Three-dimensional soliton in an ionic crystal

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We develop a translationally invariant strong-coupling theory for the Landau-Pekar polaron which is considered to be a three-dimensional soliton. We construct the theory on the basis of a rigorous account of the kinetic energy of the polarization of the crystal. We study the effect of the role played by the optical-phonon dispersion. We show that when the polaron speed increases up to a critical value, its effective mass increases and the localization is increased. If the polaron speed exceeds the critical one, a further increase in the speed is connected with a delocalization of the electron and a decrease in its effective mass.

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1. INTRODUCTION

Recently much attention has been paid to a study of non-linear wave equations in homogeneous media which have solutions corresponding to the spontaneous breaking of the local symmetry (self-localization). Particularly intensive has been the study of one-dimensional systems described by the non-linear Korteweg-de Vries, Schrödinger, and sine-Gordon equations which have particle-like solutions in the form of solitary waves—solitons.[1]

In recent years several attempts have been made to study the possibility that solitons are formed in media of two and three dimensions. Most success was achieved in the study of the so-called topological solitons which have wavefunctions with various values corresponding to the zero-point energy (degenerate vacuum). For instance, in an isotropic ferromagnet the vacuum state, i.e., the state with the lowest energy, corresponds to complete magnetization. The magnetization vector can then be in an arbitrary direction.

It was shown by Dzyaloshinskiĭ and Ivanov[2] that topological solitons which are localized in three dimensions can exist in a ferromagnet. Rebbi[3] has discussed the general conditions for the formation of topological solitons in media of various numbers of dimensions. He noted that the field which characterizes the states of two- and three-dimensional solitons must have a vector character with two and three components, respectively.

Appreciably less definite results are obtained when one studies the formation of non-topological solitons in media of two and three dimensions. The wavefunctions of non-topological solitons vanish on the infinite sphere (non-degenerate vacuum).

Recently Bogolyubskiĭ[4] has shown that the transition from a one-dimensional to a three-dimensional system leads, as a rule, to a narrowing of the stability of both scalar and spinor solitons. In particular, he showed that in the case of a complex scalar field with self-action, which is proportional to the fourth power of the field, charged three-dimensional spherically symmetric solitons are unstable in contrast to the one-dimensional ones. The instability of spherically symmetric solutions which vanish at infinity in three-dimensional space was noted by Zakharov[5] and Petviashvili[6].

We would like to draw attention to the fact that one type of stable three-dimensional non-topological soliton has been known to physicists for a relatively long time. In fact, at present one uses widely in the theory of ionic crystals the polaron concept which was introduced by Landau[7] and Pekar[8,9] more than forty years ago.

A polaron is a self-localized state of an electron in an ionic crystal and is caused by non-linear and non-local interaction of an electron with the vector field of the polarization produced in the crystal by the electron itself. Thus, the Landau-Pekar polarons are three-dimensional solitons in ionic crystals. A comprehensive study of such solitons (polarons) is thus of considerable interest from the point of view of elucidating the general conditions for the formation of non-topological solitons in a two- or three-dimensional system.

The first theoretical papers[8,9] studied the properties of a polaron at rest. The effective mass of a polaron with small translational velocity was first studied by Landau and Pekar[10] who used perturbation theory. A consistent translationally invariant adiabatic perturbation theory was developed by Bogolyubov[11] and Tyablikov.[12] They considered the kinetic energy of the ions as a small perturbation.

Bogolyubov and Tyablikov introduced three extra degrees of freedom for the description of the motion of the center of the polarization well. This required the introduction of three additional coupling conditions between the degrees of freedom of the system. The great complexity of the theory prevented it to be widely applied in practice.

Recently Gross[13] developed a translationally invariant perturbation theory in inverse powers of the dimensionless coupling parameter of the electron with the polarization field, without introducing extra variables. The state of the electron was described relative to the center of a spherically symmetric polarization well. The effect of temporal retardation of the polarization cloud relative to the spatial distribution of the electron was neglected in that paper.

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In all the mentioned theoretical studies of polarons the kinetic energy of the polarization of the crystal was taken into account through perturbation theory methods. Therefore the possible change in the spherical symmetry of the polarization cloud was neglected together with the temporal polarization retardation due to electron motion. Moreover, optical phonons without dispersion were considered. These limitations are removed in the present paper. Taking into account the dispersion of the optical phonons, we determine for the polaron energy and its other characteristics expressions which are valid for any velocity for which the continuum approximation can still be used.

