impurity centers transforms them into electrically active complexes. Milevskiĭ[10] has indicated that if the binding energy of the electron at the center exceeds the migration energy of the center, then electrically active complexes can remain in the glide planes. The existence of such complexes was observed experimentally in Ref. 11. These experiments were made on Si crystals with high concentration of oxygen (and possibly of other electrically inactive impurities). Therefore the concentration of the active centers in the glide planes was so high, that two-dimensional potential barriers were produced in them. The conductivity of such crystals in a direction perpendicular to the glide planes was much less than the conductivity in directions parallel to the glide planes. It was assumed in Ref. 11 that this fact can be attributed to detouring of the carriers around the dielectric regions produced in the glide regions (private communication from E.B. Yakimov). In our relatively pure crystals these effects could not take place. The conclusions of our paper do not depend on the nature of the electric activity of the dislocations. No matter what produces the dielectric cylinders, it can be asserted (in our opinion) that these cylinders affect the resistance of the sample because of the detour effect, and that the radii of the cylinders should depend nonmonotonically on T.

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[1]R. A. Logan, G. L. Pearson, and D. A. Kleinman, J. Appl. Phys. **30**, 885 (1959).
[2]Yu. A. Osip'yan and S. A. Shevchenko, Pis'ma Zh. Eksp. Teor. Fiz. **18**, 256 (1973) [JETP Lett. **18**, 153 (1973)].
[3]L. S. Milevskiĭ and A. A. Zolotukhin, Pis'ma Zh. Eksp. Teor. Fiz. **19**, 478 (1974) [JETP Lett. **19**, 255 (1974)].
[4]L. S. Milevskii, T. M. Tkacheva, and T. A. Pagava, Zh. Eksp. Teor. Fiz. **69**, 2132 (1975) [Sov. Phys. JETP **42**, 1084 (1975)].
[5]B. I. Shklovskiĭ and A. L. Éfros, Élektronnye svoĭstva legirovannykh poluprovodnikov (Electronic Properties of Doped Semiconductors), Nauka, 1979, p. 126.
[6]Yu. A. Osip'yan, V. M. Prokopenko, V. I. Tal'yanskii, A. A. Kharlamov, and S. A. Shevchenko, Pis'ma Zh. Eksp. Teor. Fiz. **30**, 123 (1979) [JETP Lett. **30**, 111 (1979)].
[7]Yu. A. Osip'yan, V. I. Tal'yanskiĭ, and S. A. Shevchenko, Zh. Eksp. Teor. Fiz. **72**, 1543 (1977) [Sov. Phys. JETP **45**, 810 (1977)].
[8]Yu. A. Osip'yan, V. I. Tal'yanskiĭ, A. A. Kharlamov, and S. A. Shevchenko, Zh. Eksp. Teor. Fiz. **76**, 1655 (1979) [Sov. Phys. JETP **49**, 840 (1979)].
[9]W. T. Read, Philos. Mag. **45**, 775 (1954).
[10]L. S. Milevskii, Defekty struktury v poluprovodnikakh (Structure Defects in Semiconductors), All-Union Conference, Novosibirsk, 1973, p. 120.
[11]V. G. Eremenko, V. I. Nikitenko, and E. B. Yakimov, Pis'ma Zh. Eksp. Teor. Fiz. **26**, 72 (1977) [JETP Lett. **26**, 65 (1977)].

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Self-localized excitations in the Peierls-Fröhlich state

