SOLITON SOLUTIONS IN POLARON THEORY

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Solutions are found that correspond to different states of a particle interacting with a quantum field in an ionic crystal.

The motion of an electron in an ionic crystal is described by the Hamiltonian

$$H = H_p + H_v + H_{\text{int}}, \quad H_p = -\frac{\hbar}{2\mu}\Delta_r, \quad H_v = \frac{1}{2}\sum \hbar\omega\left(b_f b_f^+ + b_f^+ b_f\right),$$
$$H_{\text{int}} = \sum_f \left\{u_f e^{i(fr)} b_f + u_f^* e^{-i\{fr\}} b_f^+\right\}, \quad u_f = \frac{e}{|f|}\sqrt{\frac{2\pi\hbar\omega c}{V}}, \qquad 1$$

where ω is the frequency of the optical phonons, c is a constant, e is the electron charge, V is the volume, and r is the electron coordinate.

The case of weak coupling of the electrons to the field of the optical phonons, when H_{int} can be treated in perturbation theory, was considered for the first time in [1]. The case of strong coupling, when H_{int} cannot be treated as a perturbation, was first considered in [2]. This paper gives a semiclassical theory of the motion of an electron in an ionic crystal, the electron being treated quantum mechanically but the field classically. A consistent solution of the quantum problem (I) in the case of strong interaction of the particle with the field was given in [3] on the basis of the adiabatic approximation with allowance for the translational degeneracy of the Hamiltonian (1). In the zeroth approximation, the wave equation has the form [3] $(H\text{-}E)\psi=0$ $\psi=e^{(i/\hbar)(pq)}\psi(\bar{\lambda})\tilde{\theta}(\ldots Q_f\ldots)$, $p=-i\hbar\partial/\partial\mathbf{q}$, where $\boldsymbol{q}$ is the part of $\mathbf{r}$ corresponding to uniform rectilinear motion, λ is the fluctuating part of r, and Q_f are the field coordinates. For $\varphi(\lambda)$, the following equation was obtained in [3]:

$$\left(-\frac{\hbar^2}{2\mu}\Delta_{\bar{\lambda}} + U(\bar{\lambda}) - W\right)\varphi(\bar{\lambda}) = 0, \qquad U(\bar{\lambda}) = -\sum_f \frac{|u_f|^2}{2\omega}\int e^{i(f\bar{\lambda}) - i(f\bar{\lambda})}\left|\varphi(\bar{\lambda}_1)\right|^2 d\bar{\lambda}_1. \qquad (2)$$

In [2, 3], the lowest energy level of the particle in the quantum field was investigated. It is of interest to consider the other possible states of the particle in the field. Using the equation $\frac{1}{|\bar{\lambda}|} = \frac{1}{2\pi^2}\int \frac{e^{-i(f\bar{\lambda})}}{f^2} df$ we can rewrite the integro-differential equation (2) in the form

$$\frac{\hbar^2}{2\mu}\Delta_{\bar{\lambda}}\varphi + e\Pi(\bar{\lambda})\varphi + W\varphi = 0, \qquad \Delta_{\bar{\lambda}}\Pi + 4\pi c e\varphi^2 = 0. \qquad (3)$$

We shall seek spherically symmetric solutions of the system (3). We go over in (3) to the new variables

$$\varphi(\bar{\lambda}) = \frac{|W|}{e\hbar}\sqrt{\frac{\mu}{2\pi c}}\, y(x), \qquad \Pi(\bar{\lambda}) = \frac{|W|}{e} z(x), \qquad |\bar{\lambda}| = \frac{\hbar}{\sqrt{2\mu|W|}}\, x. \qquad (4)$$

Substituting (4) in (3), we obtain the following system of differential equations in dimensionless variables:

$$y'' + \frac{2}{x}y' + zy - y = 0, \qquad z'' + \frac{2}{x}z' + y^2 = 0\,. \tag{5}$$

with the boundary conditions

$$y'(0) = z'(0) = 0, \qquad y(\infty) = z(\infty) = 0. \tag{5'}$$

From the normalization condition $\int \left|\varphi(\overline{\lambda})\right|^2 d\overline{\lambda} = 1$ for the wave function we obtain for the electron energy the expression

