Influence of phonon dispersion on amplitude solitons and periodic structures in a Peierls-Fröhlich system

S. A. Brazovskiĭ and S. I. Matveenko

L. D. Landau Institute of Theoretical Physics, Academy of Sciences of the USSR, Chernogolovka, Moscow Province

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An investigation is reported of the influence of the dispersion of a phonon spectrum on the ground state and spin excitations of a charge density wave in the Peierls-Fröhlich model. States with split electron energy bands, of the kind predicted by the theory of many quasi-one-dimensional compounds (for example TaS_3), are considered as a problem of behavior of a system of this kind in a strong magnetic field. It is shown that these states form a soliton lattice with a half-filled central energy band. The dispersion of the phonon spectrum causes the soliton profile to deviate from the pure amplitude type and gives rise to a fractional local electric charge.

I. INTRODUCTION

It is known that the states in a Peierls insulator, which appear as a result of formation of charge density waves in quasione-dimensional substances, have many remarkable properties (for reviews see Refs. 1 and 2). Electron-hole excitations near the edges of the spectrum at $\pm\Delta$ are unstable and can be observed only in the optical absorption effects and in some transport phenomena. Stationary elementary excitations are solitons with anomalous quantum numbers. In the case of a doubly commensurate charge density wave formed in a metal with $\rho = 1$ electrons per atom there are zero-spin solitons with a charge $\pm e$ and uncharged solitons with a spin 1/2. If $\rho \neq 1$, the pattern of elementary excitations differs even more from the situation encountered in conventional semi-conductors. In this case there are no charge excitations with a gap and charge is transported only by the collective motion of charge density waves (Fröhlich conduction) and spin excitations are, as before, amplitude solitons with an energy $W_s = 2\Delta/\pi$ and zero charge.[3,4] These predictions are supported by the experimental results obtained for materials such as TaS_3 (Ref. 5). Compounds of this type are characterized by $\rho = 1/2$ and the energy of nonstationary electron excitations is $\Delta \approx 800$ K when the effective mass is $m^* = 0.01 m_e$, whereas the energy of spin excitations[6] is $\Delta' \approx 640$ K is qualitative agreement with the formula $W_s = 2\Delta/\pi$. The mass of a soliton is estimated to be $m_s \approx 5m^*$, which can be explained by the theoretical relationship[4]

$$m^*/m_s = \lambda\bar{\omega}^2/4\Delta^2,$$

where $\bar{\omega}$ is the frequency of photons with a wave vector $2k_F$ and λ is the dimensionless form of the electron-phonon interaction constant. It is important to note that at low temperatures the activation energy of the longitudinal conductivity $E_A \approx 200$ K is much less than the half-width of the band gap $\Delta \approx 800$ K, which can be explained by the small activation of the Frölich conduction process.

However, the interest in amplitude solitons is not simply confined to the problem of spin excitations. As pointed out briefly in Ref. 7, objects equivalent to amplitude spin solitons can appear in any system which exhibits weak splitting of the electron energy bands. In this case the splitting acts in the same way as a magnetic field and the quantity $m = n_1 - n_2$, where n_1 and n_2 are the electron densities in the split bands, is equivalent to the spin moment. This formulation of the problem is particularly appropriate to systems of the MX_3 type (where M = Nb, Ta; X = S, Se) that exhibit periodically modulated charge density waves ($NbSe_3$) or coexisting charge density waves with similar periods (TaS_3). The splitting of the electron energy bands appears either because of the inequivalence of the two types of conducting chains. In the latter case we can also expect a periodically modulated charge density wave formed by domain walls representing coalescence of spin solitons.[8,9]

It is therefore clear that there are several physical situations in which an important role is played by the existence either of a low-density gas or of a periodic structure of objects equivalent to amplitude spin solitons in the one-dimensional Peierls-Fröhlich model. Clearly, the physical properties of such systems depend strongly on whether solitons have an electric charge q_s. It was shown first in Ref. 3 that the spin soliton charge is zero in the simple Peierls-Fröhlich model applicable to systems with ρ far from the integers 0, 1, or 2. However, it was shown in Ref. 7 that the appearance of a small charge is possible because of the influence of the doubly commensurate point. As the value of ρ moves away from unity, the charge decreases as follows

$$q_s \propto e \exp(-2/\lambda)/(\rho-1)^2.$$

Another source of the soliton charge may be the phonon dispersion, as shown qualitatively in Ref. 4.