2. EQUATIONS DESCRIBING A MOVING POLARON

An excess electron in a homogeneous polarizable medium causes the displacement of ions from their equilibrium positions. The Hamiltonian function of the produced vector polarization field $\mathbf{P}(\mathbf{r},t)$ can be written in the form

$$H_p=\frac{2\pi\tilde{\varepsilon}}{\Omega_0^2}\int\left[\Omega_0^2\mathbf{P}^2+\left(\frac{\partial\mathbf{P}}{\partial t}\right)^2-V_0^2\mathbf{P}\nabla_r{}^2\mathbf{P}\right]d^3r, \tag{2.1}$$

where $\tilde{\varepsilon}$ is the effective inertial permittivity, introduced by Pekar.[8,9]

The vector field $\mathbf{P}(\mathbf{r},t)$ corresponds to longitudinal optical phonons with a positive dispersion law

$$\Omega(\mathbf{k})=(\Omega_0^2+V_0^2\mathbf{k}^2)^{1/2}. \tag{2.2}$$

In the case of negative dispersion we must substitute $-V_0^2$ for V_0^2.

The Hamiltonian function of the electron in the conduction band of the crystal has in the effective mass (m^*) approximation the form

$$H_{el}=\int\Psi^*(\mathbf{r},t)\left[\mathscr{E}_0-\frac{\hbar^2}{2m^*}\nabla_r{}^2\right]\Psi(\mathbf{r},t)\,d^3r,$$
$$\int|\Psi(\mathbf{r},t)|^2\,d^3r=1, \tag{2.3}$$

where $\mathscr{E}_0$ is the energy of the bottom of the conduction band.

The interaction of the electron with the polarization produced can be written in two equivalent forms:

$$H_{int}=-e\int\varphi(\mathbf{r},t)|\Psi(\mathbf{r},t)|^2\,d^3r=-\int\mathbf{P}(\mathbf{r},t)\mathbf{D}(\mathbf{r},t)\,d^3r, \tag{2.4}$$

where $-e$ is the effective electron charge, and $\varphi(\mathbf{r},t)$ is the potential of the polarization created by the electron and is defined by the equation

$$\nabla_r\varphi(\mathbf{r},t)=4\pi\mathbf{P}(\mathbf{r},t). \tag{2.5}$$

The electron produces an electric field in the crystal with an induction vector determined by the equation

$$\mathbf{D}(\mathbf{r},t)=-e\nabla_r\int|\Psi(\mathbf{r}_1,t)|^2\frac{d^3r_1}{|\mathbf{r}-\mathbf{r}_1|}. \tag{2.6}$$

The sum of the expressions (2.1), (2.3), and (2.4) determines the complete Hamiltonian function of the system; with the its help we find the equations of motion

$$\left[i\hbar\frac{\partial}{\partial t}-\mathscr{E}_0+\frac{\hbar^2}{2m^*}\nabla_r{}^2-e\varphi(\mathbf{r},t)\right]\Psi(\mathbf{r},t)=0, \tag{2.7}$$

$$\left[\frac{\partial^2}{\partial t^2}+\Omega_0^2-V_0^2\nabla_r{}^2\right]\varphi(\mathbf{r},t)=-\frac{e\Omega_0^2}{\tilde{\varepsilon}}\int|\Psi(\mathbf{r}_1,t)|^2\frac{d^3r_1}{|\mathbf{r}-\mathbf{r}_1|}. \tag{2.8}$$

To take the translational symmetry of the problem into account we shall look for the solution of this system of equations in the form of excitations which move with constant velocities $\mathbf{V}$. We direct the z-axis of the coordinates of the system along the velocity $\mathbf{V}$ and use the equations

$$\varphi(\mathbf{r},t)=\varphi(\boldsymbol{\rho}),\quad \Psi(\mathbf{r},t)=a^{-3/2}G(\boldsymbol{\rho})\exp[i(\mathbf{kr}-\omega t)] \tag{2.9}$$

to introduce the real functions $\varphi(\boldsymbol{\rho})$ and $G(\boldsymbol{\rho})$ which depend on the dimensionless vector $\boldsymbol{\rho}$ with components determined by the equations

$$\xi=x/a,\quad \eta=y/a,\quad \zeta=(z-z_0-Vt)/a, \tag{2.9a}$$

where a is the lattice constant, $\mathbf{k}=m\mathbf{V}/\hbar$, $\hbar\omega=E_{el}+E_{int}$ is the energy (in the laboratory frame of reference) of the electron interacting with the polarization field.