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We show that stationary excited states of a one-dimensional Peierls dielectric are amplitude solitons. They originate as the result of self-trapping of an electron which is initially excited across the optical gap $2\Delta_0$. The energy of the soliton $W_s = (2/\pi)\Delta_0$, its charge $e_s = 0$, and its spin $s = 1/2$. The gap parameter has the form $\Delta(x) = \Delta_0 \tanh(\Delta_0 x/v_F)$. The soliton carries a singly occupied $\nu_0 = 1$ localized state with an energy in the center of the forbidden band $E_0 = 0$. For systems with a commensurability 1:2 the multiplicity of occupation may be arbitrary, $\nu_0 = 0$, 1, 2, and the soliton can have a charge $e_s = -e$, 0, e. We show that inclusion of electron-electron interactions conserves the property $e_s = 0$. A small local charge occurs as the result of phonon dispersion in the vicinity of $2p_F$. Interaction between the chains leads to a smoothing of the jump in the phase of the function $\Delta(x)$ at distances $l \sim v_F/T_c \gg v_F/\Delta_0$ (T_c is the three-dimensional ordering temperature). A charge $\sim e$ is localized in that region. An effective coupling between the chains or a commensurability of the order of more than two causes an attraction between solitons with a force $\sim v_F/l^2$ at distances $\lesssim l$. The presence of solitons produces spin resonance effects, absorption, or luminescence at a frequency Δ_0, and a broadening of the fundamental absorption edge $2\Delta_0$.

1. INTRODUCTION

1. It is well known that the quasi-one-dimensional gas of non-interacting electrons on a system of deformed chains at zero temperature T is in a Peierls-Fröhlich ground state (see the reviews in Refs. 1 to 3). It is characterized by a static deformation of the lattice $\varphi(x)$ and a charge density wave (CDW) $q(x)$ of the form

$$q(x) \propto \varphi(x) = \varphi_0 \cos(2p_F x + \chi),$$

where x is the coordinate along the chain, p_F the Fermi momentum for the electrons in the metallic phase, and χ the CDW phase.

The electrons occupy states with negative energies $E_k = -\varepsilon_k$, where

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$$\varepsilon_k=[(v_F k)^2+\Delta_0^2]^{1/2}, \quad \Delta_0=g\varphi_0\sim\varepsilon_F\exp\{-1/\lambda\},$$

v_F is the Fermi velocity, g the electron-phonon interaction constant, $\lambda=\nu g^2/2\pi v_F$, and ν the degree of degeneracy of the electron band.

The ground state of the system, obtained in the self-consistent-field approximation, is determined correctly due to the adiabaticity parameter

$$m/M=(u/v_F)^2=1/4\lambda\bar{\omega}^2/\Delta_0^2\ll 1,$$

where m and M are the band mass and the so-called effective CDW mass, u is the CDW phase velocity, $\bar{\omega}=\omega(2p_F)$ is the unrenormalized phonon frequency. This parameter is estimated to be $m/M\sim 10^{-3}$ for KCP and $m/M\sim 10^{-2}$ for TTF-TCNQ.[3]

2. The elementary excitations of the system contain, firstly, two phonon branches which at low temperatures can be defined conveniently as the phase χ and the amplitude δ of the mode:

$$\Delta(x,t)=[\Delta_0+\delta(x,t)]\cos(2p_F x+\chi(x,t)),$$

with the dispersion laws

$$\omega_\chi(q)=uq, \quad \omega_\delta(q)=\omega_0(1+1/12\xi_0^2q^2)^{1/2},$$
$$\omega_0=2^{1/2}(u/v_F)\Delta_0\sim 10^{12}\ \text{s}^{-1}.$$

This picture may be justified both for a system which is three-dimensional as far as the phonons are concerned, and for a one-dimensional one, regardless of the presence of a long-range order.[4] As a result of thermal and quantum fluctuations in χ and δ the parameter Δ_0 is determined with an accuracy[4,5]

$$\varepsilon_1\sim\Delta_0\max\{(T/\Delta_0)^{1/2}, (m/M)^{1/2}\}. \tag{1}$$

Apart from the phonons we must consider electron and hole excitations which determine the properties of the system as a narrow-band semiconductor. If we assume, as is usually implied, that the state of the lattice is fixed ($\Delta(x)=\Delta_0=$ const) the electron-hole excitations are constructed in the same way as the particles of the ground state — linear combinations of the waves $|\pm p_F+k\rangle$ with dispersion law ε_k. However, the excitations determined in that way are bare and must to some extent be modified under the influence of the interaction with the phonon modes-polaron effect. The present author has shown[5] that in a one-dimensional Peierls-Fröhlich system this effect is particularly strong and leads to a radical rearrangement of the picture of the electron excitations of the system. The reason is[5] that an electron or hole, excited initially into a state with momentum $k\ll\Delta_0/v_F$ and energy $\varepsilon_k\approx\Delta_0$, interacts with the deformations of the superstructure (CDW)-the renormalized phonons. When the phonon spectrum is quasi-one-dimensional this system in the units v_F, Δ_0, $\xi_0=v_F/\Delta_0$, does not contain any parameters, except the adiabaticity parameter[1)] $u/v_F\ll 1$. Because of that it is necessary to distinguish two kinds of electron effects, depending on the relation between the electron life time τ and the characteristic phonon frequency ω_0. States with $\tau\omega_0\ll 1$ are determined for a fixed spontaneous lattice configuration. States with $\tau_0\sim\Delta_0^{-1}$, corresponding to optical transitions through the gap and to virtual transitions which determine the renormalized phonon spectrum and the specific dielectric permittivity[2,3]

