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Crowdion dynamics in a nonuniformly deformed three-dimensional crystal

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Abstract. The problem of crowdion motion is formulated and analyzed as a dynamical problem of a three-dimensional crystal lattice formed by atoms of several kinds, which interact with each other by means of short-range pair potentials. It is explained that in order for the the crowdion excitations of the close-packed atomic rows to be distinguishable against the background of small dynamic deformations of the crystal as a whole, the microscopic parameters of the crystal structure must meet certain stated requirements. The equation of motion of a crowdion in an arbitrary elastic strain field of the crystal is derived in the Lagrangian formalism. Expressions are obtained which relate the effective mass and the rest energy of a crowdion with the geometric and force parameters of the crystal lattice.

PACS. 63.20.Ry Anharmonic lattice modes

1 Introduction

Many rather complex crystal structures contain close-packed atomic rows relatively weakly coupled with their surrounding environment. An intrinsic interstitial atom in such a row forms a specific configuration – a smeared clump called a crowdion, and the vacancy also becomes delocalized, forming a smeared rarefaction region that can be called an anticrowdion.

Crowdions can play an important role in the dynamics and kinetics of radiation defects, in diffusion processes, and in several other inelastic deformation phenomena in crystals [1–7].

For a qualitative description of the basic properties of a crowdion, the Frenkel–Kontorova model of a one-dimensional crystal is widely used in the physics of crystals. This model is a chain of mutually strongly interacting atoms which undergoes one-dimensional motion in a relatively weak static periodic potential [8]. Various aspects of the nonlinear dynamics in the Frenkel–Kontorova model are discussed in a recent review [9].

However, a discussion of the question of the relationship between the properties of a crowdion in a three-dimensional deformable crystal and the properties of a soliton (dislocation) in the Frenkel–Kontorova model meets with certain complexities [10]. It it not at all clear whether it is possible to distinguish a crowdion excitation from the other excitations of the crystal: free harmonic vibrations (phonons) or forced deformations of the crystal lattice.

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A special discussion and analysis is warranted for the problem of deriving the equation of motion of a crowdion and describing the interaction of a crowdion with dynamic and static deformations created by other defects or excitations of the crystal and by external forces.

In this paper we formulate and analyze the problem of crowdion motion as a dynamical problem of a three-dimensional crystal lattice. We consider a rather general case of crystal structure, formed by atoms of several different kinds, interacting with one another by means of short-ranged pair potentials. We formulate the requirements on the parameters of the crystal geometry and interatomic interaction which permit one to distinguish the crowdion excitations of the close-packed atomic rows against the background of small dynamic deformations of the crystal as a whole. We obtain expressions relating the self-energy and the effective mass of a crowdion with the microscopic parameters of the crystal. We derive an equation of motion for the center of a crowdion in an arbitrary elastic strain field of the crystal. In this work we follow the presentation in our recent work [11].

2 Statement of the model, the dynamical variables, and the Lagrangian function

Let us consider a complex multiatomic crystal lattice in which a close-packed row of identical atoms can be identified. The chemically different species of atoms are enumerated by an index α, and we assume for the sake of

definiteness that the atoms of the distinguished row have index $\alpha = 1$. The spatial orientation of the distinguished atomic row and the period of translations within it are specified by the vector $\mathbf{b}^*$, while the vector of translations of the crystal in this direction is denoted by $\mathbf{b}$; in complex crystal structures these vectors can differ in modulus. The equilibrium positions of the atoms in the ideal crystal structure are specified by a set of vectors $\mathbf{R}$, and we separate it into sets of vectors of two types: $\mathbf{R} = \{\boldsymbol{\rho}, \mathbf{R}^{(\alpha)}\}$, where $\boldsymbol{\rho}$ and $\mathbf{R}^{(\alpha)}$ are, respectively, the equilibrium positions of the atoms of the distinguished row and of the crystal matrix surrounding it. The origin of the coordinate system for the vectors $\boldsymbol{\rho}$ and $\mathbf{R}^{(\alpha)}$ is conveniently chosen to lie at one of the atoms of the distinguished row, that for which the energy of coupling with the lattice is maximum.