We shall investigate the influence of the phonon dispersion on the form of a periodic structure of spin solitons and of isolated solitons, and we shall find the magnitude and distribution of the electric charge due to the dispersion. In particular, we shall show that in the presence of the phonon dispersion a soliton is not purely of the amplitude type, i.e., the change in the phase of a charge density wave due to the passage of a soliton differs from π by an amount

$$\delta\varphi \approx 8\pi c\Delta/\bar{\omega}g^2, \quad \omega(2k_F+k) = \bar{\omega}+ck,$$

where c is the velocity of sound corresponding to $q = 2k_F$; $\bar{\omega} = \omega(2k_F)$; v_F is the Fermi velocity . An electron then acquires a charge related to the phase by[4] $q_s = e\delta\varphi/\pi$.

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By way of example, we shall consider a system consisting of two inequivalent conducting chains. The energy functional of the system is

$$W=W(\Delta_1)+W(\Delta_2)+A(\Delta_1\Delta_2^*+\Delta_2^*\Delta_1),$$

where $W(\Delta_i)$ are the energies of the individual chains given by Eq. (2) below; the last term allows for the interaction between the chains. We can readily show that in the case of a strong coupling between the chains, corresponding to $\pi v_F A \gg 1$, the deformations Δ_1 and Δ_2 are related by $\Delta_1 \approx -\Delta_2$. Therefore, a system of this kind is equivalent to a single chain subjected to a magnetic field, which is discussed below.

We shall now investigate a model describing the case of a strong coupling between the chains when the deformations are linked strictly by $\Delta_1(x)\equiv -\Delta_2(x)\equiv\Delta(x)$. We shall consider this limit in terms of the Peierls-Fröhlich problem in a magnetic field.

2. EXACT SOLUTION OF THE PERIODIC PROBLEM

We shall consider a system of noninteracting electrons in a deformable chain. The wave functions of the electrons and the lattice deformation can be described by

$$\begin{aligned}\psi(x)&=\psi_1(x)\exp(ip_Fx)+\psi_2\exp(-ip_Fx),\\ \varphi(x)&=g^{-1}[\Delta(x)\exp(2ip_Fx)+\Delta^*(x)\exp(-2ip_Fx)],\end{aligned}\tag{1}$$

where p_F is the Fermi momentum and g is the electron–phonon interaction constant ($\lambda=g^2/v_F$).

Any stationary state of the system can be found from the condition for an extremum of the energy functional of the system $W\{\Delta(x),\psi(x)\}$. If we assume that the electron spectrum near the Fermi surface is linear, we can find by analogy with Ref. 4 that

$$\begin{aligned}W\{\Delta(x),\psi_1(x),\psi_2(x)\}&=\int dx\Big\{\frac{|\Delta(x)|^2}{g^2}\\ &+\frac{c}{\bar\omega g^2}(-i)(\Delta^*\Delta'-\Delta'^*\Delta)\\ &+\sum_{E<\mu}-iv_F(\psi_1^*\psi_1-\psi_2^*\psi_2)+\Delta(x)\psi_1^*\psi_2+\Delta^*\psi_2^*\psi_1\Big\},\end{aligned}\tag{2}$$

where μ is the chemical potential and the prime denotes differentiation with respect of x. The first two terms in Eq. (2) represent the lattice deformation energy written down allowing for the phonon dispersion near $2p_F$.

