New method of finding dynamic solutions in the Peierls model

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(Submitted 16 February 1988)
Zh. Eksp. Teor. Fiz. **94**, 344–354 (July 1988)

We develop a new and more lucid method of finding dynamic solitons in quasi-one-dimensional metals in the Peierls limits. The method yields, in addition to the known soliton and polaron solutions, also breather-type solutions and solutions that are not related at all to changes of the electron spectrum.

We investigate here a nonstationary continual model of a Peierls dielectric (PD). By using a unified approach[1] we not only account for the heretofore known solutions (soliton, polaron, bipolaron), but also obtain a new solution that has no stationary analog. A remarkable feature of the proposed method is that it avoids the algebraic-geometric approach to the spectral theory of periodic operators.[2]

The determination of finite-gap potentials of a number of equations is the subject of an extensive literature (as applied to continual PD models see, e.g., Ref. 2). The periodic (Bloch) wave functions and potentials are fully determined by specifying the beginnings $E_1, \ldots, E_{2q+1}$ and the ends $E_2, \ldots, E_{2q+1}$ of the band gaps. The band boundaries define a Riemann surface that is equivalent to a sphere with q "handles" (where the number of handles corresponds to the number of solitons[1]). It was shown earlier in Ref. 2 that to solve the problem of spin excitations it is necessary to use doubly-periodic solutions ($q=2$) superimposed on a periodic structure. The second period l_2 appears in the lattice deformation as a result of the onset of a spin moment m in the system. The formation of the new period l_2 is due to splitting off of a pair of additional bands in the electron spectrum. They appear in the forbidden bands $E_- < |E| < E_+$, one of them being empty and all the states of the other ν-fold filled by particles with polarized spin. The excittion spectrum was investigated in the limit $m \to 0$ corresponding to $l_2 \to 0$ (i.e., the order q of the Riemann surface Γ decreases as a result of the collapse of the additional bands). The method proposed by us permits, in contrast, e.g., to Refs. 2 and 3, a complete analysis of the nonstationary continual model of a PD without resorting to the finite-gap integration formalism.

We proceed now to an exposition of our model. Assuming the electron spectrum to be linear near the Fermi surface, we can express the Lagrangian of the nonstationary Peierls model in the adiabatic approximation in the form

$$\mathscr{L} = i\int d\Gamma\left\{\psi^+ \frac{\partial}{\partial t}\psi - \psi^+\sigma_3\frac{\partial}{\partial x}\psi + \psi^+(\sigma_-\Delta^* - \sigma_+\Delta)\psi\right\}$$
$$-\lambda|\Delta|^2 - \lambda_2\left|\frac{\partial\Delta}{\partial x}\right|^2 + \mu\left|\frac{\partial\Delta}{\partial t}\right|^2$$
$$-i\lambda_1\left(\Delta^*\frac{\partial\Delta}{\partial x} - \Delta\frac{\partial\Delta^*}{\partial x}\right) - \frac{1}{2}\lambda_3|\Delta|^4, \qquad (1)$$

where the terms in the curly brackets constitute the energy of the electron subsystem, and the remaining terms the energy of the lattice subsystem; $\psi^+ = (\psi_1^*, \psi_2^*)$ is a two-component Dirac spinor; $\sigma_\pm = 1/2(\sigma_1 \pm i\sigma_2)$, σ_k are Pauli matrices; λ, $\lambda_1, \lambda_2, \lambda_3, \mu$ are constants whose values are determined from experiment; $d\Gamma = \nu L dp/2\pi\langle\psi^+\psi\rangle_x$ is the density of states, ν the multiplicity of electron-band filling, L the length of the system, dp the differential of the quasimomentum, and $\langle\ldots\rangle_x$ denotes averaging over x.

Varying (1) with respect to ψ^+ we obtain the equations

$$\frac{\partial}{\partial t}\psi - \sigma_3\frac{\partial}{\partial x}\psi + [\sigma_-\Delta^*(x,t) - \sigma_+\Delta(x,t)]\psi = 0. \qquad (2)$$

Varying (1) with respect to Δ^* we obtain the self-consistency equations

$$i\int d\Gamma\,\psi^+\sigma_-\psi = \lambda\Delta - \mu\frac{\partial^2\Delta}{\partial t^2} + \lambda_2\frac{\partial^2\Delta}{\partial x^2} + 2i\lambda_1\frac{\partial\Delta}{\partial x} + \lambda_3\Delta|\Delta|^2. \qquad (3)$$

To find the soliton solution of Eqs. (2) with the self-consistency conditions (3), we use a generalization of the method proposed in Ref. 1. The integrable potentials of Eqs. (2) are taken to mean such $\Delta(x,t)$ for which Eqs. (2) have solution of the form (see Ref. 1)

$$\psi(x,t,k) = \left\{r_\infty + \sum_{i=0}^{N}\frac{r_i(x,t)}{k-\varkappa_i}\right\}\exp\left[i\left(kz_+ + \frac{z_-}{k}\right)\right], \qquad (4)$$

where $|\varkappa_0|^2 = 1$, $z_\pm = 1/2(t \pm x)$ (r_∞ is defined below).