We assume that the interatomic interaction in the crystal is described by a set of short-ranged pair potentials $U_{\alpha\alpha'}(\mathbf{r}-\mathbf{r}')$ ($\mathbf{r}$ and $\mathbf{r}'$ are the coordinates of two arbitrary atoms), and each individual atom with coordinate $\mathbf{r}$ can also be acted on by time-varying external forces, which correspond to potentials $U_\alpha^{(e)}(\mathbf{r}, t)$.

The atomic displacements $\boldsymbol{\eta}(\mathbf{R}, t)$ from the equilibrium positions in the ideal crystal are written in the form

$$\boldsymbol{\eta}(\mathbf{R}, t) = \mathbf{u}(\mathbf{R}, t) + \frac{bz(\boldsymbol{\rho}, t)}{b^*}[\mathbf{b}^* + \mathbf{u}(\boldsymbol{\rho}, t) - \mathbf{u}(\boldsymbol{\rho} - \mathbf{b}^*, t)]\delta_{\mathbf{R}\boldsymbol{\rho}}. \tag{1}$$

Here δ_{ik} is the Kronecker delta; $\mathbf{u}(\mathbf{R}, t)$ are arbitrary small displacements satisfying the condition $|\mathbf{u}(\mathbf{R}, t) - \mathbf{u}(\mathbf{R}', t)| \ll |\mathbf{R}-\mathbf{R}'|$; z stands for additional dimensionless displacements describing the propagation of a crowdion excitation along the distinguished atomic row $\mathbf{R} = \boldsymbol{\rho}$. The nucleation and motion of a crowdion are accompanied by changes in the dimensionless displacement z by an amount $|z| \leq 1$.

We write a general expression for the Lagrangian of the problem in the form

$$\begin{aligned}\mathcal{L} = {} & \frac{1}{2}\sum_{\alpha,\mathbf{R}^{(\alpha)}} m_\alpha[\dot{\mathbf{u}}(\mathbf{R}^{(\alpha)}, t)]^2 + \frac{1}{2}\sum_{\boldsymbol{\rho}} m_1[\dot{\boldsymbol{\eta}}(\boldsymbol{\rho}, t)]^2 \\ & -\frac{1}{2}\sum_{\alpha,\mathbf{R}^{(\alpha)}}\sum_{\alpha',\mathbf{R}^{(\alpha')}} U_{\alpha\alpha'}[\mathbf{R}^{(\alpha)} - \mathbf{R}^{(\alpha')} + \mathbf{u}(\mathbf{R}^{(\alpha)}, t) \\ & -\mathbf{u}(\mathbf{R}^{(\alpha')}, t)] - \frac{1}{2}\sum_{\boldsymbol{\rho}}\sum_{\boldsymbol{\rho}'} U_{11}[\boldsymbol{\rho} - \boldsymbol{\rho}' + \boldsymbol{\eta}(\boldsymbol{\rho}, t) \\ & -\boldsymbol{\eta}(\boldsymbol{\rho}', t)] - \sum_{\boldsymbol{\rho}}\sum_{\alpha,\mathbf{R}^{(\alpha)}} U_{1\alpha}[\boldsymbol{\rho} - \mathbf{R}^{(\alpha)} + \boldsymbol{\eta}(\boldsymbol{\rho}, t) \\ & -\mathbf{u}(\mathbf{R}^{(\alpha)}, t)] - \sum_{\alpha,\mathbf{R}^{(\alpha)}} U_\alpha^{(e)}[\mathbf{R}^{(\alpha)} + \mathbf{u}(\mathbf{R}^{(\alpha)}, t), t] \\ & -\sum_{\boldsymbol{\rho}} U_1^{(e)}[\boldsymbol{\rho} + \boldsymbol{\eta}(\boldsymbol{\rho}, t), t].\end{aligned} \tag{2}$$