Variation of Eq. (2) with respect to ψ_1 and ψ_2 gives the following equations for the eigenfunctions ψ_1 and ψ_2 corresponding to the energy E:

$$\hat H\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}=\begin{pmatrix}-i\dfrac{\partial}{\partial x} & \Delta(x)\\ \Delta^*(x) & i\dfrac{\partial}{\partial x}\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}=E\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix},$$
$$\psi_{1,2}=\psi_{1,2}(E,x).\tag{3}$$

Variation of Eq. (2) with respect to $\Delta(x)$ and $\Delta^*(x)$ gives the matching conditions

$$\sum_{E<\mu}\psi_1^*\psi_2+\frac{\Delta^*}{g^2}+\frac{2ic}{\bar\omega g^2}\Delta'^*=0,\tag{4a}$$

$$\sum_{E<\mu}\psi_1\psi_2^*+\frac{\Delta}{g^2}-\frac{2ic}{\bar\omega g^2}\Delta'=0.\tag{4b}$$

It readily follows from Eq. (3) that

$$J(E)=|\psi_1(x)|^2-|\psi_2(x)|^2$$

is independent of x. Eliminating $\psi_2(x)$ from Eq. (3), we obtain the following equation for $\psi_1(x)$:

$$-\psi_1''+\frac{\Delta'}{\Delta}\psi_1'-\frac{i\Delta'}{\Delta}E\psi_1=(E^2-|\Delta|^2)\psi_1\tag{5}$$

or

$$-i\tilde\chi'+\tilde\chi^2+\frac{i\Delta'}{\Delta}(\tilde\chi-E)=E^2-|\Delta|^2,\qquad \tilde\chi\equiv -i\psi_1'/\psi_1.\tag{6}$$

We shall describe the quasimomentum p for the function $\psi_1(x)$ by

$$p=\frac{1}{L}\int_0\tilde\chi(x)\,dx,\tag{7}$$

where L is the length of the system. In the vicinity of $E\to\infty$, Eq. (6) gives the following expansion for the quasimomentum p in powers of the energy E:

$$p=E-\frac{I_1}{E}-\frac{I_2}{E^2}-\ldots,\tag{8}$$

where

$$I_1=\frac{1}{L}\int\frac{|\Delta|^2}{2}dx,\qquad I_2=-\frac{i}{8L}\int(\Delta^*\Delta'-\Delta^{*\prime}\Delta)\,dx.$$

It should be noted that the lattice deformation energy in Eq. (2) can be written in the form

$$W_{ph}=\frac{2I_1}{g^2}+\frac{8c}{\bar\omega g^2}I_2.\tag{9}$$

We shall need later also a different form of Eq. (5). Making the substitution $\psi=\Delta^{1/2}(x)\,(x)$, we find from Eq. (5) that

$$-\varphi''+q\varphi=0,\tag{10}$$

$$q=-E^2-iE(\ln\Delta)'-{}^1/_2(\ln\Delta)''+{}^1/_4(\ln\Delta)'^2+|\Delta|^2.\tag{10a}$$

For a system of great length L we can, without loss of generality, introduce periodic boundary conditions for the function $\Delta(x)$. Then, a solution of Eq. (10) can be sought in the form of a Bloch function:

$$\Delta(x+L)=\Delta(x),\ \varphi(x+L)=e^{ipL}\varphi(x),\ \varphi(0)=1.$$

Following the method of finite-band potentials (see, for example, Ref. 10), we can obtain the expression for the function $\varphi(x)$ and for the variational derivative of the quasimomentum $\delta p/\delta\Delta\,(x)$. The function $\varphi(x)$ is a single-valued meromorphic function on a Riemann surface

$$Z=R^{1/2}(E),\qquad R(E)=\prod_{i=1}^{2n}(E-E_i),$$

where E_i are the terminal points of the spectrum, so that the allowed bands correspond to the intervals $(-\infty, E_1)$, (E_2, E_3), $\ldots$, $(E_{2n}+\infty)$. We shall use φ_+ and φ_- to denote the values of the function $\varphi(x)$ on the upper and lower sheets of the Riemann surface. We shall define the functions $\chi_\pm$ by

$$\varphi_\pm(x)=\exp\left\{i\int_{x_0}^{x}\chi_\pm(x)\,dx\right\}. \tag{11}$$

The following Riccati equation for $\chi_\pm$ follows from Eq. (11):