With the aid of (2.9), Eq. (2.8) is transformed to the form

$$\mathscr{R}\varphi(\boldsymbol{\rho})=-\frac{e}{\tilde{\varepsilon}a}\int\frac{G^2(\boldsymbol{\rho}_1)\,d^3\rho_1}{|\boldsymbol{\rho}-\boldsymbol{\rho}_1|}, \tag{2.10}$$

where the operator $\mathscr{R}$ is defined by the formula

$$\mathscr{R}=1+\sigma^2\frac{\partial^2}{\partial\xi^2}-\sigma_0{}^2\nabla_\rho{}^2, \tag{2.11}$$

in which we have used the notation

$$\sigma_0{}^2=V_0{}^2/a^2\Omega_0{}^2,\quad \sigma^2=V^2/a^2\Omega_0{}^2. \tag{2.12}$$

We shall be interested only in the self-localized states of an electron. In that case the right-hand side of Eq. (2.10) decreases faster than $|\boldsymbol{\rho}|^{-1}$. Thus, we need the particular solutions of Eq. (2.10) which satisfy the boundary condition

$$\varphi(|\boldsymbol{\rho}|\to\infty)=0. \tag{2.13}$$

The condition (2.13) can be satisfied in the $\boldsymbol{\rho}$ by coordinate system by considering the $\boldsymbol{\rho}$-space in the form of a cube of edge length $2L$ moving together with an electron, located in the region $\boldsymbol{\rho}\approx 0$, at a constant velocity V relative to an unbounded dielectric at rest. In this case the particular solution of (2.10) which satisfies the condition (2.13) will have the form

$$\varphi(\boldsymbol{\rho})=\int\limits_{(2L)^3}\frac{W(\boldsymbol{\rho}-\boldsymbol{\rho}_2)G^2(\boldsymbol{\rho}_1)\,d^3\rho_1\,d^3\rho_2}{|\boldsymbol{\rho}_1-\boldsymbol{\rho}_2|} \tag{2.14}$$

with

$$W(\boldsymbol{\rho})=\frac{a^3}{L^3}\operatorname{Re}\sum_{\mathbf{q}}\frac{\exp(i\mathbf{q}\boldsymbol{\rho})}{1-\sigma^2q_z{}^2+\sigma_0{}^2\mathbf{q}^2}. \tag{2.15}$$

The summation in (2.15) is over all values of the components of the dimensionless wavevector

$$q_i=\frac{\pi a}{L}n_i,\ n_i=0,\ \pm1,\ldots;\ i=x,y,z, \tag{2.16}$$

which are eigenvalues of the operator $\mathscr{R}$ defined on the set of differentiable functions in the closed volume $(2L)^3$ with zero boundary conditions.

As $L\to\infty$ the wavevector q runs through a quasi-continuous number of values with discreteness interval $a\pi/L\to 0$. Therefore the sum in (2.15) can be replaced by an integral so that

$$W(\rho)=\frac{1}{(2\pi)^3}\int\frac{\exp(i\mathbf{q}\boldsymbol{\rho})\,d^3q}{1-\sigma^2q_z^2+\sigma_0^2\mathbf{q}^2}. \tag{2.17}$$

When evaluating (2.17) the rule for going round the poles $q_z=\pm(\sigma^2-\sigma_0^2)^{-1/2}$ when $\sigma^2>\sigma_0^2$ must be chosen in accordance with the causality principle.

The function $W(\boldsymbol{\rho}-\boldsymbol{\rho}_2)$ in (2.14) takes into account the non-locality of the interaction between the electron and the polarization field. This non-locality is caused by the phonon dispersion ($\sigma_0\neq 0$) and the temporal retardation due to the motion of the electron ($\sigma\neq 0$).

Using (2.17), Eq. (2.7) is transformed into an integro-differential equation

$$\left\{\frac{\hbar^2}{2m^*a^2}\nabla_\rho^2+\Lambda+\frac{e^2}{a\tilde{\varepsilon}}\int\frac{W(\boldsymbol{\rho}-\boldsymbol{\rho}_2)G^2(\boldsymbol{\rho}_1)\,d^3\rho_1 d^3\rho_2}{|\boldsymbol{\rho}_1-\boldsymbol{\rho}_2|}\right\}G(\boldsymbol{\rho})=0; \tag{2.18}$$

$$\Lambda=E_{el}+E_{int}-\mathscr{E}_0-\frac{1}{2}m^*V^2$$

$$=\frac{\hbar^2}{2m^*a^2}\int(\nabla_\rho G)^2\,d^3\rho-\frac{e^2}{a\tilde{\varepsilon}}\int\frac{G^2(\boldsymbol{\rho})W(\boldsymbol{\rho}-\boldsymbol{\rho}_2)G^2(\boldsymbol{\rho}_2)}{|\boldsymbol{\rho}_1-\boldsymbol{\rho}_2|}d^3\rho\,d^3\rho_1\,d^3\rho_2 \tag{2.18a}$$

is the energy of the electron in the potential well $\varphi(\boldsymbol{\rho})$ which is moving with the velocity V.