3 Simplified Lagrangian

Let us begin by discussing the main approximation of crowdion theory, without the use of which it would be altogether impossible to introduce correctly the concept of a crowdion excitation: the qualitative assumption that the energy of interaction of the atoms within the distinguished row (the fourth term in (2)) is large compared to the energy of interaction of this row with the external matrix (the fifth term in (2)). In our model this postulate allows us to assume that, like the elastic strains of the crystal, the crowdion deformations are also small, *i.e.*, we have the two simultaneous inequalities:

$$\begin{aligned}&|\mathbf{u}(\mathbf{R}, t) - \mathbf{u}(\mathbf{R}', t)| \ll |\mathbf{R} - \mathbf{R}'|, \\ &b^*|z(\boldsymbol{\rho}, t) - z(\boldsymbol{\rho}', t)| \ll |\boldsymbol{\rho} - \boldsymbol{\rho}'|.\end{aligned} \tag{3}$$

Satisfaction of inequalities (3), as we know, allows one to pass from a discrete (lattice) to a continuum approximation in the description of the dynamical processes or static deformations in a crystal, by replacing the finite differences of the displacements by derivatives:

$$\begin{aligned}&u_i(\mathbf{R}, t) - u_i(\mathbf{R}', t) = (R_k - R'_k)u_{ik}(\mathbf{R}, t), \\ &u_{ik}(\mathbf{R}, t) = \frac{\partial u_i(\mathbf{R}, t)}{\partial R_k}; \\ &z(\boldsymbol{\rho}, t) - z(\boldsymbol{\rho}', t) = (\rho_i - \rho'_i)\nu_i z'(\boldsymbol{\rho}, t), \\ &z' \equiv \frac{\partial}{\partial x}z, \quad \boldsymbol{\rho} = \boldsymbol{\nu}x.\end{aligned} \tag{4}$$

Here $u_{ik}(\mathbf{R}, t)$ is the tensor of elastic distortions of the crystal, b^*z' is the local crowdion deformation of the distinguished atomic row, x is the axis which is parallel to the distinguished close-packed row of atoms, and $\boldsymbol{\nu}$ is the unit vector in the direction of that row; summation over repeated coordinate indices is implied.

The short-range character of the interatomic potentials and the smallness of the deformations allow us to represent the Lagrangian (2) in the form of a Taylor series expansion in the derivatives u_{ik}, z', $\dot{u}_i$, and $\dot{z}$ or the finite differences corresponding to them.

Expanding expression (2) in the derivatives u_{ik}, z', $\dot{u}_i$, and $\dot{z}$ to terms of second order, taking into account the consequences of the translational symmetry of the crystal, and regrouping the terms for our future convenience, we obtain

$$\begin{aligned}\mathcal{L} = {} & \frac{1}{2}\sum_{\alpha,\mathbf{R}} m_\alpha[\dot{\mathbf{u}}(\mathbf{R}, t)]^2 - \frac{1}{2}\sum_{\alpha,\mathbf{R}}\sum_{\alpha',\mathbf{R}'} A_{ik}^{(\alpha\alpha')}(\mathbf{R} - \mathbf{R}') \\ & \times u_i(\mathbf{R}, t)u_k(\mathbf{R}', t) - \sum_{\alpha,\mathbf{R}} U_\alpha^{(e)}[\mathbf{R} + \mathbf{u}(\mathbf{R}, t), t] \\ & + \frac{1}{2}\sum_{\boldsymbol{\rho}}\{m_1 b^2[\dot{z}(\boldsymbol{\rho}, t)]^2 - wb^2[z'(\boldsymbol{\rho}, t)]^2 - 2\Phi[z(\boldsymbol{\rho}, t)]\} \\ & + \sum_{\boldsymbol{\rho}}\{m_1 b_i \dot{u}_i(\boldsymbol{\rho}, t)\dot{z}(\boldsymbol{\rho}, t) - bw_{ik}u_{ik}(\boldsymbol{\rho}, t)z'(\boldsymbol{\rho}, t) \\ & - u_{ik}(\boldsymbol{\rho}, t)\Phi_{ik}[z(\boldsymbol{\rho}, t)] + b_i F_i^{(e1)}[\boldsymbol{\rho} + \mathbf{u}(\mathbf{R}, t), t]z(\boldsymbol{\rho}, t)\}.\end{aligned} \tag{5}$$