$$\varepsilon(q)=\omega_p^2/[6\Delta_0^2+(v_F q)^2] \tag{2}$$

(ω_p is the plasma frequency) belong to this class. Among the thermo-activated excitations there are also states for which the recombination proceeds faster than over a time ω_0^{-1}. For all these short-lived states one can take the spectrum ε_k, smeared out by an amount $\sim\varepsilon_1$ given by (1). The corresponding theory was given in Refs. 4 and 5.

Long-lived excitations with $\tau\gg\omega_0^{-1}$ must be studied as stationary states of the electron-phonon system. It was shown in Ref. 5 that they can be considered as strong coupling polarons with a constant $\alpha\sim(v_F/u)^{1/2}\gg 1$, with an intermediate radius $\sim\xi_0$, and with an energy W inside the forbidden band $-\Delta_0<W<\Delta_0$, and with an effective mass $M_p\sim m^*M/m\sim\Delta_0/u^2$ ($m^*=\Delta_0/v_F^2$). For the simple model of non-interacting electrons on an isolated chain, an exact solution was indicated with deformations of the domain wall type carrying a localized electron state. Notwithstanding the localization of the wavefunction of the additional electron and the lattice deformation the total charge and energy densities of this excited state turned out to be delocalized and constant along the length of the system. In what follows, we shall call these excitations solitons in accord with the established terminology.

3. In the present paper we give a detailed theory of the stationary excited states of a Peierls-Fröhlich system. We consider the effect of weak electron-electron interactions, coupling between chains, and phonon dispersion on the soliton charge. We study the interaction between solitons. We establish a correspondence with quasi-classical solutions in two-dimensional models of interacting fermions in field theory.[6-8] It allows us to state that the solitons considered are the only possible kind of stationary excited states for a system of spin-$\frac{1}{2}$ electrons. For a system with a single conduction electron per elementary cell, a soliton solution can exist and with an unoccupied or doubly occupied localized state. For a system with spinless fermions corresponding to an infinite repulsion of real electrons at a single site excited stationary states are in general not present.

2. SINGLE-SOLITON SOLUTION FOR AN ISOLATED CHAIN

1. We consider a system of non-interacting electrons on a deformed chain which is in the Peierls-Fröhlich ground state. We add to the system $\nu_0\leqslant\nu$ electrons, where ν is the degree of degeneracy of the original band. As a result of the interaction $\Delta(x)$ of these electrons with the deformations of the superstructure the system goes over into a stationary state: the ground state or an excited state. It follows from the analysis

given in Ref. 5 that one may expect self-trapping of the additional electrons in a region $\sim\xi_0$ when the binding energy is $W_b \sim \Delta_0$. Since $W_b/\omega_0 \sim v_F/u \gg 1$ one can solve the problem in the approximation which is quasi-classical in the lattice degrees of freedom, corresponding to the strong-coupling polaron theory. (This theory is given in Refs. 9 and 10 for one-dimensional problems.) In the zeroth approximation in the parameter ω_0/W_b in the trapping region and in the parameter u/v_F outside it[4] one can consider the lattice deformation to be a classical quantity

$$\varphi(x)=g^{-1}[\Delta(x)\exp[i(2p_Fx+\chi)]+\text{c.c.}], \tag{3}$$

where $\Delta(x)=\Delta_1(x)+i\Delta_2(x)$ is a complex function, and χ = const is an arbitrary phase. Far from the localization region ($|x|\gg\xi_0$), the system must go over into one of the possible ground states, i.e.,

$$\Delta(x)\xrightarrow[x\to\pm\infty]{}\Delta_\pm=\text{const},\quad |\Delta_\pm|=\Delta_0.$$