Without solving Eq. (2.18) we can evaluate the function $G(\boldsymbol{\rho})$ by a variational method, minimizing the functional

$$J\{G\}=-\frac{\hbar^2}{2m^*a^2}\int d^3\rho G(\boldsymbol{\rho})\Big[\nabla_\rho^2G(\boldsymbol{\rho})+\gamma G(\boldsymbol{\rho})\int\frac{W(\boldsymbol{\rho}-\boldsymbol{\rho}_1)G^2(\boldsymbol{\rho}_1)}{|\boldsymbol{\rho}_1-\boldsymbol{\rho}_2|}d^3\rho_1\,d^3\rho_2\Big]; \tag{2.19}$$

$$\gamma=\frac{e^2}{a\tilde{\varepsilon}}\frac{m^*a^2}{\hbar^2} \tag{2.20}$$

is a dimensionless parameter which is proportional to the ratio of the Coulomb energy to twice the energy of an electron with momentum $\hbar/a$ in the conduction band.[1)]

When there is no dispersion and the polaron is at rest ($\sigma_0=\sigma=0$), the function (2.17) reduces to a δ-function. In that case the functional (2.19) changes into Pekar's functional[8,9] and the zeroth-approximation functional from the papers by Bogolyubov and Tyablikov.[11,12]

The energy of the polarization of the crystal (2.1) changes, when we change to the $\boldsymbol{\rho}$ variables and use the relation

$$\frac{\partial\mathbf{P}}{\partial t}=-\frac{V\,\partial\mathbf{P}}{a\,\partial\zeta}$$

to the form

$$E_p(V)=\frac{2\pi\tilde{\varepsilon}a^3}{\Omega_0^2}\int\left[V^2\left(\frac{\partial\mathbf{P}}{\partial\zeta}\right)^2+\Omega_0^2\mathbf{P}^2+\frac{V_0^2}{a^2}(\nabla_\rho\mathbf{P})^2\right]d^3\rho. \tag{2.21}$$

If the function $G_0(\rho)$ minimizes the functional (2.19) under the condition $\int G_0^2(\boldsymbol{\rho})d^3\rho=1$, the vector field of the polarization is determined according to (2.5) and (2.14) by the expression

$$\mathbf{P}(\boldsymbol{\rho})=-\frac{e}{\tilde{\varepsilon}a^2 4\pi}\nabla_\rho\int\frac{W(\boldsymbol{\rho}-\boldsymbol{\rho}_2)G_0^2(\boldsymbol{\rho}_1)}{|\boldsymbol{\rho}_1-\boldsymbol{\rho}_2|}d^3\rho_1\,d^3\rho_2. \tag{2.22}$$

The total energy $(E_{el}+E_{int}+E_p)$ of a polaron moving with a constant velocity V is, when we use the identity

$$\int W(\boldsymbol{\rho}-\boldsymbol{\rho}_1)W(\boldsymbol{\rho}-\boldsymbol{\rho}_2)d^3\rho=\mathscr{L}W(\boldsymbol{\rho}_1-\boldsymbol{\rho}_2),$$

in which we have the operator

$$\mathscr{L}=1+\sigma^2\frac{\partial}{\partial\sigma^2}+\sigma_0^2\frac{\partial}{\partial\sigma_0^2},$$

expressed by the formula

$$E(V)=\mathscr{E}_0+\frac{1}{2}m^*V^2+\frac{\hbar^2}{2m^*a^2}\int d^3\rho(\nabla_\rho G(\boldsymbol{\rho}))^2+\frac{a^3}{8\pi\tilde{\varepsilon}}\int d^3\rho_1\,d^3\rho_2\Big\{\mathbf{D}(\boldsymbol{\rho}_1)\mathbf{D}(\boldsymbol{\rho}_2)[\mathscr{L}-2]+\sigma^2\frac{\partial\mathbf{D}(\boldsymbol{\rho}_1)}{\partial\zeta_1}\frac{\partial\mathbf{D}(\boldsymbol{\rho}_2)}{\partial\zeta_2}\mathscr{L}+\sigma_0^2\nabla_{\rho_1}\mathbf{D}(\boldsymbol{\rho}_1)\nabla_{\rho_2}\mathbf{D}(\boldsymbol{\rho}_2)\mathscr{L}\Big\}W(\boldsymbol{\rho}_1-\boldsymbol{\rho}_2). \tag{2.23}$$

The expressions obtained are valid for any velocities of the polaron for which we can still use the continuum approximation.

3. DIRECT VARIATIONAL METHOD

We can perform the minimization of the functional (2.19) by a direct variational method. Bearing in mind that when the electron moves the polarization accompanying it has cylindrical symmetry, we use as trial function the normalized function

$$G(\rho)=\left(\frac{2}{\pi}\right)^{3/4}\alpha^{1/2}\beta\exp(-\alpha^2\zeta^2-\beta^2\mathbf{R}^2),\quad \mathbf{R}^2=\xi^2+\eta^2, \tag{3.1}$$

which depends on two variational parameters: α and β.