To construct integrable potentials, we specify a set of different complex numbers $\varkappa_1, \varkappa_2, \ldots, \varkappa_N, c_{ij}$ $(i,j = 1, \ldots, N)$ that play the role of the construction parameters. Given the parameters, it is possible to determine the function (4) of k, stipulating that its residues with respect to k satisfy the following conditions:

$$i\operatorname*{res}_{\varkappa_i}\psi(x,t,k)(k-\varkappa_0)(k-\varkappa_0^*)\frac{1}{k^2} = \sum_{j=1}^{N}c_{ij}\psi(x,t,\varkappa_j^*). \qquad (5)$$

Note that (5) corresponds to the conditions for the collapse of the additional bands in the finite-band approach.[2]

We denote by $\psi(x,t,k)$ a function having the form (4), satisfying the condition (5), and so normalized that $r_\infty = 1$, $\psi_1(0) = 0$:

$$\psi_1(x,t,k) = \left\{\frac{k}{k-\varkappa_0} + \sum_{i=1}^{N}\frac{\tilde{r}_i(x,t)k}{(k-\varkappa_i)(k_0-\varkappa_0)}\right\}\exp\left[i\left(kz_+ + \frac{z_-}{k}\right)\right]. \qquad (6)$$

We normalize similarly $\psi_2(x,t,k)$ by the condition $r_\infty = 0$, $\psi_2(0) = 1$:

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$$\psi_2(x,t,k)=\left\{-\frac{\varkappa_0}{k-\varkappa_0}+\sum_i^N\frac{\tilde{r}_i(x,t)k}{(k-\varkappa_i)(k-\varkappa_0)}\right\}\times\exp\left[i\left(kz_+ +\frac{z_-}{k}\right)\right]. \quad (7)$$

Since the functions (6) and (7) must satisfy (2), we obtain for the potentials $\Delta(x,t)$ and $\Delta^*(x,t)$

$$\Delta(x,t)=\frac{i}{\varkappa_0}\left\{-1+\sum_j\frac{\tilde{r}_j(x,t)}{\varkappa_j}\right\},\ \Delta^*(x,t)=i\left\{\varkappa_0-\sum_j\tilde{\tilde{r}}_j(x,t)\right\}.$$

We formulate now without proof the necessary and sufficient conditions under which the function (4) has no singularities.[1] Let the construction parameters $\varkappa_1,\ldots,\varkappa_N$, c_{ij}, which specify together with the conditions (5) the functions $\psi(x,t,k)$, meet the following requirements.

1. The matrix c_{ij} is Hermitian, $c_{ij}=c_{ij}^*$.

2. We number the points $\varkappa_1,\ldots,\varkappa_N$ such that $\operatorname{Im}\varkappa_i>0$, $i=1,\ldots,p$; $\operatorname{Im}\varkappa_i<0$, $i=p+1,\ldots,N$. We require that the Hermitian matrix c_{ij}, $1\leqslant i,j\leqslant p$ be non-positive-definite, and the Hermitian matrix c_{ij}, $p+1\leqslant i,j\leqslant N$ be non-negative-definite. The function (4) with $k\neq\varkappa_i$ has then a smooth dependence on x and t and is an eigenfunction for the operator (2) with a smooth potential and with a zero eigenvalue.

The integrable potential $\Delta(x,t)$ specified within the framework of our construction by the parameters $\varkappa_1,\ldots,\varkappa_N$ together with the $N\times N$ matrix c_{ij} will be called the N-soliton potential.

It is easy to note that the constructed function of form (4) has, besides the poles at the points $k=\varkappa_i$ $(i=1,\ldots,N)$, have also singularities at $k=0$ and $k=\infty$. In the vincinity of the point $k=\infty$ the functions $\psi(x,t,k)$ defined by (6) and (7) can be represented in the form

$$\psi_1(x,t,k)=\left\{1+\sum_{s=1}^{\infty}\xi_s^{11}(x,t)k^{-s}\right\}\exp(ikz_+),$$
$$\psi_2(x,t,k)=\left\{\sum_{s=1}^{\infty}\xi_s^{21}(x,t)k^{-s}\right\}\exp(ikz_+). \quad (8)$$

The expansions at the point $k=0$ have analogously the form

$$\psi_1(x,t,k)=\left\{\sum_{s=1}^{\infty}\xi_s^{12}(x,t)k^{s}\right\}\exp\left(i\frac{z_-}{k}\right),$$
$$\psi_2(x,t,k)=\left\{1+\sum_{s=1}^{\infty}\xi_s^{22}(x,t)k^{s}\right\}\exp\left(i\frac{z_-}{k}\right). \quad (9)$$

For the quantities $\xi_1^{kl}(x,t)$ we obtain with the aid of (8), (9), and (2)

$$i\xi_1^{21}=-\Delta^*(x,t),\quad \partial_-\xi_1^{11}=i(|\Delta|^2-1),$$
$$i\xi_{s+1}^{21}+\partial_+\xi_s^{21}=-\Delta^*(x,t)\xi_s^{11},\quad i\xi_1^{12}=\Delta(x,t),$$
$$\partial_+\xi_1^{22}=i(|\Delta|^2-1),\quad i\xi_{s+1}^{12}+\partial_-\xi_s^{12}=\Delta(x,t)\xi_s^{22},$$
$$s=1,2,\ldots, \quad (10)$$

where we have introduced the symbol $\partial_\pm=(\partial/\partial t\pm\partial/\partial x)$. Relations (10) serve as the basis for the construction of the solutions of (2) with self-consistency equations (3).

Before proceeding with their derivation, we formulate a statement which we shall need hereafter. Let the parameters $\varkappa_i$, $\varkappa_i^*$, and c_{ij} satisfy the above conditions that guarantee non-singularity of $\Delta(x,t)$; then

$$\delta(x-y)=\int_{\Lambda_-}^{\Lambda_+}d\Omega\,\psi_1(x,t,k)\psi_2^+(y,t,k)-2\pi\sum_{i=1}^{N}c_{ii}\psi_1(x,t,\varkappa_i^*)\psi_2^*(y,t,\varkappa_i^*), \quad (11)$$

where

$$\psi^+(x,t,k)=\psi^*(x,t,k^*),\qquad d\Omega=\frac{dk}{k^2}(k-\varkappa_0)(k-\varkappa_0^*).$$