The electron wavefunctions $\psi_\mu(x)$ in the field $\Delta(x)$ can be written in two equivalent representations:

$$\psi_\mu(x)=\psi_{\mu+}(x)\exp[i(p_Fx+\chi)]+\psi_{\mu-}(x)\exp[-i(p_Fx+\chi)] \tag{4a}$$

or

$$\psi_\mu(x)=2^{1/2}[u_\mu(x)\cos(p_Fx)+iv_\mu(x)\sin(p_Fx)], \tag{4b}$$

where

$$\psi_{\mu\pm}=2^{-1/2}(u_\mu\pm v_\mu)e^{\pm i\chi/2}.$$

Any stationary state of the system, including the ground state, is determined by the condition that the functional of the energy of the system $W\{\Delta(x),\psi_\mu(x)\}$ is an extremum. Assuming the electron spectrum near the Fermi points $\pm p_F$ to be linear we can write

$$\begin{aligned}W\{\Delta(x),\psi_{\mu\pm}(x)\}&=\frac{\Delta(x)\Delta^*(x)}{g^2}\\&+\sum_\mu\{-iv_F[\psi_{\mu+}^*(x)\psi_{\mu+}'(x)-\psi_{\mu-}^*(x)\psi_{\mu-}'(x)]\\&+\Delta(x)\psi_{\mu+}^*(x)\psi_{\mu-}(x)+\Delta^*(x)\psi_{\mu-}^*(x)\psi_{\mu+}(x)\},\end{aligned} \tag{5a}$$

where $\psi'_{\mu\pm}(x)=d\psi_{\mu\pm}(x)/dx$ and the summation is taken over all occupied states.[2)] The first term in (5a) is the lattice deformation energy. Since we want to obtain solutions with a well defined parity we shall use the representation (4b) in which

$$\begin{aligned}&W\{\Delta_1(x),\Delta_2(x),u_\mu(x),v_\mu(x)\}\\&=\frac{\Delta_1^2(x)+\Delta_2^2(x)}{g^2}+\sum_\mu\{-i[u_\mu^*(x)v_\mu'(x)+v_\mu^*(x)u_\mu'(x)]\\&+\Delta_1(x)[u_\mu^*(x)u_\mu(x)-v_\mu^*(x)v_\mu(x)]\\&+i\Delta_2(x)[v_\mu^*(x)u_\mu(x)-u_\mu^*(x)v_\mu(x)]\}.\end{aligned} \tag{5b}$$

Varying (5b) with respect to $u_\mu(x)$, $v_\mu(x)$ we get Dirac type equations for the eigenfunctions corresponding to the energies E_μ:

$$u_\mu'-\Delta_2u_\mu-i(E_\mu+\Delta_1)v_\mu=0, \tag{6a}$$

$$v_\mu'+\Delta_2v_\mu-i(E_\mu-\Delta_1)u_\mu=0. \tag{6b}$$

Varying (5b) with respect to $\Delta_1(x)$, $\Delta_2(x)$ we get the self-consistency conditions:

$$\frac{\delta W}{\delta\Delta_1}=2\frac{\Delta_1}{g^2}-\sum_\mu(u_\mu^*u_\mu-v_\mu^*v_\mu)=0, \tag{7}$$

$$\frac{\delta W}{\delta\Delta_2}=2\frac{\Delta_2}{g^2}+\frac{1}{i}\sum_\mu(u_\mu^*v_\mu-v_\mu^*u_\mu)=0. \tag{8}$$