$$-i\chi_\pm'+\chi_\pm^2+q=0, \tag{12}$$

where the function $q=q(x)$ is defined by Eq. (10a). We can readily show[10] that the Wronskian of Eq. (10) has the following form for the allowed bands:

$$J(\varphi_+,\varphi_-)=\varphi_+'\varphi_--\varphi_+\varphi_-'$$
$$=2i\chi_R(x_0,E)=2iR^{1/2}(E)\left[\prod_{k=1}^{n-1}(E-\gamma_k(x_0))\right]^{-1}, \tag{13}$$

where the function χ_R is found from the relationship

$$\chi_\pm=\chi_{\pm R}+{}^1/_2 i(\ln\chi_{\pm R})', \tag{14}$$

and the functions $\gamma_i(x)$ satisfy the equations

$$\gamma_k'(x)=\pm R^{1/2}(\gamma_k)\left[\prod_{j\neq k}(\gamma_k-\gamma_j)\right]^{-1}. \tag{15}$$

Using Eqs. (13) and (14), we obtain the following expression for the wave function:

$$\psi_1(x)=\left[\frac{\Delta(x)\prod_k(E-\gamma_k(x))}{\Delta(x_0)\prod_k(E-\gamma_k(x_0))}\right]^{1/2}$$
$$\times\exp\left\{\pm i\int_{x_0}^{x}\frac{R^{1/2}(E)\,dy}{\prod_k(E-\gamma_k(y))}\right\}. \tag{16}$$

Equations (10) and (16) yield the trace identities:

$$\sum_1^{n-1}\gamma_k=\frac{i}{2}\frac{\partial}{\partial x}\ln\Delta+\frac{s}{2},\qquad s=\sum_{i=1}^{2n}E_i, \tag{17}$$

$$\sum_1^{n-1}\gamma_k^2=-|\Delta|^2+\frac{1}{2}\frac{\partial^2}{\partial x^2}\ln\Delta+\frac{1}{4}\left(\frac{\partial}{\partial x}\ln\Delta\right)^2+\frac{1}{2}\sum_{i=1}^{2n}E_i^2.$$

Equations (16) and (17) were obtained earlier by Its[11] in connection with the solution of the nonlinear Schrödinger equation

$$i\Delta_t+\Delta_{xx}-2|\Delta|^2\Delta=0. \tag{18}$$

It is found that all the finite-band solutions $\Delta(x,t)$ of Eq. (18) are also solutions of the equations for the eigenvalues of the operator $\hat{H}$ of Eq. (3) for an arbitrary value of the parameter t. A general solution $\Delta(x,t)$ of Eq. (18) is found in Ref. 11 for a spectrum with an arbitrary number of the allowed bands and we shall use this solution later. We note that the relationship between the solution of the nonlinear Schrödinger equation (18) and the problem of finding an extremum of the functional of the type (2) was first pointed out by Fateev[12] in a study of the Gross–Neveu chiral model.

We shall now write down the equation for the variational derivative of the quasimomentum $p(E)$ with respect to the potential $\Delta(x)$ for a fixed period T:

$$\delta p=-\frac{1}{T}\int_{x_0}^{x_0+T}\frac{\delta q(x)\prod_k(E-\gamma_k(x))}{2R^{1/2}(E)}=\sum_{j=0}^{n}\frac{l_jE^{n-j-1}}{R^{1/2}}. \tag{19}$$

We can obtaine Eq. (18) in the conventional wave, such as that described in Ref. 10.