We consider now an integral along the contour $\partial\Gamma$ drawn around the cut from Λ_- to Λ_+ in the k-plane:

$$\oint_{\partial\Gamma}E(k)\psi_1\psi_2^+\,d\Omega.$$

Here $E(k)$ is a function equal to

$$E(k)=\ln\frac{k-\Lambda_+}{k-\Lambda_-}+\gamma+\gamma_1k+\frac{\gamma_2}{k}+\gamma_3k^2, \quad (12)$$

where γ, γ_1, γ_2, and γ_3 are constants. We apply the residue theorem to the above contour integral. The self-consistency conditions take then, with the aid of (11), the form

$$\int_{\Lambda_-}^{\Lambda_+}d\Omega\,\psi_1\psi_2^+=\gamma(\xi_1^{12}+\gamma_1^{*21})+\gamma_1(\xi_2^{*21}+\xi_1^{*21}\xi_1^{11})+\gamma_2(\xi_2^{12}+\xi_1^{12}\xi_1^{*22})+\gamma_3\xi_1^{*21}+\gamma_3(\xi_3^{*21}+\xi_2^{*21}\xi_1^{11}+\xi_1^{*21}\xi_2^{11}), \quad (13)$$

$$E(\varkappa_m^*)-E(\varkappa_n)=i\pi(\nu_m-n_0)\delta_{nm}, \quad (14)$$

where ν_m are the occupation factors of the mth local level $(0\leqslant\nu_m\leqslant2)$, and n_0 is an arbitrary integer (the phase of the complex value logarithm). We have assumed in the derivation of (14) that the electron band is completely filled $(\nu=2)$. The quantities $\xi_s^{kl}(x,t)$ are defined in (10):

$$\xi_2^{*21}+\xi_1^{*21}\xi_1^{11}=-\partial_+\Delta(x,t),\quad \xi_2^{12}+\xi_1^{12}\xi_1^{*22}=\partial_-\Delta(x,t),$$
$$I_3=\xi_3^{*21}+\xi_2^{*21}\xi_1^{11}+\xi_1^{*21}\xi_2^{11}=i\partial_+^2\Delta+\Delta\partial_+\xi_1^{11}-i\Delta(\xi_2^{*11}+\xi_2^{11}+\xi_1^{11}\xi_1^{*11}).$$

It is impossible in the general case to obtain for I_3 an expression that depends only on $\Delta(x,t)$ and its derivatives. Such an expression will be obtained later on, since its derivation calls for additional information on the solutions themselves.

We confine ourselves in the present paper to solutions of Eqs. (2) with condition (3), constructed with the aid of a 2×2 matrix c_{ij} (i.e., $N\leqslant2$), with the aid of the parameters $\varkappa_i$, $\varkappa_i^*(i=1,2)$. Leaving out the straightforward but cumbersome manipulations, we present directly the final expression:

$$\Delta(x,t)=-i\left[1+A_{11}\left(\frac{\varkappa_1^*}{\varkappa_1}\right)+A_{22}\left(\frac{\varkappa_2^*}{\varkappa_2}\right)+A_{12}\left(\frac{\varkappa_2^*}{\varkappa_1}\right)+A_{21}\left(\frac{\varkappa_1^*}{\varkappa_2}\right)+A\left(\frac{\varkappa_1^*\varkappa_2^*}{\varkappa_1\varkappa_2}\right)\right]\Big/\varkappa_0(1+A_{11}+A_{22}+A_{12}+A_{21}+A), \quad (15)$$

in which the following notation is introduced:

$$A_{11}=\frac{ic_{11}|\varkappa_1|^2\exp[i(\omega_1^*-\omega_1)]}{(\varkappa_1^*-\varkappa_1)(\varkappa_1^*-\varkappa_0)(\varkappa_1-\varkappa_0^*)},\quad A_{22}=\frac{ic_{22}|\varkappa_2|^2\exp[i(\omega_2^*-\omega_2)]}{(\varkappa_2^*-\varkappa_2)(\varkappa_2^*-\varkappa_0)(\varkappa_2-\varkappa_0^*)},$$

$$A_{12}=\frac{ic_{12}\varkappa_1\varkappa_2^*\exp[i(\omega_2^*-\omega_1)]}{(\varkappa_2^*-\varkappa_1)(\varkappa_2^*-\varkappa_0)(\varkappa_1-\varkappa_0^*)},\quad A_{21}=\frac{ic_{21}\varkappa_1^*\varkappa_2\exp[i(\omega_1^*-\omega_2)]}{(\varkappa_1^*-\varkappa_2)(\varkappa_1^*-\varkappa_0)(\varkappa_1-\varkappa_0^*)},$$

$$A=\frac{(c_{11}c_{22}-c_{12}c_{21})|\varkappa_1|^2|\varkappa_2|^2(\varkappa_1-\varkappa_2)(\varkappa_1^*-\varkappa_2^*)\exp[i(\omega_1^*-\omega_1+\omega_2^*-\omega_2)]}{(\varkappa_1^*-\varkappa_1)(\varkappa_2^*-\varkappa_2)(\varkappa_1^*-\varkappa_0)(\varkappa_1-\varkappa_0^*)(\varkappa_2^*-\varkappa_0)(\varkappa_2-\varkappa_0^*)(\varkappa_1^*-\varkappa_2)(\varkappa_2^*-\varkappa_1)},$$

$$\omega_i=(\varkappa_i+1/\varkappa_i)t+(\varkappa_i-1/\varkappa_i)x,\quad \omega_i^*\equiv\omega_i(\varkappa_i^*). \tag{16}$$

As the first example, we consider a solution of the kink type. Such a solution is obtained in the framework of our construction with the aid of the parameters $\varkappa_1$, $\varkappa_1^*$, and c_{11} [where $\varkappa_1$ is of the form $\varkappa_1=\rho\exp(i\varphi)$]. To be specific, we assume that $\operatorname{Im}\varkappa_1>0$, and then $c_{11}<0$. Without loss of generality, we choose φ in the interval $\langle 0,\pi/2\rangle$. After some calculations, expression (15) for $\Delta(x,t)$ takes the form

$$\Delta(x,t)=-i\Delta_0\cos\varphi+\Delta_0\sin\varphi\,\mathrm{th}[\alpha_s(x-\bar{x}-v_st)]. \tag{17}$$

Here

$$\bar{x}=-\frac{1}{2\alpha_s}\ln\left|\frac{c_{11}\rho}{2\sin\varphi(\rho^2+1+2\rho\cos\varphi)}\right|,\quad \alpha_s=\frac{\Delta_0\sin\varphi}{(1-v_s^2)^{1/2}},$$

$\bar{x}$ is an arbitrary parameter that describes the center of the soliton, and Δ_0 is the solution of (2) in the case of homogeneous PD (it corresponds to the limit $\varphi=0$). The soliton velocity v_s is connected with the modulus of the parameter $\varkappa_1$ by the relation $v_s=(\rho^2-1)/(\rho^2+1)$.