2. Equations (6) to (8) correspond to the self-consistent field approximation for a non-uniform state of the system or, strictly speaking, to the zeroth quasi-classical approximation. Their applicability is, as we indicated above, based upon the existence of the adiabaticity parameter $v_F/u\gg1$. One knows also another physical system described by approximately equivalent equations. That is the model of a two-dimensional relativistic field theory with a large number of interacting fermions $\nu\gg1$ which was studied in Refs. 6 to 8. The large parameter ν was necessary for the use of the quasi-classical approach. However, the approximate equations which were derived were studied already exactly for arbitrary ν and the results obtained can be used in the cases of interest to us, $\nu=2$ or $\nu=1$. In view of the necessity of a more detailed study and also because of the different dynamics of these systems we give below an independent derivation of the soliton solution. The results of Refs. 6 to 8 indicate the uniqueness of the solution given here.[3)]

3. We shall look for a solution such that in the region of the soliton $\Delta(x)$ changes in the complex plane along a chord of the circle $|\Delta|=\Delta_0$. Through the choice of the phase χ in the definitions (3)(4a) we can assume that Δ_1 = const, $\Delta=\Delta_1+i\Delta_2(x)$, as shown in Fig. 1. We define the parameters $0\leqslant\theta\leqslant\pi$ and $k_0\geqslant0$ in such a way that

$$\Delta_1=\Delta_0\cos\theta,\quad k_0=(\Delta_0^2-\Delta_1^2)^{1/2}=\Delta_0\sin\theta.$$

It is clear from Eqs. (6a) and (6b) that when $\Delta_1=$ const there exists always a localized, normalized solution which in what follows will be indicated by the index $\mu=0$.

a) If $\Delta_2(\pm\infty)=\mp k_0$, as shown by the arrow in Fig. 1, we have $E_0=\Delta_1$, $v_0(x)\equiv0$,

$$u_0(x)\propto\exp\left\{\int_0^x\Delta_2(y)dy\right\}. \tag{9a}$$

b) If $\Delta_2(\pm\infty)=\pm k_0$, we have $E_0=-\Delta_1$, $u_0(x)\equiv0$,

$$v_0(x)\propto\exp\left\{-\int_0^x\Delta_2(y)dy\right\}. \tag{9b}$$

It is clear from a comparison with the results of Ref.

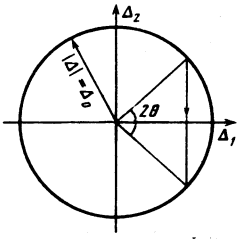

FIG. 1.

5 that the cases a) and b) correspond to electron and hole polarons. To fix the ideas we shall in what follows consider the case a).

When $\mu \neq 0$ it follows from (6b) that

$$u_\mu(x) = (v_\mu' + \Delta_2 v_\mu)/i(E_\mu - E_0). \tag{10}$$

Substituting (10) into (7), (8) we get

$$\frac{\delta W}{\delta \Delta_1} = 2\frac{\Delta_1}{g^2} + 2\sum_{\mu \neq 0} v_\mu^* v_\mu - \rho(x), \tag{11}$$

where

$$\rho(x) = \sum_\mu (u_\mu^* u_\mu + v_\mu^* v_\mu) \tag{12}$$

is the particle number density, and

$$\frac{\delta W}{\delta \Delta_2} = 2\frac{\Delta_2}{g^2} + \sum_{\mu \neq 0} \left(2\Delta_2 + \frac{d}{dx}\right)\frac{v_\mu^* v_\mu}{E_\mu - E_0}. \tag{13}$$

Substituting (10) into (6a) we get an equation for $v_\mu(x)$ when $\mu \neq 0$:

$$v_\mu'' + [\Delta_2'(x) - \Delta_2^2(x) + E_\mu^2 - E_0^2] v_\mu = 0. \tag{14}$$

As $x \to \pm\infty$ we have $\Delta_2' \to 0$, $\Delta_2^2 + E_0^2 \to \Delta_0^2$, i.e., (14) changes to the equation

$$v_\mu'' + (E_\mu^2 - \Delta_0^2) v_\mu = 0, \tag{14a}$$

corresponding to the unperturbed ground state. The solutions of (14a) are plane waves, numbered by the quasi-momentum $\mu = k$:

$$E_k = -\varepsilon_k = -[(v_F k)^2 + \Delta_0^2]^{1/2}, \quad v_k(x) = (N_k L)^{-1/2} e^{ikx}, \tag{15}$$

where L is the length of the chain, and N_k a normalizing factor. We require that (15) be a solution also of the exact Eq. (14) for all x. For this it is necessary that