Comparing Eqs. (18) and (19), we find the relationship between the coefficients l_j and δI_k:

$$l_i=\sum_{j=0}^{n}\alpha_{ij}\delta I_j,\qquad \alpha_{ij}=-1. \tag{20}$$

Next, using Eq. (19) we can write the condition for an extremum of the functional (2) in the form

$$\delta W=-\frac{2}{\pi}\int_{E<\mu}\delta p(E)\,dE+\frac{2}{g^2}\delta I_1+\frac{8c}{\bar{\omega}g^2}\delta I_2=0. \tag{21}$$

Equating to zero the coefficients for independent variations δI_k, we obtain the following system of algebraic equations:

$$\int_{E<\mu}\frac{E^k}{R^{1/2}(E)}dE=0,\qquad k=0,1,\ldots,n-3,\qquad n>1, \tag{22a}$$

$$-\frac{2}{\pi}\int\frac{E^{n-2}}{R^{1/2}(E)}dE=\frac{8c}{\bar{\omega}g^2}\equiv B, \tag{22b}$$

$$-\frac{2}{\pi}\int\frac{E^{n-1}-{}^1/_2sE^{n-2}}{R^{1/2}(E)}dE=\frac{2}{g^2}. \tag{22c}$$

The variation of Eq. (21) is incomplete, because it is assumed in Eq. (19) that the numbers of states m_j are constant for each of the $n+1$ allowed bands. It is shown in Refs. 13 and 14 that the variation of the parameters m_j leads to a condition that the chemical potential should always lie within an allowed band.

A method similar to that described in Ref. 13 makes it easy to show that the system of equations (22a) is solvable only if $n\leqslant 3$. Moreover, we can show that, in the case of low values of B, Eq. (22b) cannot be solved for $n=2$ or 3. Therefore, at low values of B the only possible case is $n=1$ (we shall give later the criterion of smallness of B). If $n=1$, it readily follows from Eqs. (10), (15), and (17) that the lattice deformation and the electron spectrum are described by

$$\Delta(x)=\rho e^{isx},\quad \rho={}^1/_2(E_2-E_1),\quad s=E_1+E_2,\quad p={}^1/_2 s+R^{1/2}(E). \tag{23}$$

The formulas in Eq. (23) can be used to calculate quite easily the total energy of the system. The levels E_1 and E_2 are found by minimization of the energy allowing for the fact that the total number of particles in a system is conserved. We can easily show that if B is small, then the total energy of the system has a minimum at $s=0$. The derivative $\partial W/\partial s$ is given by

$$\left.\frac{\partial W}{\partial s}\right|_{s=0}=\frac{2\rho}{\pi}\operatorname{sgn}s+\frac{1}{4}B\rho^2. \tag{24}$$

We can use Eq. (24) to determine $c_{\max}$ which is the maximum value of the velocity of sound below which the system is in

the ground state with a homogeneous charge density wave. We then find that

$$n=1,\ E_2=-E_1=\Delta_0\sim E_F e^{-1/\lambda},$$

so that

$$c_{max}=\frac{2}{\pi}\frac{\omega_0 g^2}{\Delta_0}\sim c\lambda e^{-1/\lambda}. \tag{25}$$

It follows from Eq. (25) that in systems with $\lambda>1$ we always have $c<c_{\max}$. If $\lambda\sim 1$, our continuum model ceases to be valid.

We have thus established that in the ground state at $T=0$ the deformation $\Delta(x)$ is homogeneous: $\Delta(x)=\text{const}$, whereas the electron spectrum is $E^2=p^2+\Delta^2$. Using the matching condition in the form of Eq. (4a) and (4b), we readily obtain the following expression for the charge distribution in a chain[4]:

$$\rho(x)-\bar{\rho}=-{}^1/_2 B(|\Delta|^2-\langle|\Delta|^2\rangle). \tag{26}$$

In the case under consideration we find that $\rho(x)=\bar{\rho}$.

We shall now tackle the problem of the ground state of a system with split bands formulated in the Introduction. As demonstrated above, this problem can be described most naturally in terms of the Peierls–Fröhlich model[7] in a magnetic field h. The state of the system can be studied most conveniently for a fixed "spin concentration" m. As usual, the value of m is defined in terms of the magnetic field: $h=\partial W/\partial m$, where $W=W(m)$ is the ground-state energy. We recall that in the problem of two types of chain the initial splitting of the spectrum equivalent to h is specified.