The self-consistency equations (14) reduce to the following:

$$\varphi+(\gamma_2/\rho-\gamma_1\rho)\sin\varphi-\gamma_3\rho^2\sin 2\varphi=\pi(\nu_1-n_0)/2, \tag{18}$$

where ν_1 is the occupation factor of the local level ($\nu_1=1,2,3$), and n_0 is an arbitrary integer.

Equation (18) does not have solutions for arbitrary values of n_0. The admissible values of n_0 are simplest to determine if the constants γ_1, γ_2, and γ_3 are set equal to zero. It follows then from (18) that for a solution $\varphi[\varphi\in(0,\pi/2)]$ to exist, n_0 must take on values -1, 0, and 1 for $\nu_1=0,1,2$, respectively. (We have discarded the value $\varphi=0$, since it corresponds to the homogeneous case.)

We consider now Eq. (18). We denote $\gamma_1\rho-\gamma_2/\rho$ by γ_4. We have then, depending on the values of $\gamma_3\rho^2$ and γ_4, the following possibilities:

1. $\gamma_3\geqslant 0$, $\gamma_4\geqslant 0$. This case is special, inasmuch as for any value of the constants there exists only the solution $\varphi=\pi/2$ [the real $\Delta(x,t)$, which coincides with the solution obtained by Brazovskiĭ and Kirova[3] in the weak-binding limit]. In the remaining cases listed below, except $\varphi=\pi/2$, there can exist also other solutions of Eq. (18).

2. $\gamma_3<0$, $\gamma_4<0$ or $\gamma_3>0$, $\gamma_4<0$. For given signs of the constants there exists always a solution of Eq. (18), in the limit of both weak and tight binding.

3. $\gamma_3<0$, $\gamma_4>0$. A solution exists only for $|\gamma_3|^2\rho>\pi/4+\gamma_4/\sqrt{2}$ (i.e., the tight-binding limit).

The self-consistency equation (13) takes the form

$$\int_{\Lambda_-}^{\Lambda_+}d\Omega\,\psi_1\psi_2^+=-i\Delta(x,t)(\gamma+\gamma_3)-\gamma_1\partial_+\Delta+\gamma_2\partial_-\Delta+\gamma_3I_3. \tag{19}$$

Using the connnection between the derivatives of $\Delta(x,t)$ with respect to ∂_+ and ∂_-, we obtain for I_3

$$I_3=i\partial_+^2\Delta(x,t)+i\Delta\frac{v_s-1}{v_s+1}\partial_-\xi_1^{11}-i\Delta(\xi_2^{*11}+\xi_2^{11}+\xi_1^{11}\xi_1^{*11}),$$

where v_s is the soliton velocity.

$$\beta(1-|\Delta|^2)+\alpha(1+I_2)=i\sum_{i,j}^{N}[F(\varkappa_i)-F(\varkappa_j^*)]\psi_1(\varkappa_j^*)\psi_1^*(\varkappa_i^*).$$

To determine $I_2=\xi_2^{*11}+\xi_2^{11}+\xi_1^{11}\xi_1^{*11}$ we use the following procedure. We specify a function $F=\alpha k+\beta/k$ (α and β are arbitrary constants) and consider the expression for $F_1\psi_1\psi_1^+\,d\Omega$. With the aid of the residue theorem, we get

We require now satisfaction of the equality $F(\varkappa_i)=F(\varkappa_j^*)$ ($i,j=1,2$), which makes it possible to determine the constants α and β. For a solution in the form (17) we have, after simple calculations

$$I_2=(|\Delta|^2-1)/\alpha-1,\quad \alpha=|\varkappa_1|^{-2}=(1+v_s)/(1-v_s)$$

or ultimately for I_3:

$$I_3=i\partial_+^2\Delta-2i\Delta|\Delta|^2(1-v_s)/(1+v_s)+i\Delta(3-v_s)/(1+v_s).$$

Having determined I_3, we can write the self-consistency equation (13) in the form

$$\int_{\Lambda_-}^{\Lambda_+}d\Omega\,\psi_1\psi_2^+=-2i\Delta(\gamma+\gamma_3)-{}^1/_2\gamma_1(1-v_s)\partial_x\Delta-{}^1/_2\gamma_2(1+v_s)\partial_x\Delta$$
$$-{}^1/_4i\gamma_3(1-v_s)^2\partial_x^2\Delta-2i\gamma_3\Delta|\Delta|^2(1-v_s)/(1+v_s).$$