$$-\Delta_2'(x) + \Delta_2^2(x) + E_0^2 \equiv \Delta_0^2,$$

whence

$$\Delta_2(x) = -k_0 \operatorname{th}(k_0 x). \tag{16}$$

Substituting (16) into (9a) and (10) we get a complete set of electron states in the field $\Delta(x)$:

$$\begin{aligned} &\mu = 0: \ E_0 = \Delta_0 \cos\theta, \quad v_0(x) \equiv 0, \\ &\quad u_0 = (k_0/2)^{1/2}/\operatorname{ch}(k_0 x), \\ &\mu = k: E_k = -\varepsilon_k, \quad v_k(x) = \frac{1}{(N_k L)^{1/2}} e^{ikx}, \\ &\quad u_k = \frac{1}{(N_k L)^{1/2}} \frac{-k + ik_0 \operatorname{th}(k_0 x)}{E_0 + \varepsilon_k}, \end{aligned} \tag{17}$$

where

$$N_k = \frac{2\varepsilon_k}{E_0 + \varepsilon_k}\left(1 - \frac{k_0}{\varepsilon_k (E_0 + \varepsilon_k)}\frac{1}{L}\right) \tag{18}$$

[an accuracy $O(1/L)$ is necessary in (18) for a correct isolation of the single-particle effect].

We substitute Eqs. (16) to (18) in Eqs. (11) to (13). When summing we must assume the states with $\mu = k$, $E_\mu = -\varepsilon_k$ to be ν-fold occupied states, those with $\mu = k$, $E_\mu = +\varepsilon_k$ to be unoccupied, while we assign to the localized states $\mu = 0$ an arbitrary occupation number ν_0: $0 \leq \nu_0 \leq \nu$. We get

$$\frac{\delta W}{\delta \Delta_2} = 2\Delta_2(x) X, \tag{19}$$

$$\frac{\delta W}{\delta \Delta_1} = 2E_0 X + \frac{k_0}{2\operatorname{ch}^2(k_0 x)}\left[\nu_0 - \frac{\nu}{L}\sum_k \frac{k_0}{\varepsilon_k (E_0 + \varepsilon_k)}\right], \tag{19a}$$

where

$$X = \frac{1}{g^2} - \frac{\nu}{L}\sum_k \frac{1}{2\varepsilon_k}. \tag{20}$$

In equilibrium we must have $X = 0$. This condition determines for the ground state ($\theta = 0$, $\nu_0 = 0$) the equilibrium value of the gap parameter

$$\Delta_{00} \sim \varepsilon_F \exp\{-1/\lambda\}.$$

If there is a soliton present the sum in (20) is changed by an amount $\sim O(1/L)$ due to the change in the density of states because of the existence of scattering phases in $u_k(x)$ and due to the accuracy of the normalization (18). We thus have always

$$X = X(\theta) = O(1/L).$$

The sum in (19a) can be evaluated to order $O(1)$, as it occurs with a factor which is integrated over x. We get

$$\frac{\delta W}{\delta \Delta_1} = \frac{\Delta_0 k_0}{2\operatorname{ch}^2(k_0 x)}\left[\nu_0 - \nu\frac{\theta}{\pi}\right] + 2E_0 X. \tag{21}$$

In the equilibrium position

$$\delta W/\delta \Delta_1 = \delta W/\delta \Delta_2 = 0$$

and we have from (19) and (21) $\Delta_0 = \Delta_{00} + O(1/L)$, $\theta = \theta_0 = \pi\nu_0/\nu$, or $\theta = 0$.