In contrast to the $m=0$ case discussed above, we now have two Fermi levels of the system: $\mu_{\uparrow\downarrow}=\mu\mp h$, so that the bands located in the range $E<\mu_\uparrow$ are doubly filled, whereas those lying in the range $\mu_\uparrow<E<\mu_\downarrow$ are singly filled. The self-consistency conditions of the system in question are still given by Eq. (22), expect that the integral over the singly filled energy bands should have the coefficient 1/2 in front of it. We can show that in this case the system (22) is solvable only for $n=2$ and the equations in this system become

$$-\frac{2}{\pi}\int\frac{E-s/2}{R^{1/2}(E)}dE=\frac{2}{g^2},\qquad s=E_1+E_2+E_3+E_4, \tag{27}$$

$$-\frac{2}{\pi}\int\frac{dE}{R^{1/2}(E)}=B,\qquad R=(E-E_1)(E-E_2)(E-E_3)(E-E_4). \tag{28}$$

Then, the energy band $(-E_F, E_1)$ is doubly filled, whereas the band (E_2, E_3) is singly filled (see Fig. 1 below). Another equation is obtained by equating the number of states in the (E_2, E_3) band to the spin concentration m:

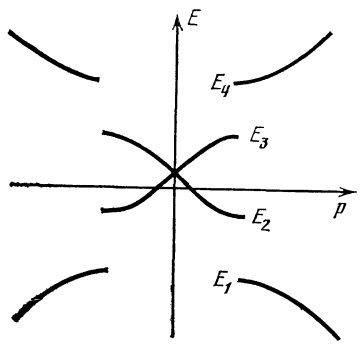

FIG. 1.

$$\frac{1}{\pi}\int_{E_2}^{E_3}dp=m. \tag{29}$$

The fourth self-consistency condition reflects conservation of the total particle concentration $n=n_\uparrow+n_\downarrow$ when the difference $m=n_\uparrow-n_\downarrow$ is established:

$$p(E_1)=-{}^1/_2\pi m. \tag{30}$$

We recall that the differential dp is of the form

$$dp=\frac{E^2+ME+N}{R^{1/2}(E)}dE, \tag{31}$$

where the coefficients M and N are found from the conditions

$$\int_{E_1}^{E_2}\frac{dp}{dE}dE=\int_{E_3}^{E_4}\frac{dp}{dE}dE=0. \tag{32}$$

We shall also give an explicit expression for the field $\Delta(x)$ consisting of the general formula form Eq. (11) when $n=2$

$$\Delta(x)=\frac{\vartheta_2(\varkappa(x-x_0)-2r_1)}{\vartheta_2(\varkappa(x-x_0))}\exp[i(s-2K_1)+\Omega], \tag{33}$$

$$|\Delta(x)|^2=-2R_1-\frac{\partial^2}{\partial x^2}\ln[\exp\{-i\pi\varkappa(x-x_0)\}\vartheta_2(\varkappa(x-x_0))], \tag{34}$$

where $\vartheta_2(\xi)\equiv\vartheta_2(\xi|q)$ is the ϑ Jacobi function

$$k=\left[\frac{(E_3-E_2)(E_4-E_1)}{(E_4-E_2)(E_3-E_1)}\right]^{1/2},$$

$$\varkappa=-i\frac{[(E_4-E_2)(E_3-E_1)]^{1/2}}{2K(k)}, \tag{35}$$

$$r_1=\frac{-F(\nu,k)}{2K(k)},\qquad q=\exp\left(\frac{-\pi K(k')}{K(k)}\right),$$

$$\nu=\arcsin\left[\frac{E_3-E_1}{E_4-E_2}\right]^{1/2},$$

$$K_1=\frac{E_3-E_4}{K(k)}\Pi\left(\frac{\pi}{2},\frac{E_3-E_2}{E_3-E_1},k\right)+E_4,$$

$$R_1=N+Ms+\frac{3}{4}\sum E_i^2+\frac{1}{2}\sum_{i>j}E_iE_j,$$

and F, K, and Π are elliptic integrals.

