. Thus it is possible to connect the equations of motion (3.4) with microscopic Lorentz equations. Such an approach could make possible a description of the interaction between the electromagnetic field and the crystal for a wider range of the parameters $\mathbf{k}$ and ω.

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