Substituting (3.1) in the functional (2.19) we get the function

$$J(\alpha,\beta)=\frac{\hbar^2}{2m^*a^2}[\alpha^2+2\beta^2-\gamma\alpha^2\beta^4\pi^{-3}j(\alpha,\beta)], \tag{3.2}$$

in which

$$j(\alpha,\beta)=\int d^2\rho_1 d^2\rho_2 d^3\rho_3\frac{W(\rho_3)}{|\rho_1|}\exp\left\{-\frac{\alpha^2}{2}[(\zeta_1+\zeta_2+\zeta_3)^2+(\zeta_2-\zeta_1-\zeta_3)^2]-\frac{\beta^2}{2}[(\mathbf{R}_1+\mathbf{R}_2+\mathbf{R}_3)^2+(\mathbf{R}_2-\mathbf{R}_1-\mathbf{R}_3)^2]\right\}. \tag{3.3}$$

The explicit evaluation of all expressions given above depends on the form of the function (2.17) which depends on σ, σ_0, and the ratio

$$s^2=V^2/V_0^2=\sigma^2/\sigma_0^2. \tag{3.4}$$

When $\sigma_0^2>0$ and $0\leqslant s^2<1$ the function (2.17) is given by the formula

$$W(\rho)=[4\pi\sigma_0^2(\zeta^2+(1-s^2)\mathbf{R}^2)^{1/2}]^{-1}\exp\left(-\frac{(\zeta^2+(1-s^2)\mathbf{R}^2)^{1/2}}{\sigma_0(1-s^2)^{1/2}}\right). \tag{3.5}$$

When $\sigma_0^2>0$ and $s^2>1$ the function (2.17) takes the form

$$W(\rho)=\cos\frac{(\zeta^2-(s^2-1)\mathbf{R}^2)^{1/2}}{\sigma_0(s^2-1)^{1/2}}[2\pi\sigma_0^2(\zeta^2-(s^2-1)\mathbf{R}^2)^{1/2}]^{-1}, \tag{3.6}$$

provided the inequalities

$$\zeta<0 \text{ and } \zeta^2>(s^2-1)\mathbf{R}^2, \tag{3.7}$$

are satisfied and it vanishes if these inequalities are not satisfied.

The exact expressions (3.5) and (3.6) are very complicated for analytical calculations so that we shall use approximate values which are valid under some limitations on the parameters of the system.

In connection with the employed continuum approximation we study only excitations in a localization region which appreciably exceeds the lattice constant. In that case the dispersion of the optical phonons is always small, so that the inequality

$$|\sigma_0^2|\ll 1. \tag{3.8}$$

holds. Therefore, when $\sigma^2>\sigma_0^2$, we can replace the function (2.17) by the approximate expression

$$W(\rho)\approx\left[1+\sigma_0^2\left(\frac{\partial^2}{\partial\xi^2}+\frac{\partial^2}{\partial\eta^2}\right)\right]\delta(\xi)\delta(\eta)W(\zeta), \tag{3.9}$$

where

$$W(\zeta)=\begin{cases}\dfrac{\sin(|\zeta|(\sigma^2-\sigma_0^2)^{-1/2})}{(\sigma^2-\sigma_0^2)^{1/2}}, & \text{if } \zeta<0\\ 0, & \text{if } \zeta\geqslant 0\end{cases} \tag{3.10}$$

We must bear in mind that due to the quasi-continuity of the wavevector (2.16) the quantity $(\sigma^2-\sigma_0^2)^{-1/2}$ also takes on quasi-continuous values

$$(\sigma^2-\sigma_0^2)^{-1/2}=\frac{\pi a}{L}n_z,\quad n_z=1,2,\ldots, \tag{3.11}$$

with a discreteness interval which tends to zero as $L\to\infty$.

If at the same time as the inequality (3.8) the inequality

$$\sigma^2\ll 1 \tag{3.12}$$

is satisfied, we can use for $W(\rho)$ the even simpler expression

$$W(\rho)=1-\sigma^2\frac{\partial^2}{\partial\xi^2}+\sigma_0^2\nabla_\rho^2+\sigma^4\frac{\partial^4}{\partial\xi^4}-2\sigma^2\sigma_0^2\nabla_\rho^2\frac{\partial^2}{\partial\xi^2}. \tag{3.13}$$

Although Eqs. (3.9) and (3.13) are written down for the case of positive phonon dispersion, when $\sigma_0^2>0$, they are also valid in the case of negative dispersion, when $\sigma_0^2<0$.

In the following sections we give the calculations of $G(\rho)$, $E(V)$, and other quantities which characterize a moving polaron for the case when Eqs. (3.9) and (3.13) are valid.

4. SMALL DISPERSION, SLOW POLARON

We shall assume the polaron motion to be slow when inequality (3.12) holds. For characteristic ionic crystals $a\Omega_0\approx 2.5\times 10^6$ cm/s. Hence, the inequality (3.12) is satisfied even for not very small electron velocities.