Note that this equation determines the connection between the constants γ, γ_1, γ_2, γ_3 and the constants λ, λ_1, λ_2, λ_3, μ in the Lagrangian (1). It follows hence that no soliton solution of Eqs. (2) is possible in the case of arbitrary constants. It follows from the expressions above that are related by a strictly defined relation:

$$v_s=\pm[(\lambda_2-\lambda_3/2)/(\mu-\lambda_3/2)]^{1/2},$$

i.e., a soliton cannot be immobile at finite μ and λ. Our next task is to calculate the physical characteristics of a soliton moving with velocity v_s. It is known that the charge is determined with the aid of the equation

$$q=e\sum_n\psi_n^*\psi_n,$$

so that we must obtain explicit expressions for the wave functions. We use for this purpose expressions (6) and (7) for the ψ functions. We calculate first the wave functions of the continuous spectrum. In the case of physical interest $\varphi = \pi/2$ (i.e., $\varkappa_1 = i\rho$), the expressions for $\psi_1(x, t, k)$ and $\psi_2(x, t, k)$ take the form

$$\psi_1(x,t,k)=\frac{i\rho k}{(k-\varkappa_0)(k-i\rho)}\left\{\operatorname{th}[\alpha_s(x-\bar{x}-v_st)]-\frac{i}{\rho}k\right\}\times\exp\left[i\left(kz_++\frac{z_-}{k}\right)\right],$$

$$\psi_2(x,t,k)=\frac{\varkappa_0 k}{(k-\varkappa_0)(k-i\rho)}\left\{\operatorname{th}[\alpha_s(x-\bar{x}-v_st)]+i\frac{\rho}{k}\right\}\times\exp\left[i\left(kz_++\frac{z_-}{k}\right)\right].$$

For the discrete-spectrum wave functions (recall that $\omega_0 = 0$) we have for $\varphi = \pi/2$

$$\psi_1^{(0)}(x,t)=\frac{1}{2}\Delta_0^{1/2}\left(\frac{1-v_s}{1+v_s}\right)^{1/4}\operatorname{sech}[\alpha_s(x-\bar{x}-v_st)],$$
$$\psi_2^{(0)}(x,t)=\frac{1}{2}\Delta_0^{1/2}\left(\frac{1+v_s}{1-v_s}\right)^{1/4}\operatorname{sech}[\alpha_s(x-\bar{x}-v_st)].$$

Note that the wave functions are normalized by the condition

$$\int\{|\psi_1|^2-|\psi_2|^2\}dx=1.$$

Let the local electron density in the valence band be equal to $1/2\pi$ in the homogeneous state. In the presence of an inhomogeneous deformation (a kink), the change of the local charge density can then be written in the form

$$\Delta q(x,t)=e\nu_1 q_0(x,t)+e\sum_k\rho_k(x,t), \qquad (20)$$

where $q_0(x, t)$ is the contribution of the state with an occupation number ν_1, and $\rho_k(x, t)$ is the contribution of the continuum states. The total charge is equal to

$$q=\int d\xi\,\Delta q(\xi).$$

With the aid of (20) we obtain for the total charge of the soliton

$$q=e\left\{\nu_1-\frac{2}{\pi}\left[\operatorname{arctg}\left(\frac{\Lambda}{\sin\varphi}\left(\frac{1+v_s}{1-v_s}\right)^{1/2}\right)\right]\sin\varphi\right\},$$

i.e., the soliton can carry a non-integer electric charge.

As the next example, we consider a polaron (bipolaron) solution of Eqs. (2) with the self-consistency condition (3). To obtain such a solution within the framework of our construction, we must consider already a two-soliton case, i.e., $N=2$ in (15). Let the matrices c_{ij} ($c_{12}=c_{21}=0$) and two complex numbers $\varkappa_1$ and $\varkappa_2$ be given. We choose both numbers with positive imaginary part, and then $c_{11}<0$, $c_{22}<0$ so that $\varkappa_1=\rho\exp(i\varphi)$, $\varkappa_2=\rho\exp[i(\pi-\varphi)]$ (see Fig. 1a). With this choice of the parameters, the general expression for $\Delta(x, t)$ goes over after some calculations into the known equation

$$\Delta(x,t)=\Delta_0-k_0\left\{\tanh\frac{k_0(x+x_0-v_pt)}{(1-v_p^2)^{1/2}}-\tanh\frac{k_0(x-x_0-v_pt)}{(1-v_p^2)^{1/2}}\right\}. \qquad (21)$$

Here $k_0 = \Delta_0 \sin\varphi$ (the definitions of Δ_0 and φ are similar to

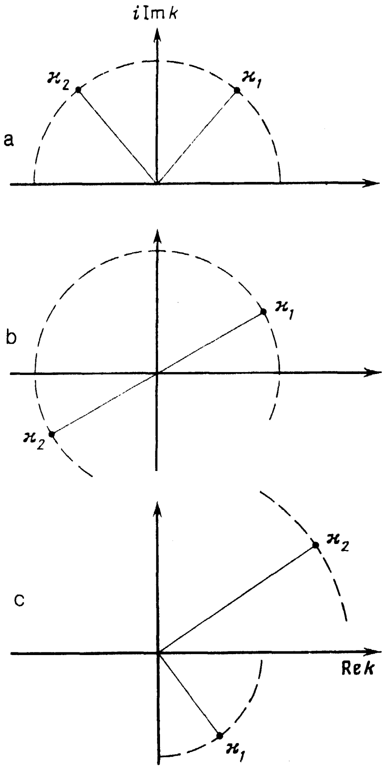

FIG. 1. Choice of the construction parameters $\varkappa_1$ and $\varkappa_2$: a—for a polaron-type solution (21), b—for solution (24), c—for solution (27).

those for the case of the soliton). The parameter x_0 is determined from the equation $k_0 = \Delta_0\tanh(2k_0x_0)$. In the derivation of (21) we have subjected c_{22}, for simplicity, to the additional condition $\bar{x}=0$ (i.e., the polaron has a center at the point $\bar{x}=0$), where

$$\bar{x}=\frac{1}{\alpha_p}\ln\left|\frac{c_{22}\rho\operatorname{ctg}\varphi}{2(\rho^2+1+2\rho\sin\varphi)}\right|,$$
$$\alpha_p=\frac{\Delta_0\sin\varphi}{(1-v_p^2)^{1/2}}.$$

The parameter ρ is connected with the polaron velocity by the relation $v_p = (\rho^2-1)/(\rho^2+1)$. If $x_0 \ll 1$ expression (21) describes a shallow polaron. If $x_0 \gg 1$, the solution (21) takes the form of two domain walls spaced $d \approx x_0$ apart.