In writing expression (5) we have used the following notation:

$$A_{ik}^{(\alpha\alpha')}(\mathbf{R}) = -\frac{\partial^2 U_{\alpha\alpha'}(\mathbf{R})}{\partial R_i \partial R_k},$$

$$w = -\frac{1}{2}\sum_{\boldsymbol{\rho}} A_{ik}^{(11)}(\boldsymbol{\rho})\rho_i\rho_k,$$

$$w_{ik} = -\frac{1}{2}\sum_{\boldsymbol{\rho}} A_{ni}^{(11)}(\boldsymbol{\rho})\rho_n\rho_k,$$

$$\Phi(z) = \sum_{\alpha,\mathbf{R}^{(\alpha)}} [U_{1\alpha}(\mathbf{R}^{(\alpha)} + \mathbf{b}z) - U_{1\alpha}(\mathbf{R}^{(\alpha)})],$$

$$\Phi_{ik}(z) = \sum_{\alpha,\mathbf{R}^{(\alpha)}} \left[\frac{\partial U_{1\alpha}(\mathbf{R}^{(\alpha)} + \mathbf{b}z)}{\partial(R_i^{(\alpha)})}(R_k^{(\alpha)} + b_k z) - \frac{\partial U_{1\alpha}(\mathbf{R}^{(\alpha)})}{\partial R_i^{(\alpha)}} R_k^{(\alpha)}\right]. \quad (6)$$

4 Crowdion in a rigid crystal matrix

As a zeroth approximation of perturbation theory it is natural to treat the crowdion as a topological soliton on the distinguished row of atoms in the absence of external forces ($\mathbf{F}^{(e\alpha)}(\mathbf{r}) \equiv 0$), assuming that the crystal matrix is absolutely rigid ($\mathbf{u}(\mathbf{R}, t) \equiv 0$). This approximation corresponds to the Lagrangian

$$\mathcal{L}_0 = \frac{1}{2}\sum_{\boldsymbol{\rho}} [m_1 b^2 (\dot{z})^2 - w b^2 (z')^2 - 2\Phi(z)] \quad (7)$$

and the equation of motion that follows from it:

$$m_1 b^2 \ddot{z} - w b^2 z'' + \frac{\mathrm{d}}{\mathrm{d}z}\Phi(z) = 0. \quad (8)$$

The topological soliton of interest is a solution of equation (8) in the form $z(\boldsymbol{\nu}x, t) = z_s[\boldsymbol{\nu}(x - x_s)]$ ($x_s = v_s t$, $v_s = \text{const.}$), which satisfies the following boundary conditions at the ends of the atomic row:

$$z_s(-\infty) \equiv 0, \quad z_s(\infty) = s, \quad z_s'(\pm\infty) \equiv 0. \quad (9)$$

The symbol $s = \pm 1$ denotes the sign of the soliton (crowdion): the value $s = 1$ corresponds to a delocalized vacancy, and $s = -1$ to a delocalized interstitial in the atomic row.

We easily obtain the asymptotic expressions for the displacements $z_s[\boldsymbol{\nu}(x - x_s)]$ for the slow crowdion:

$$s z_s[\boldsymbol{\nu}(x - x_s)] = \begin{cases} \frac{1}{2}\exp(\frac{x - x_s}{\lambda_s}), & x < x_s - \lambda_s; \\ 1 - \frac{1}{2}\exp(-\frac{x - x_s}{\lambda_s}), & x > x_s + \lambda_s, \end{cases}$$

$$\lambda_s = b\left(\frac{w}{\kappa}\right)^{1/2}, \quad \kappa = \left.\frac{\partial^2\Phi(z)}{\partial z^2}\right|_{z=n=0,\pm1,\pm2,\ldots}. \quad (10)$$

The parameter λ_s has the meaning of the half-width of the crowdion: the relative local deformation of the atomic row, $b^* z_s'[\boldsymbol{\nu}(x - x_s)]$ is appreciably different from zero only near its center, on an interval $x_s \pm \lambda_s$, and reaches its maximum value at the center of the crowdion:

$$\max|b^* z_s'| = \frac{b^*}{\lambda_s} = \frac{b^*}{b}\left(\frac{\kappa}{w}\right)^{1/2}.$$