If we use in (2.19) the approximate expression (3.13), the wavefunction (3.1) minimizes the functional (3.2) at the values

$$\beta=\alpha_0(1-6\alpha_0^2\sigma_0^2)+{}^{12}/_{7}\alpha_0^3\sigma^2, \tag{4.1}$$

$$\alpha=\beta(1+{}^{12}/_{7}\alpha_0^2\sigma^2)^{1/2},\quad \alpha_0\equiv\gamma/3\pi^{1/2}. \tag{4.2}$$

Hence, the square of the wavefunction (3.1) has the form

$$G_0^2(\rho)=\left(\frac{2}{\pi}\right)^{3/2}\alpha\beta^2\exp\left[-2\beta^2\left(\rho^2+\frac{12}{7}\alpha_0^2\sigma^2\zeta^2\right)\right]. \tag{4.3}$$

The spatial probability distribution of the electron is thus spherically symmetric in the case of a polaron at rest ($\sigma=0$). According to (4.1) positive dispersion ($\sigma_0^2>0$) leads to a smaller and negative dispersion to a greater localization of the electron.

At nonzero polaron velocity ($\sigma^2\neq 0$) the constant values of $G_0^2(\rho)$ are situated on surfaces which have the form of an oblate ellipsoid of revolution with an axis of symmetry directed along the polaron velocity. An increase in the velocity, while inequality (3.12) remains valid, is accompanied by an increase of its localization. The total energy of the polaron (including the polarization energy) can be written in the form

$$E(V)=E(0)+{}^{1}/_{2}m_{eff}V^2, \tag{4.4}$$

where the energy of a polaron at rest is

$$E(0)=\mathscr{E}_0-\frac{a^3}{8\pi\varepsilon}\int[\mathbf{D}^2-\sigma_0^2(\nabla_\rho\mathbf{D})^2]d^3\rho\approx\mathscr{E}_0-0{,}053E_a\frac{m^*}{m\varepsilon}(1-0.142\gamma^2\sigma_0^2), \tag{4.5}$$

m is the mass of a free electron and $E_a=me^4/\hbar^2$ is the atomic unit of energy.

The effective polaron mass is

$$m_{eff}=m^*+\frac{a}{4\pi\varepsilon\Omega_0^2}\int\left[\left(\frac{\partial\mathbf{D}}{\partial\zeta}\right)^2-2\sigma_0^2\left(\frac{\partial}{\partial\zeta}\nabla_\rho\mathbf{D}\right)^2+3\sigma^2\left(\frac{\partial^2\mathbf{D}}{\partial\zeta^2}\right)^2\right]d^3\rho\approx m^*+\frac{4e^2\gamma^2}{(9\pi)^2a^3\Omega_0^2}\left[1+\frac{\gamma^2}{5\pi}\left(\frac{181}{21}\sigma^2-18\sigma_0^2\right)\right]. \tag{4.6}$$

When the polaron velocity increases its effective mass increases in correspondence with the increase of its localization.

5. FAST ELECTRON

If the condition (3.12) for small velocities is not satisfied, but the dispersion of the optical phonons is small ($|\sigma_0^2| \ll 1$) we must perform the calculation with a value of $W(\rho)$ given by Eq. (3.10). In that case the function (3.2) takes the form

$$J(\alpha,\beta)=\frac{\hbar^2}{2m^*a^2}\left\{\alpha^2+2\beta^2-\frac{6\alpha_0 fF}{\sigma}+12\sigma_0^2\alpha_0\beta^2\left[\frac{F}{\sigma}+\frac{F-\alpha\sigma}{\alpha\sigma^3}\right]\frac{f\alpha^2-\beta^2}{\alpha^2-\beta^2}\right\}, \tag{5.1}$$

where α_0 is given by Eq. (4.2),

$$f=(\alpha^2-\beta^2)^{-1/2}\operatorname{arctg}(\alpha^2-\beta^2)^{1/2}, \tag{5.2}$$

and the function

$$F(x)=e^{-x^2}\int_0^x e^{t^2}dt \tag{5.3}$$

at the value $x \equiv 1/2\alpha\sigma$.

For small dispersion ($\sigma_0 \approx 0$) minimization of the function (5.1) is realized at values of α and β shown in Fig. 1 as functions of the variable

$$\alpha_0\sigma=\gamma V/3\pi^{1/2}a\Omega_0 \tag{5.4}$$

which is proportional to the velocity. The dependences of the parameters α and β on the velocity undergo a considerable change on going through the critical value $\alpha_0\sigma_{cr} \approx 0.14$.

An increase in the subcritical velocities is accompanied by an increase in the self-localization of the electron, especially in the longitudinal direction ($\alpha > \beta$). On going through the critical value, an increase of velocity is accompanied by delocalization and by a diminution of the longitudinal-transverse asymmetry. The medium does not manage to get completely polarized due to the fast motion of the electron.