We proceed now to a discussion of the self-consistency equations (3). Expression (21) satisfies Eq. (13) (just as in the case of a kink). The matching conditions (14) are in the case of a polaron

$$E(\varkappa_1^*)-E(\varkappa_1)=i\pi(\nu_1-n_0),$$
$$E(\varkappa_2^*)-E(\varkappa_2)=i\pi(\nu_2-n_0). \qquad (22)$$

Here ν_1 and ν_2 are the occupation numbers of the upper and lower discrete levels, respectively. Equations (22) are equivalent to the following equation (with the above choice of the parameters $\varkappa_1$ and $\varkappa_2$)

$$\varphi={}^1/_4\pi(\nu_1-\nu_2+2)+\gamma_3\rho^2\sin 2\varphi. \qquad (23)$$

The matching condition (23) is in a certain sense simpler than the condition (18) for a soliton (in the case of a polaron there is no dependence on the constants γ_1 and γ_2 and on the variable n_0). In the two-soliton case, however, there are now two possibilities:

1. $\nu_1 - \nu_2 = 1$, polaron-type solution.
2. $\nu_1 - \nu_2 = 0$, bipolaron-type solution.

Before we proceed to anlayze Eq. (23), we note that in the limit $\gamma_0 = 0$, i.e., $\varphi = \pi/4$, we obtain the known expression for a symmetric polaron.[3]

We consider thus first Eq. (23) for a polaron. It has a solution for any sign of the constant γ_3. In the case $\gamma_3 \rho^2 \gg 1$, i.e., as $\varphi \to \pi/2$, the polaron is unstable to decay into two domain walls (see, e.g., Ref. 2).

Let $\nu_1 = \nu_2$ be a solution of the bipolaron type. It follows from (23) that a solution exists only if $\gamma_3 \rho^2 < 0$, $|\gamma_3|\rho^2 > 1$ (i.e., only in the tight-binding limit). Note that for the discrete model of a PD this result was obtained in Ref. 4. For $\gamma_3 \rho^2 \ll 1$ (as $\varphi \to \pi/2$), the bipolaron decays into two domain walls.

We proceed now to consider the self-consistency equation (13). In the derivation of the equation for I_3 in terms of $\Delta(x,t)$, $\partial_x \Delta$, $\Delta|\Delta|^2$, we proceed just as in the case of a soliton. Leaving out these simple calculations, we note that the equation for I_3 is the same as for a soliton (in which v_s must now be substituted by the polaron velocity v_p). The restrictions on the constants γ_1, γ_2, and γ_3 are the same as in the case of the soliton.

Our next task is to calculate the physical characteristics of a slowly moving polaron. Since we shall proceed exactly as in the soliton case, we present as a rule only the final result. In contrast to the soliton, we have now two local levels $\pm\omega_0$ ($\omega_0 = \Delta_0 \cos\varphi$). For the wave functions of the discrete spectrum ($E = \omega_0$) we have

$$\psi_1^{(0)}(x,t) = \frac{iN_0}{\rho} \exp[i\theta_0(x,t)] \times \{(1+i)\operatorname{sech}\beta_+ + (1-i)\operatorname{sech}\beta_-\},$$

$$\psi_2^{(0)}(x,t) = iN_0 \exp[i\theta_0(x,t)]\{(1-i)\operatorname{sech}\beta_+ + (1+i)\operatorname{sech}\beta_-\},$$
$$\beta_\pm = \alpha_p(x \pm x_0 - v_p t).$$

Here $N_0 = \frac{1}{4}(k_0\rho)^{1/2}$ is a normalization constant. For the level $E = -\omega_0$ we have

$$\psi_{1-}^{(0)}(x,t) = -i\psi_2^{(0)}(x,t), \qquad \psi_{2-}^{(0)}(x,t) = i\psi_1(x,t).$$

Before we write down the continuum wave functions, we note that in the direct calculation of the physical characteristics of the polaron it is more convenient to change to true momentum variables $[p = \frac{1}{2}\Delta_0(k - 1/k)]$. Since this cannot lead to misunderstanding, we use the symbol k for the momentum. The wave functions ψ_1 and ψ_2 of the continuum are equal to

$$\psi_1(x,t,k) = \frac{iN_k}{\rho} \exp[i\theta_k(x,t)] \times \{A_- - \gamma_-(1+i)t_+ + \gamma_+(1-i)t_-\},$$

$$\psi_2(x,t,k) = -iN_k \exp[i\theta_k(x,t)] \times \{A_+ - \gamma_-(1-i)t_+ + \gamma_+(1+i)t_-\}.$$

Here

$$t_\pm = \operatorname{th}\beta_\pm, \quad \gamma_\pm = {}^1/_2 k_0\{1 \pm ik/(\omega_k - \Delta_0)\},$$
$$N_k = \frac{1}{2^{3/2}}\left\{\frac{(\omega_k-\Delta_0)(1+v_p)}{(\omega_k - kv_p)(k^2+k_0^2)}\right\}^{1/2},$$

$$\omega_k = (k^2+\Delta_0^2)^{1/2}, \qquad A_\pm = \omega_k + \Delta_0 \pm k.$$

We calculate now the local charge density corresponding to the contribution of the discrete level. Proceeding as in the soliton case, we have for $\rho_0(x,t)$

$$\rho_0(x,t) = \alpha_p(\operatorname{sech}^2\beta_+ + \operatorname{sech}^2\beta_-).$$

The contribution of the continuous spectrum is

$$\rho_k(x,t) = -\frac{k_0^2\omega_k}{4\pi(\omega_k - kv_p)(k^2+k_0^2)}(\operatorname{sech}^2\beta_+ + \operatorname{sech}^2\beta_-).$$