The additional energy of the atomic row due to the appearance in it of a crowdion wave $z_s[\boldsymbol{\nu}(x - x_s)] = z_s(\boldsymbol{\rho} - \boldsymbol{\rho}_s)$, where $\boldsymbol{\rho}_s = \boldsymbol{\nu}x_s = \boldsymbol{\nu}v_s t$, is given by

$$E_0 = \frac{1}{2}m_{s0}v_s^2 + \varepsilon_{s0};$$

$$\varepsilon_{s0} = \frac{b}{b*}\int_0^1 [2w\Phi(z)]^{1/2}\mathrm{d}z, \quad m_{s0} = m_1\frac{\varepsilon_{s0}}{w}. \quad (11)$$

The parameters ε_{s0} and m_{s0} have the meaning of the self-energy and the effective mass of the crowdion, and the center of the crowdion can be treated as a pseudoparticle endowed with those properties. This equation coincides with equation (10) in §43 of the book [12].

5 Crowdion as a source of elastic fields

We shall assume that the interaction of such a crowdion with a deformable crystal matrix and a system of sufficiently weak external forces preserves the soliton properties of the crowdion excitation but can lead to changes in the shape of the crowdion and disrupt the steady motion of its center, *i.e.*, it can lead to a change in the velocity v_s of the crowdion during its motion. This assumption allows us to consider the coordinate of the center of the crowdion to be some, in general nonlinear, function of time $x_s(t)$ and to consider, in addition to the elastic displacements $\mathbf{u}(\mathbf{R}, t)$, velocities $\dot{\mathbf{u}}(\mathbf{R}, t)$, and distortions $u_{ik}(\mathbf{R}, t)$, the functions $x_s(t)$ and $v_s(t) = \dot{x}_s(t)$ as dynamical variables of the crystal. The formal substitution of the soliton $z = z_s[\boldsymbol{\rho} - \boldsymbol{\rho}_s(t)]$ described in the previous section into the function (5) converts it to a function of the set of dynamical variables indicated above:

$$\mathcal{L} = \mathcal{L}_{cs}\{\mathbf{u}(\mathbf{R}, t), \dot{\mathbf{u}}(\mathbf{R}, t), u_{ik}(\mathbf{R}, t), x_s(t), v_s(t)\}.$$

The expression thus obtained will be considered as the Lagrangian of a crystal containing a crowdion and will determine the combined space–time evolution of the elastic displacements of the atoms of the crystal $\mathbf{u}(\mathbf{R}, t)$ and of the crowdion center $x_s(t)$.

Substituting $z = z_s[\boldsymbol{\rho} - \boldsymbol{\rho}_s(t)]$ into equation (5), we obtain

$$m_\alpha \ddot{u}_i(\mathbf{R}, t) + \sum_{\alpha',\mathbf{R}'} A_{ik}^{(\alpha\alpha')}(\mathbf{R} - \mathbf{R}')u_k(\mathbf{R}', t) = F_i^{(e\alpha)}[\mathbf{R} + \mathbf{u}(\mathbf{R}, t), t] + F_i^{(s)}(\mathbf{R}, t), \quad (12)$$

$$F_i^{(s)} = \delta_{\mathbf{R}\boldsymbol{\rho}}\left\{m_1 b_i \dot{v}_s z_s'(\boldsymbol{\rho} - \boldsymbol{\rho}_s) + \frac{\partial}{\partial\rho_k}\Phi_{ik} z_s(\boldsymbol{\rho} - \boldsymbol{\rho}_s)] + b w_{ik}\frac{\partial}{\partial\rho_k} z_s'(\boldsymbol{\rho} - \boldsymbol{\rho}_s)\right\}. \quad (13)$$

The long-wavelength character of the forces $\mathbf{F}^{(e\alpha)}$ and the relatively small values of the phonon and crowdion displacements allow us to assume that $\mathbf{F}^{(e\alpha)} \approx \mathbf{F}^{(e\alpha)}(\mathbf{R} + \mathbf{u}^{(e)}(\mathbf{R},t),t)$. In this approximation the general solution of equation (12) can be written in the form of a superposition of three types of displacements:

$$\mathbf{u} = \mathbf{u}^{(ph)} + \mathbf{u}^{(e)} + \mathbf{u}^{(s)}. \tag{14}$$