Using the expression foir the wave function ψ_1 of Eq. (16), we obtain the following general expression for the quasimomentum:

$$p=\frac{1}{2T}\int_0^T\frac{\Delta'}{\Delta}dx+R^{1/2}(E)\int_0^T\frac{dy}{E-\gamma_k(y)}. \tag{36}$$

Substituting Eq. (36) into Eq. (30) and applying Eq. (34), we obtain the equivalent condition:

$$4\pi r_1+s-2K_1=-\pi. \tag{37}$$

3. PROPERTIES OF AN ISOLATED SOLITON

We shall now consider the case of a low concentration m. It follows from Eqs. (27)–(30) and (37) that

$$-E_1=E_4=\Delta_0,\qquad \Delta_0\sim E_F e^{-1/\lambda}, \tag{38}$$

$$\pi-4\,\mathrm{arctg}\frac{\Delta_0+E_0}{(\Delta_0^2-E_0^2)^{1/2}}=-\pi B(\Delta_0^2-E_0^2)^{1/2}. \quad (39)$$

Equation (37) describes the position of a local level E_0. If B is small, it follows from Eq. (37) that

$$E_0\approx\pi B\Delta_0^2/4>0. \quad (40)$$

In the limit $m\to 0$, i.e., when $E_2\to E_3\to E_0$ the general expression for the deformation (33) gives the isolated soliton profile:

$$\Delta(x)=-e^{i\alpha/2}\{E_0-i(\Delta_0^2-E_0^2)^{1/2}\,\mathrm{th}[(\Delta_0^2-E_0^2)^{1/2}x]\}, \quad (41)$$

$$|\Delta(x)|^2=\Delta_0^2-(\Delta_0^2-E_0^2)/\mathrm{ch}^2[(\Delta_0^2-E_0^2)^{1/2}x], \quad (42)$$

where

$$\alpha=4\arcsin[(\Delta_0+E_0)/2\Delta_0]^{1/2}\geqslant\pi. \quad (42a)$$

It is clear from Eq. (39) that $\Delta(x)$ varies along a chord of a circle of radius Δ_0; we then have

$$\Delta(x)\to\Delta_0,\quad x\to-\infty;\qquad \Delta(x)\to\Delta_0 e^{i\alpha},\quad x\to\infty.$$

Figure 2 shows the complete path representing variation of the complex function $\Delta(x)$ in the case of a lattice of relatively few solitons; here, $\theta=\pi-\alpha/2$.

We shall now find the charge distribution in a soliton. Substituting Eq. (40) into Eq. (26), we find from Eq. (39) that

$$\rho(x)-\bar{\rho}=e\frac{B}{2}\frac{\Delta_0^2-E_0^2}{\mathrm{ch}^2[(\Delta_0^2-E_0^2)^{1/2}x]}. \quad (43)$$

The soliton charge is

$$q_s=eB(\Delta_0^2-E_0^2)^{1/2}. \quad (44)$$

Equations (42a) and (44) and the condition (39) yield an equivalent expression $q_s=e(\alpha-\pi)/\pi$, which corresponds to a general formula for a chord soliton of Ref. 4.

In the approximation of a strong coupling of the electron and phonon spectra we can use the results of Ref. 13 and obtain from Eq. (42) the following approximate expression:

$$q_s\approx e\frac{8}{\pi^2e^2}\frac{\sin(\pi|\rho-1|/2)}{\cos^3(\pi|\rho-1|/2)}\frac{e^{-2/\lambda}}{\lambda|\rho-1|},\quad e^{-1/\lambda}\ll|\rho-1|\ll 1. \quad (45)$$

In the limit $\rho\to 1$, Eq. (45) gives $q\propto e^{-2/\lambda}/\lambda$.