The change of the local charge density in the presence of the polaron deformation (21) is ultimately

$$\Delta\rho(x,t) = \alpha_p(\operatorname{sech}^2\beta_+ + \operatorname{sech}^2\beta_-) \times \Bigg\{\nu_1 + \nu_2 - \frac{4}{\pi}(1-v_p^2)^{1/2}\operatorname{arctg}\left(\frac{\Lambda}{\Delta_0\sin\varphi}\right) + \frac{4v_p^2\sin^2\varphi}{\pi[(1-v_p^2)\sin^2\varphi - 1]}\left[\frac{1}{\sin\varphi}\operatorname{arctg}\left(\frac{\Lambda(1-v_p^2)^{1/2}}{\Delta_0\sin\varphi}\right) - (1-v_p^2)^{1/2}\operatorname{arctg}\left(\frac{\Lambda}{\Delta_0\sin\varphi}\right)\right]\Bigg\}.$$

In the physically interesting case of trans-$(CH)_x$ ($\gamma_3 = 0$) we obtain for $\Delta \to \infty$, $v_p = 0$, and $\nu_2 = 2$ the well-known result of the static theory[2]:

$$\Delta\rho(x) = {}^1/_4\nu_1 k_0\{\operatorname{sech}^2[k_0(x+x_0)] + \operatorname{sech}^2[k_0(x-x_0)]\}.$$

The total charge is equal to $q = e\nu_1$. The case $\nu_1 = 2$ (doubly occupied level) corresponds to a soliton-antisoliton pair with large spacing between them. In the presence of one additional electron (or hole), the excitation carries a charge $q = \pm e$ and a spin 1/2. In the general case ($\gamma_3 \neq 0$) it follows from the equation for Δq that the charge can take on any value in the intervals $0 < q < e$ for the polaron and $0 < q < 2e$ for the bipolaron.

By way of a nontrivial example we consider the solution of Eqs. (2) in the case of an antidiagonal matrix c_{ij} ($c_{11} = c_{22} = 0$, $c_{12} = c_{21}^*$). Note that the solution obtained below is not a true soliton, for at the given choice of the matrix c_{ij} there is no contribution from the discrete spectrum. It follows from (15) that the solution $\Delta(x,t)$ will be nonsingular if the imaginary parts of $\varkappa_1$ and $\varkappa_2$ are different. For the sake of argument, we choose the parameters $\varkappa_1 = \rho\exp(i\varphi)$, $\varkappa_2 = \rho\exp[i(\pi+\varphi)]$ (see Fig. 1b). After some calculations, the general expression for $\Delta(x,t)$ takes the form

$$\frac{\Delta(x,t)}{\Delta_0}=1-\left[1+\left(\frac{\sin 2\varphi}{2}\right)^2\right]^{-1}$$
$$\times\left\{\left(\frac{\sin 2\varphi}{2}\right)^2\left[\cos 2\varphi+\frac{2}{\sin^2\varphi}\right]\cdot\right.$$
$$\left.+i\sin 2\varphi\left[\left(\frac{\sin 2\varphi}{2}\right)^2-1\right]\right\}$$
$$\times\left\{1+\left[\left(\frac{\sin 2\varphi}{2}\right)^2+1\right]^{-1}\sin\varphi\sin 2\varphi\right.$$
$$\left.\times i\,\mathrm{ch}\left[\frac{2\Delta_0\cos\varphi}{(v^2-1)^{1/2}}(x-vt)\right]\right\}^{-1}, \tag{24}$$

where $v=(\rho^2\pm 1)/(\rho^2-1)$ is the polaron velocity ($v^2-1>0$); the parameter φ is determined from the self-consistency equations (14); c_{12} is chosen such that A_{12} [see Eq. (16)] is equal to $\exp[i(\omega_2^*-\omega_1)]/\cos\varphi(A_{12}=A_{21}^*)$.

The solution (24) has the same value (Δ_0) as $x\to\pm\infty$, i.e., is indeed a polaron. Note that if φ is zero or $\pi/2$, the solution (24) goes over into the homogeneous one [$\Delta(x,t)=\Delta_0$].

The self-consistency equation (13) remains the same as in the case of a diagonal matrix c_{ij}, and only the matching conditions (14) are changed. In our case they are equal to

$$E(\varkappa_1^*)=E(\varkappa_2),\ E(\varkappa_2^*)=E(\varkappa_1) \tag{25}$$

where the function $E(k)$ is defined by Eq. (12). The equalities (25) are equivalent to the following conditions:

$$(\gamma_1\rho+\gamma_2/\rho)\cos\varphi=0,\quad \varphi=-\pi/2+\gamma_3\rho^2\sin 2\varphi. \tag{26}$$

For $\varphi\neq\pi/2$ we obtain from the first equation of (26) the connection $\gamma_1\rho^2=-\gamma_2$ between the constants, and from the second we get the condition $\gamma_3>0$ ($\gamma_3\rho^2>3\pi/4$). We put $\varphi=\pi/2-\delta$ ($\delta\ll 1$) and consider (24) in the vicinity of $\varphi=\pi/2$. Then, using the second equation of (26), we have in first order in δ,

$$\delta=\pi/\gamma_3\rho^2\ll 1.$$

It follows hence that such a solution exists for $\gamma_3\rho\gg 1$ (i.e., in the tight-binding limit). In this aproximation, the expression for $\Delta(x,t)$ ($\Delta=\Delta_{\mathrm{Re}}+i\Delta_{\mathrm{Im}}$ simplifies to:

$$\frac{\Delta(x,t)}{\Delta_0}=1-(\delta^2-2i\delta)\left\{1+\delta\,\mathrm{ch}\left[\frac{2\Delta_0\delta}{(v^2-1)^{1/2}}(x-vt)\right]\right\}^{-1}.$$

It follows from this expression for $\Delta(x,t)$ that the excitation constitutes a shallow well incapable of trapping particles. Taking into account the connection between the quantities δ,ρ, and v we obtain for the polaron width ξ the estimate

$$1/\xi\sim\delta(v^2-1)^{-1/2}\sim(v-1)^{1/2},$$

from which it follows that the well is very wide, and in the limit $v=1$ the solution (24) becomes homogeneous. In addition, we see that for such a well to exist it is necessary that it move faster than with the Fermi velocity v_F ($v_F=1$). This is in fact the difference (together with the aforementioned absence of a contribution from the discrete spectrum) from the usual polaron solution (21).