Here $\mathbf{u}^{(\mathrm{ph})}$ are the free vibrations of the crystal (acoustical and optical phonons), $\mathbf{u}^{(e)}$ are the displacements under the influence of the external forces $\mathbf{F}^{(e\alpha)}$, and $\mathbf{u}^{(s)}$ are the displacements arising as a result of the presence of the crowdion in the crystal.

An explicit relation between these displacements and the coordinate and velocity of the center of the crowdion can be obtained at distances $|\mathbf{R} - \boldsymbol{\rho}_s| \gg \lambda_s$, taking into account the exponential localization of the functions $z_s'(\boldsymbol{\rho} - \boldsymbol{\rho}_s)$ and $\Phi_{ik}[z_s(\boldsymbol{\rho} - \boldsymbol{\rho}_s)]$ on the $0x$ axis around the center of the crowdion $\boldsymbol{\rho}_s$ (see the asymptotic expressions (10) and the smooth (power-law) character of the coordinate dependence of the Green function and its derivative:

$$\begin{aligned} u_i^{(s)}(\mathbf{R},t) &= q_s m_1 v_k G_{ik}^{(\alpha 1)}(\mathbf{R} - \boldsymbol{\rho}_s)\dot{v}_s \\ &\quad + (q_s w_{kn} + \varphi_{kn})\frac{\partial}{\partial R_n} G_{ik}^{(\alpha 1)}(\mathbf{R} - \boldsymbol{\rho}_s), \\ &|\mathbf{R} - \boldsymbol{\rho}_s| \gg \lambda_s; \end{aligned} \tag{15}$$

$$q_s = \frac{sb}{b^*} = b\sum_{\boldsymbol{\rho}} z_s'(\boldsymbol{\rho}), \quad \varphi_{ik} = \frac{bw^{1/2}}{b^*}\int_0^1 \frac{\Phi_{ik}(z)}{\sqrt{2\Phi(z)}}\mathrm{d}z.$$

6 Crowdion equation of motion

We consider a crowdion as a particle whose motion in the bulk of the crystal can be described by the dynamical variables $\boldsymbol{\rho}_s = \boldsymbol{\nu} x_s(t)$ and $\dot{\boldsymbol{\rho}}_s = \boldsymbol{\nu} v_s$. We assume that the crystal contains free vibrations (acoustical and optical phonons) $\mathbf{U}^{(\mathrm{ph})}(\mathbf{R},t)$ and driven displacements excited by external forces, $\mathbf{u}^{(e)}(\mathbf{R},t)$, and we treat these fields as specified functions of the coordinates and time. Substituting the expression $z = z_s(\boldsymbol{\rho} - \boldsymbol{\rho}_s)$, the general expression for the displacement fields (14), and the expression for the displacement field created by the crowdion into the Lagrangian (5), we can separate off from it the last two terms as a separate unit $\mathcal{L}_s$, which will depend on the dynamical variables of the crowdion and will include the external fields and forces as parameters. Some of the terms of this separate unit can be interpreted as the energy of interaction of a crowdion with the external fields, while the terms due to the displacements $\mathbf{u}^{(s)}$ describe its self-effect. The quantity $\mathcal{L}_s$ assumes the usual form of the Lagrangian of a particle in classical mechanics, $\mathcal{L}_s = \mathbf{L}_s\{x_s, v_s; \mathbf{u}^{(\mathrm{ph})} + \mathbf{u}^{(e)}, \mathbf{F}^{(e1)}\}$, if it is constructed in the quadratic approximation in the velocities v_s.