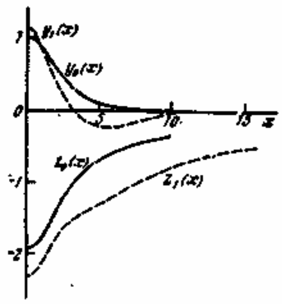

Fig. 1

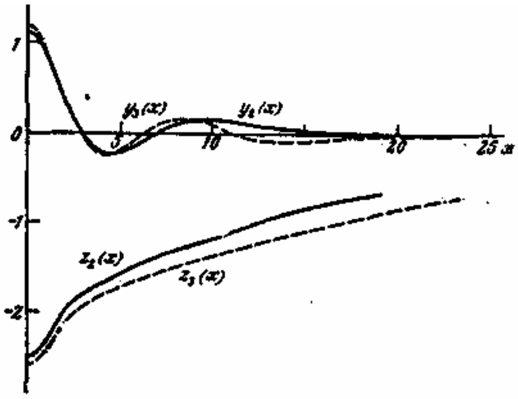

Fig. 2

$$W = -2\Gamma^{-2}\frac{e^4c^2\mu}{\hbar^2}, \qquad \Gamma = \int y^2x^2dx. \tag{6}$$

Solutions of the system of equations (5) with the boundary conditions (5') can be found numerically on a computer. The method to be used is described in [4]. First, one writes down power expansions for a family of solutions of the system (5) near x = 0 satisfying only some of the conditions (5') for x = 0. The family of such solutions depends on two parameters. Specifying their values, one can solve numerically the Cauchy problem on the given interval $[0, x_f]$. For the system (5), one can analyze how a given solution behaves as $x \to \infty$. It was found that there exist different values of the parameters for which the conditions (5') are satisfied as $x \to \infty$. These values of the parameters (and the solutions to the Cauchy problem for the ordinary differential equations corresponding to them) can be found to a given accuracy on a computer. In Figs. 1 and 2, we show four solutions describing different states of the electron. In the general case for the (n+1)-*th* solution (n-*th* mode) $y_n(x)$ intersects the x axis n times. The solutions can be readily reconstructed if y(0) and z(0) for them are given. For the zeroth and first mode (Fig.1): $y_0(0)=1.021$, $z_0(0)=-1.938$ and $y_1(0)=1.091$, $z_1(0)=-2.320$; for the second and the third mode (Fig.2): $y_2(0)=1.118$, $z_2(0)=-2.502$ and $y_3(0)=1.13$, $z_3(0)=-2.61$. Note that the case n=0 corresponds to the one considered in [2]. The agreement is very good. The deviation of our solution for the zeroth mode from the solution found by Pekar by the direct variational method does not exceed $1\cdot10^{-3}$ in absolute magnitude. For the first four modes we obtain $\Gamma_0=3.5052$, $\Gamma_1=8.060$, $\Gamma_2=12.66$, $\Gamma_3=17.24$.

We calculate the effective masses of the particles in the states we have found. The effective mass of a particle in the ground state was calculated for the first time by Landau and Pekar in [5]. The expression obtained in [5] for the effective mass is valid for any nondegenerate state. Therefore, the effective mass of an electron in state n is

$$M_n = \frac{1}{3\omega^2 c}\left[\int_0^\infty \left(\frac{d^2\Pi_n}{d|\bar{\lambda}|^2}\right)^2 |\bar{\lambda}|^2 d|\bar{\lambda}| + \int_0^\infty \left(\frac{d\Pi_n}{d|\bar{\lambda}|}\right)^2 d|\bar{\lambda}|\right]. \tag{7}$$

Going over in (7) to the dimensionless variables (4), we obtain instead of (7) the expression

$$M_n = 32\mu / 3\Gamma_n^5, \qquad L_n = \int y_n^4 x^2 dx, \tag{8}$$

where $\alpha = \frac{e^2 c}{\hbar}\sqrt{\frac{\mu}{2\hbar\omega}}$ is the electron-phonon coupling constant. For the first four modes, we have L=1.1264, L_1=0.969, L_2=0.873, L_3=0.81. It follows from (8) that for $\Gamma_n^5 L_n^{-1} > 32/3\alpha^4$ the effective mass M_n of the "dressed" particle becomes less than the "bare" mass μ. For example, for coupling constant б=8.9 (NaCl) the polaron mass is in accordance with (8) already less than the electron mass μ for n=2.

We are grateful to E. E. Shnol' for discussing the questions considered in this paper and to K. M. Borisyuk for assistance in the numerical calculations.

We are particularly grateful to A. M. Molchanov for pointing out to us the asymptotic Hamiltonicity of some types of differential equations.

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