We proceed now to consider one more nontrivial example. We construct in the most general form a solution $\Delta(x,t)$ that does not reduce to a moving stationary solution, using the same matrix c_{ij} as in the preceding examples. We choose the parameters $\varkappa_1$ and $\varkappa_2$ in the form $\varkappa_1=\rho_1\exp(i\varphi_1)$, $\varkappa_2=\rho_2\exp(i\varphi_2)$, $\rho_1\neq\rho_2$ (see Fig. 1c). The expression obtained for $\Delta(x,t)$ in the case of different ρ_1,ρ_2,φ_1, and φ_2 is quite unwieldy. In addition, it is difficult to analyze the self-consistency equations (14) in this case. To simplify the subsequent calculations, we put therefore $\varphi_1=-\varphi$, $\varphi_2=\pi/2-\varphi$ (the parameter φ takes on values in the interval from zero to $\pi/2$). After straightforward but cumbersome calculations, expression (15) takes the form

$$\frac{\Delta(x,t)}{\Delta_0}=\{e^\sigma\,\mathrm{sh}[\mathrm{Im}(\omega_1+\omega_2)+\sigma+2i\varphi]$$
$$+i\,\mathrm{ch}[\varepsilon+i\,\mathrm{Re}(\omega_2-\omega_1)]\}$$
$$\times\{e^\sigma\,\mathrm{ch}[\mathrm{Im}(\omega_1+\omega_2)+\sigma]+\cos[\mathrm{Re}(\omega_2-\omega_1)]\}^{-1}, \tag{27}$$

where we have introduced the notation

$$\mathrm{Im}(\omega_1+\omega_2)=[(\rho_1+1/\rho_1)\sin\varphi-(\rho_2+1/\rho_2)\cos\varphi](x-v_1t),$$
$$\mathrm{Re}(\omega_2-\omega_1)=[(1/\rho_2-\rho_2)\sin\varphi-(1/\rho_1-\rho_1)\cos\varphi](x-v_2t),$$
$$v_1=\frac{(\rho_2-1/\rho_2)\cos\varphi-(\rho_1-1/\rho_1)\sin\varphi}{(\rho_2+1/\rho_2)\cos\varphi-(\rho_1+1/\rho_1)\sin\varphi},$$
$$v_2=\frac{(\rho_2+1/\rho_2)\sin\varphi-(\rho_1+1/\rho_1)\cos\varphi}{(\rho_2-1/\rho_2)\sin\varphi-(\rho_1-1/\rho_1)\cos\varphi},$$
$$e^{2\sigma}=2/\sin 2\varphi,\quad \varepsilon=\ln(\rho_2/\rho_1).$$

This choice of the parameters $\varkappa_1$ and $\varkappa_2$ ensures non-singularity of $\Delta(x,t)$.

The velocities v_1 and v_2 satisfy now the conditions $1-v_1^2>0$, $1-v_2^2<0$, i.e., just as in the preceding example, the velocity v_2 exceeds the Fermi velocity v_F. We obtain hence for the quantities Im ($\omega_1+\omega_2$) and Re ($\omega_2-\omega_1$)

$$\mathrm{Im}(\omega_2+\omega_1)=2\Delta_0(1-\mathrm{ch}\,\varepsilon\sin 2\varphi)^{1/2}(x-v_1t)(1-v_1^2)^{-1/2},$$
$$\mathrm{Re}(\omega_2-\omega_1)=2i\Delta_0(1-\mathrm{ch}\,\varepsilon\sin 2\varphi)^{1/2}(x-v_2t)(v_2^2-1)^{-1/2}.$$

To be specific, we consider hereafter only solutions for which $1-\cosh\varepsilon\sin 2\nu>0$. In view of the presence of the two velocities v_1 and v_2, the self-consistency equation (13) cannot be solved in the general case of arbitrary constants γ_1, γ_2, and γ_3. We confine ourselves therefore to the case $\gamma_1=\gamma_2$ and $\gamma_3=0$ [see (12)]. The matching conditions (14) are then

$$\ln(\rho_2/\rho_1)+\gamma_1(\rho_1+1/\rho_1)\cos\varphi-\gamma_1(\rho_2+1/\rho_2)\sin\varphi=0,$$
$$\pi/4-\varphi+{}^1/_2\gamma_1(1/\rho_2-\rho_2)\cos\varphi+{}^1/_2\gamma_1(\rho_1-1/\rho_1)\sin\varphi=0.$$

The equations reduce to the following:

$$\varphi=\pi/4+B\cos\varphi, \tag{28}$$

where

$$B=\frac{\gamma_1}{2}\left\{\frac{1}{\rho_2}-\rho_2+\frac{\rho_2(\rho_1^2-1)}{\rho_1(\rho_2^2+1)}\left[\frac{1}{\gamma_1}\ln\frac{\rho_2}{\rho_1}+\rho_1+\frac{1}{\rho_1}\right]\right\}.$$

A graphic analysis of Eq. (28) yields the conditions for the existence of a solution. In the case $B>0$, a solution exists in the interval ($\pi/4$, $\pi/2$). The points $\varphi=\pi/2$ and $\pi/4$ must be excluded, for at $\varphi=\pi/2$ the solution $\Delta(x,t)$ becomes $\Delta_0=\mathrm{const}$. Note that in the vicinity of the point $\varphi=\pi/4$ the conditions $1-v_1^2>0$, $1-v_2^2<0$ are no longer valid, i.e., there is no longer a solution in the form (27). For $B < 0$, the solution (28) exists only if $|B| < \pi/4$. The quantity φ itself lies in the interval $(0, \pi/4)$. For $\varphi = 0$ the solution $\Delta(x, t)$ is equal to Δ_0 (becomes homogeneous).

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Translated by J. G. Adashko