4. We determine the total excitation energy $W(\theta)$ from the relation

$$\frac{dW}{d\theta} = \int dx \left[\frac{\delta W}{\delta \Delta_1}\frac{d\Delta_1}{d\theta} + \frac{\delta W}{\delta \Delta_2}\frac{d\Delta_2}{d\theta}\right], \tag{22}$$

whence

$$\frac{dW}{d\theta} = \int dx \left[\sin 2\theta \frac{x \operatorname{th}(k_0 x)}{\operatorname{ch}^2(k_0 x)} X(\theta) + \frac{k_0^2}{2\operatorname{ch}^2(k_0 x)}\left(\nu\frac{\theta}{\pi} - \nu_0\right)\right]. \tag{22a}$$

The quantity $X(\theta)$ occurs in (22a) with a factor integrated over x, i.e., one can with an accuracy $O(1)$ assume that $X(\theta) \equiv 0$. We get

$$\frac{dW}{d\theta} = \Delta_0 \sin\theta \left(\nu\frac{\theta}{\pi} - \nu_0\right). \tag{22b}$$

Integrating (22b) with the boundary condition $W(0) = \nu_0 \Delta_0$, corresponding to electrons at the point $k = 0$ when the superstructure is not deformed, we get, in agreement with the results from Refs. 6 to 8[4)]

$$W(\theta) = \Delta_0\left[\left(\nu_0 - \nu\frac{\theta}{\pi}\right)\cos\theta + \frac{\nu}{\pi}\sin\theta\right], \tag{23}$$

$$W_s = W(\theta_0) = \frac{\nu}{\pi}\sin\left(\pi\frac{\nu_0}{\nu}\right)\Delta_0, \quad \theta_0 = \pi\frac{\nu_0}{\nu}. \tag{23a}$$

It is clear from (22b) and (23) that the positions $\theta = 0$ and $\theta = \theta_0$ correspond to a maximum and a minimum of the energy of the system. We show the function $W(\theta)$ in Fig. 2 for $\nu = 2$, $\nu_0 = 0, 1, 2$.

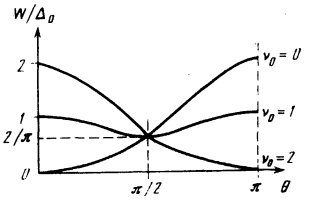

FIG. 2.

5. We consider different cases for the occupation numbers ν and ν_0.

a) $\nu_0=0:\theta_0=0, W_s=0, k_0=0$, and we have the undeformed system in its ground state.

b) $\nu_0=\nu:\theta_0=\pi, W_s=0, k_0=0$, and we have the undeformed system with an occupied ν-fold degenerate level in the ground state.

When $\nu=1$ the trivial cases a) and b) exhaust all possibilities. Hence we conclude that when $\nu=1$ (infinite repulsion of the electrons on one site) there are no stationary excited states. Any electron excited across the gap will after a time $\tau \gtrsim \omega_0^{-1}$ be continuously absorbed into the ground state. This non-radiative recombination proceeds, as follows from the qualitative analysis given in Ref. 5, through intermediate non-stationary polaron states.

We now consider the most important case of electrons with spin degeneracy $\nu=2$. Here there is already a non-trivial stationary state:

$$\nu=2,\quad \nu_0=1,\quad \theta_0=\frac{\pi}{2},$$
$$k_0=\frac{\Delta_0}{v_F},\quad E_0=\Delta_1=0,$$
$$W_s=\frac{2}{\pi}\Delta_0, \tag{24}$$

which we shall study in what follows. We note that this solution with $\theta_0=\pi/2$ has an electron-hole symmetry, i.e., self-trapping both of an electron, and of a hole leads to the same result.

6. We show that the soliton charge is delocalized. It follows from Eqs. (17), (18) that the density distributions $\rho_\mu(x)$ in the states $\mu=0,k$ are equal to

$$\rho_0(x)=\frac{1}{2\operatorname{ch}^2(k_0x)},\quad \rho_k(x)=\left[-\rho_0(x)+\frac{1}{L}\right]\frac{k_0}{\varepsilon_k(E_0+\varepsilon_k)}\frac{1}{L}.$$

The total change in density in the system has the form

$$\delta\rho(x)=\nu_0\rho_0+\nu\sum_k\rho_k(x)=\left(\nu_0-\nu\frac{\theta}{\pi}\right)\rho_0(x)+\frac{\nu_0}{L}. \tag{25}$$

In equilibrium $\theta=\pi\nu_0/\nu$ and we find from (25) that

$$\delta\rho(x)=\nu_0/L=\text{const}. \tag{25a}$$

An exact compensation of local charges has taken place. We shall show in section 4 that the effects of coupling between chains, and also commensurability again produces a local charge around the soliton, but at distances $l\gg\xi_0$.