We shall compare the charge q_s due to the phonon dispersion with the residual charge q_s^* of a spin soliton due to the influence of the umklapp processes,[7] i.e., we shall compare the former charge width

$$q_s^*\approx\frac{8e^{-2/\lambda}}{\pi^3|\rho-1|^2}. \quad (46)$$

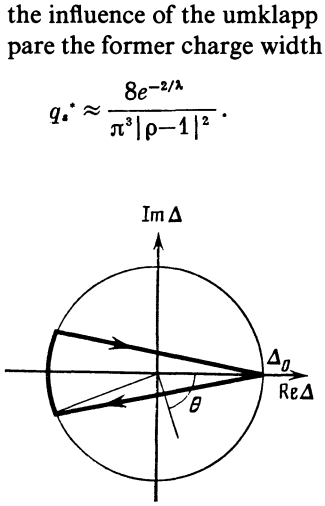

FIG. 2.

It follows from Eqs. (45) and (46) that in the range $|\rho-1|>\lambda^{1/2}$ we have $q_s>q_s^*$, i.e., the soliton charge is mainly due to the phonon dispersion near $\pm 2p_F$ In the limit $\rho\to 0$, Eq. (45) becomes

$$q_s\approx\frac{4}{\pi\lambda}\exp\left(-\frac{\pi\rho}{\lambda}\right),\quad \lambda\ll\rho\ll 1. \quad (47)$$

Following Ref. 4, we can obtain the soliton energy as a function of the angle θ:

$$W_s=\Delta\left\{\left(1-\frac{2\theta}{\pi}\right)\cos\theta+\frac{2\sin\theta}{\pi}\right\}+B\Delta^2\left(\frac{\theta}{2}-\frac{1}{4}\sin 2\theta\right)$$
$$=\Delta\left\{\left(1-\frac{2\theta}{\pi}\right)\left(\frac{\cos\theta}{2}+\frac{\theta}{2\sin\theta}\right)+\frac{2}{\pi}\sin\theta\right\}, \quad (48)$$

where $\theta=\pi-\alpha/2$ is governed by the self-consistency condition (37), equivalent to the condition for a minimum of the function $W_s(\theta)$.

4. CONCLUSIONS

There are quasione-dimensional compounds (for example, those with the formula MX_3) in which charge density waves with similar vectors propagate along chains. This situation occurs if the Fermi surface can be divided into planar symmetric regions with different wave vectors. The following are examples: a) a system of two inequivalent chains; b) a system with a smooth dependence of the spectrum on $k_\perp$, where $k_\perp$ is the wave vector perpendicular to the chain directions.[8] At low temperatures we can expect interference between similar charge density waves to produce modulated superstructures (soliton lattices). When the coupling between the chains is weak, the charge density waves are subject to a weak modulation of the 2π-phase soliton type; no significant changes take place in the electron spectrum. When the coupling is strong, modulation of the charge density waves produces a lattice of solitons similar to amplitude solitons and it alters both electronic and optical properties. The problem which then arises is readily formulated and solved on the basis of Peierls theory with a magnetic field.

It is known[7] that amplitude solitons of the type of interest to us are characterized by a half-filled local level in the middle of the band gap and carry no electric charge. We solved exactly the problem of a soliton lattice allowing for the dispersion of the phonon spectrum near $2p_F$. We found that the dispersion produces the following effects: 1) a change in the topological nature of a soliton so that a change in the phase $\Delta(x)$ at one soliton differs from π; 2) appearance of a fractional electric charge $q_s\propto(\lambda^{-1}e^{-2/\lambda})$e; 3) a shift of the local level out of the middle of the band gap. All these effects are characterized by a smallness order Δ_0/E_F, but in partice they need not be small if $\Delta_0\sim E_F$.

We shall conclude by noting that a fractional electric charge of solitons, discussed frequently in the literature, may be exhibited by various systems manifesting the Peierls effect (for a review see Ref. 1). In systems with a fractional occupancy of the electron energy bands $\rho\neq 0$, 1, and 2, a fractional charge is either due to the dispersion of the phonon spectrum or due to second-order umklapp processes.[7] These two effects are discussed above and they may be comparable,

but they are characterized by different dependences on ρ. A special case of solitons with fractional charges is encountered in the orthogonal case of a combined Peierls insulator which is known as the $(AB)_x$ polymer case.

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