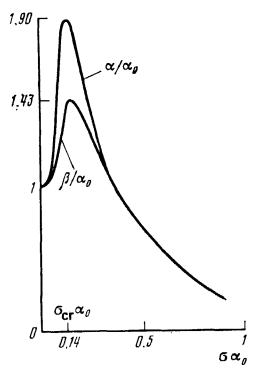

FIG. 1. Along the axes are plotted $\sigma\alpha_0$ and α/α_0 (upper curve), β/α_0 (lower curve). The maximum values 1.90 and 1.43 are reached, respectively, for $\sigma\alpha_0 = 0.13$ and $\sigma\alpha_0 = 0.15$.

The energy of the polaron is determined by the values of α and β which we have found through the expression

$$E(V)=\mathscr{E}_0+\frac{1}{2}m^*V^2+\frac{\hbar^2}{2m^*a^2}\left\{\alpha^2+2\beta^2-3\alpha_0 f\left[\frac{2F}{\sigma}+\frac{(1-2\alpha\sigma^2)F-\alpha\sigma}{\alpha^2\sigma^3}\right]\right\}, \tag{5.5}$$

where the functions f and F are given by (5.2) and (5.1).

The energy (5.5) of the polaron is proportional at low to the square of the velocity. When the velocity increases further this dependence becomes more complicated. One can, however, retain Eq. (4.4) for the energy provided the deviation from the quadratic dependence is characterized by the velocity-dependence of the polaron effective mass.

Using an electronic computer to evaluate the energy (5.5), we find the velocity-dependence of the effective mass $m_{eff}(V)$ shown in Fig. 2. The polaron effective mass thus increases steeply when the polaron velocity approaches its critical value, which corresponds to the maximum self-localization of the electron.

6. POLARIZATION OF THE CRYSTAL ACCOMPANYING THE ELECTRON MOTION

The motion of an electron in an ionic crystal is accompanied by a local polarization which is given by Eq. (2.21) with the appropriate values of the wavefunction (3.1).

When the polaron is at rest the wavefunction (3.1) is spherically symmetric ($\alpha = \beta = \alpha_0$) and the function $W(\rho)$ becomes a delta-function. In that case the projection of the polarization vector along any direction away from the center of the polaron ($\rho = 0$) is given by the expression

$$P_{\zeta,0}^{(\alpha_0)}(0,0,\zeta)=\frac{e}{4\pi a^2\varepsilon\zeta}\left\{2\left(\frac{2}{\pi}\right)^{1/2}\exp(-2\alpha_0^2\zeta^2)-\frac{\Phi(\alpha_0\zeta\sqrt{2})}{\zeta}\right\}, \tag{6.1}$$

where $\Phi(x)$ is the probability function. The polarization field (6.1) has the symmetry

$$P_{\zeta,0}^{(\alpha_0)}(0,0,\zeta)=-P_{\zeta,0}^{(\alpha_0)}(0,0,-\zeta), \tag{6.2}$$

vanishes for $\zeta = 0$ and, decreases like ζ^{-2} at large values of ζ.

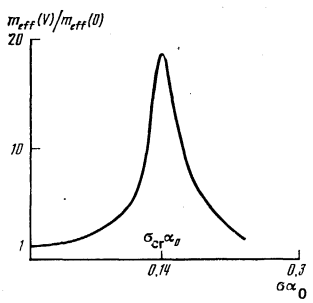

FIG. 2. Along the axes are plotted $\sigma\alpha_0$ and the effective mass of the moving polaron divided by the effective mass of a polaron at rest.

For low polaron velocities when one can use the first terms of the expansion (3.13), the component of the polarization vector along the direction of the motion (ζ-axis) can be written in the form

$$P_{\zeta,\sigma}(0,0,\zeta)\approx\{1+4\alpha^2(\sigma^2-\sigma_0^2)[1-4\alpha^2\zeta]\}P_{\zeta,0}^{(\alpha)}(0,0,\zeta), \tag{6.3}$$

in which $P_{\zeta,0}^{\alpha}(0,0,\zeta)$ is given by (6.1) with

$$\alpha\approx\alpha_0(1-6\sigma_0^2\alpha_0^2)+{}^{12}/_{7}\alpha_0^3\sigma^2. \tag{6.4}$$

For values $\sigma\approx\sigma_0$ the radial dependence of the potential energy of the interaction of the electron with the polarization field is given by the expression

$$e\varphi_0(\rho)=-e^2\Phi(2^{1/2}\alpha\rho)/a\tilde{\varepsilon}\rho. \tag{6.5}$$