Taking into account the self-effect of the crowdion through a crystal having a finite elastic compliance leads to a renormalization of the bare values of the effective mass m_{s0} and rest energy ε_{s0}:

$$\begin{aligned} \mathcal{L}_s = \frac{1}{2}m_s v_s^2 - \varepsilon_s - \sum_{\boldsymbol{\rho}}\{ & m_1 v_s b_i[\dot{u}_i^{(ph)}(\boldsymbol{\rho},t) + \dot{u}_i^{(e)}(\boldsymbol{\rho},t)] \\ & \times z_s'(\boldsymbol{\rho} - \boldsymbol{\rho}_s) + [u_{ik}^{(ph)}(\boldsymbol{\rho},t) + u_{ik}^{(e)}(\boldsymbol{\rho},t)] \\ & \times [b w_{ik} z_s'(\boldsymbol{\rho} - \boldsymbol{\rho}_s) + \Phi_{ik}(z_s)] \\ & + b_i F_i^{(e)}[\boldsymbol{\rho} + \mathbf{u}^{(e)}(\boldsymbol{\rho},t),t] z_s(\boldsymbol{\rho},t)\}. \end{aligned} \tag{16}$$

$$\begin{aligned} m_s = m_{s0} + 2m_1 b \sum_{\boldsymbol{\rho},\boldsymbol{\rho}'} & \frac{\partial^2 G_{ik}^{11}(\boldsymbol{\rho} - \boldsymbol{\rho}')}{\partial\rho_n \partial\rho_m}\nu_i\nu_m z_s'(\boldsymbol{\rho}) \\ & \times \{b w_{kn} z_s'(\boldsymbol{\rho}') + \Phi_{kn}[z_s(\boldsymbol{\rho}')]\}; \end{aligned} \tag{17}$$

$$\begin{aligned} \varepsilon_s = \varepsilon_{s0} + \sum_{\boldsymbol{\rho},\boldsymbol{\rho}'} & \frac{\partial^2 G_{ik}^{11}(\boldsymbol{\rho} - \boldsymbol{\rho}')}{\partial\rho_n \partial\rho_m}\{b w_{im} z_s'(\boldsymbol{\rho}) \\ & + \Phi_{im}[z_s(\boldsymbol{\rho})]\}\{b w_{kn} z_s'(\boldsymbol{\rho}') + \Phi_{kn}[z_s(\boldsymbol{\rho}')]\}. \end{aligned} \tag{18}$$

In going to the Newtonian form of the equation of motion it is helpful to take into account the exponentially "sharp" character of the functions $z_s'(\boldsymbol{\rho} - \boldsymbol{\rho}_s)$ and $\Phi_{ik}[z_s'(\boldsymbol{\rho} - \boldsymbol{\rho}_s)]$ against the background of the smooth coordinate dependences of the external fields, as this was done in the derivation formula (15). This lets us take the values of the external fields at the point $\boldsymbol{\rho} = \boldsymbol{\rho}_s$ out from under the summation over $\boldsymbol{\rho}$. As a result, the equation of motion of the crowdion takes the final form

$$\begin{aligned} m_s\dot{v}_s = & -q_s\nu_i F_i^{(e1)}[\boldsymbol{\rho}_s + \mathbf{u}^{(e)}(\boldsymbol{\rho}_s,t),t] \\ & + q_s m_1 \nu_i \frac{\partial^2}{\partial t^2}[u_i^{(ph)}(\boldsymbol{\rho}_s,t) + u_i^{(e)}(\boldsymbol{\rho}_s,t)] - (q_s w_{ik}) \\ & + \varphi_{ik}\frac{\partial}{\partial x_s}[u_{ik}^{(ph)}(\boldsymbol{\rho}_s,t) + u_{ik}^{(e)}(\boldsymbol{\rho}_s,t)]. \end{aligned} \tag{19}$$

Expressions for the constants of the lattice–crowdion interaction w_{ik} and φ_{ik} are given in (6) and (15).

Let us conclude with the discussion of another important question that has direct bearing on the dynamical properties of a crowdion. Taking the discreteness into account leads to a correction to the crowdion energy which is periodic in the coordinate $x_s = v_s t$ and is analogous to the Peierls energy for a dislocation [9]. The problem of crowdion mobility in such potential relief appears. The question of a quantum tunneling of the crowdion through barriers of this relief and appearance of a band spectrum is of a special interest [12–17].

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