This potential well has a depth $-e^2\alpha 2^{3/2}/a\tilde{\varepsilon}\pi^{1/2}$ and has the symmetry

$$\varphi_0(\rho)=\varphi_0(-\rho).$$

When the polaron moves with a velocity $V=a\sigma\Omega_0>V_0$ in the frame of reference moving with the polaron, the ζ-dependence of the potential energy along the symmetry axis is given by the integral

$$e\varphi_0(0,0,\zeta)=-\frac{e^2}{a\tilde{\varepsilon}(\sigma^2-\sigma_0^2)^{1/2}}\int_0^{\infty}\frac{\sin(x/(\sigma^2-\sigma_0^2)^{1/2})}{x+\zeta}\Phi(2^{1/2}\alpha(x+\zeta))\,dx. \tag{6.6}$$

The depth of this well in the region $\zeta=0$ is equal to

$$e\varphi_0(0,0,0)=-\frac{4\alpha e^2 z}{a\tilde{\varepsilon}\pi^{1/2}}F(z), \tag{6.7}$$

where $F(z)$ is given by Eq. (5.3) with the value $z=1/2^{3/2}\alpha(\sigma^2-\sigma_0^2)^{1/2}$. Thus, when the polaron velocity increases the depth (6.7) of the well first increases somewhat and later decreases. As $\zeta\to\infty$ the function (6.6) has a simple asymptotic form:

$$e\varphi_0(0,0,\zeta)\to e^2/a\tilde{\varepsilon}\zeta,\quad \zeta\to\infty. \tag{6.8}$$

The asymptotic form of the function (6.6) contains in the region of large ζ-values, apart from $e^2/a\tilde{\varepsilon}|\zeta|$, a small oscillating term

$$-4(\sigma^2-\sigma_0^2)^{1/2}\exp\left(-\frac{1}{4(\sigma^2-\sigma_0^2)}\right)\sin\frac{\zeta}{(\sigma^2-\sigma_0^2)^{1/2}}, \tag{6.9}$$

which vanishes when (3.11) is taken into account.

7. CONCLUSION

The method proposed in this paper for solving the problem of a moving polaron (three-dimensional soliton) does not, in contrast to known methods, use perturbation theory with regard to the ion kinetic energy. Taking the dispersion of the optical phonons into account, it allows to study the effect of the non-local character of the interaction which is caused by spatial dispersion. This method can be applied for a study of strong-Coulomb-interaction systems which consist of vector and scalar fields which possess dispersion.

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[1)] Our parameter γ is connected with the dimensionless parameter α_F introduced by Fröhlich, which characterizes the interaction between the electron and the optical phonons, by the simple relation

$$\gamma=\alpha_F\hbar^{1/2}\Omega_0^{1/2}(\hbar^2/2m^*a^2)^{-1/2}.$$

For crystals of the NaCl, NaI type ($\Omega\approx 5\times10^{13}$ Hz, $a=5\times10^{-8}$ cm, $m^*\approx 3m$, $\alpha_F\approx 9$) we have $\gamma\approx 0.8\alpha_F\approx 7.2$.

[1]A. Scott, F. Y. F. Chu, and D. W. McLaughlin, Proc. IEEE **61**, 1443 (1973).
[2]I. E. Dzyaloshinskiĭ and B. A. Ivanov, Pis'ma Zh. Eksp. Teor. Fiz. **29**, 592 (1979) [JETP Lett. **29**, 540 (1979)].
[3]C. Rebbi, Sci. Am. **240**, Nr 2, 76 (1979).
[4]N. L. Bogolyubskiĭ, Teor. Mat. Fiz. **43**, 378 (1980).
[5]V. E. Zakharov, Zh. Eksp. Teor. Fiz. **62**, 1745 (1972) [Sov. Phys. JETP **35**, 908 (1972)].
[6]V. I. Petviashvili, in Nelineĭnye volny (Non-linear waves), Nauka, Moscow, 1979, p. 5.
[7]L. D. Landau, Collected Papers, Vol. 1, Nauka, Moscow, 1969, p. 90; Phys. Z. Sowjetunion **3**, 664 (1933) [Collected Papers of L. D. Landau, Pergamon, Oxford, 1965, p. 67].
[8]S. I. Pekar, Zh. Eksp. Teor. Fiz. **16**, 335 (1946).
[9]S. I. Pekar, Issledovaniya po elektronnoĭ teorii kristallov (Studies in the electron theory of crystals) Gostekhizdat, Moscow, 1951 [German translation published by Akademie Verlag, Berlin; English translation published as US AEC Report AEC-tr-5575 (1963)].
[10]L. D. Landau and S. I. Pekar, Zh. Eksp. Teor. Fiz. **18**, 419 (1948) [Collected Papers of L. D. Landau, Pergamon, Oxfor, 1965, p. 478].
[11]N. N. Bogolyubov, Ukr. Mat. Zh. **2**, 3 (1950).
[12]S. V. Tyablikov, Zh. Eksp. Teor. Fiz. **21**, 377 (1951).
[13]E. Gross, Ann. Phys. **99**, 1 (1976).

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