The properties obtained can also be established without turning to the explicit form of the solution. We differentiate (12) with respect to x and use Eqs. (6) to (8). We get

$$\frac{1}{2}\frac{d\rho}{dx}=\Delta_1\frac{\delta W}{\delta\Delta_2}-\Delta_2\frac{\delta W}{\delta\Delta_1}. \tag{26}$$

Hence it follows that in equilibrium $\rho(x)=\text{const}$ and we are led to (25a). A similar investigation for a more general model is performed in section 3.

7. We show that the total soliton energy is delocalized. There is a lattice part of the energy density

$$w_{lat}=\frac{\Delta^2(x)}{g^2}-\frac{\Delta_0^2}{g^2}=-\frac{k_0^2}{g^2\operatorname{ch}^2(k_0x)},$$

a bound state energy density

$$w_b=E_0\rho_0(x),$$

and also an energy density of the states of the continuous spectrum

$$w_c(x)=-\sum_k\varepsilon_k\rho_k(x)=-\frac{\theta}{\pi}E_0\rho_0(x)+O\left(\frac{1}{L}\right).$$

The total energy density is equal to

$$w(x)=w_{lat}+\nu_0w_b+\nu w_c=\Delta_0(\nu_0-\nu\theta/\pi)\cos\theta\rho_0(x)+O(1/L). \tag{27}$$

We see from (27) that in equilibrium when $\theta=\theta_0=\pi\nu_0/\nu$ we have $w(x)\propto 1/L$ and from a comparison with (24) we get

$$w(x)=\frac{2}{\pi}\Delta_0\frac{1}{L}.$$

Thus, local changes in the electron and lattice energies are fully compensated. The total soliton energy (23a) is $W_s=(2/\pi)\Delta_0$ and is determined by the volume effects of the density of states[6] although the equilibrium conditions (19a), (20b) are defined locally.

8. The kinetic energy of a soliton moving with a velocity $v\ll u$ is basically determined, as for strong coupling polarons, by the lattice inertia. The electron contribution to the mass M_s is small in the ratio $\sim(u/v_F)^2\ll 1$. We have

$$W_{kin}=\int dx\frac{|\dot\Delta(x,t)|^2}{g^2\bar\omega^2}. \tag{28}$$

Neglecting the change in the shape of the soliton when it moves with a small velocity we can substitute into (28) $\Delta(x,t)=\Delta_0\tanh(x-vt)$. We obtain

$$W_s={}^1/_2M_sv^2,\quad M_s=\Delta_0/\pi u^2=m^*M/\pi m. \tag{28a}$$

9. In concluding this part we consider the special case of a system with two-fold commensurability when in the metallic phase there is one electron in the elementary cell. For the well known compounds of organic origin[2] the Peierls transition is in this case suppressed by the Mott–Hubbard effect (Ref.5).[5)] However, the model considered here can be applied to the K(*def*)TCP compound.[12] Moreover, as a result of recent studies[13] of polyacetylene $(CH)_x$ and interpretation of this system as a Peierls dielectric with a doubling of the period was proposed. In view of the large band width ($\approx$10 eV) Coulomb effects may be insignificant when $\Delta=0.7$ eV.

In all its complexity, the case considered can, according to Ref. 14, be reduced to a determination of the phase of the function $\Delta(x)$. By an appropriate choice of the constant χ in the definitions (3) and (4a), (4b) we can put in the functional (5b) $\Delta_1\equiv 0$, which corresponds to the condition $\theta=\pi/2$. After variation we get Eqs. (6a), (6b), and (8) for $\Delta_1=0$ but we need not take into account Eq. (7) and its consequences (19a) and (21). To sum up, we obtain all results described above for $\nu=2$, except the connection (23a) between θ_0 and ν_0. In the case considered we have $\theta=\pi/2$ automatically for any ν_0.

We arrive at the conclusion that the soliton can now

carry any number of localized electrons $\nu_0 = 0, 1, 2$. Correspondingly, the charge of the soliton will be $e_s = -e, 0, e$, where e is the charge of the carriers in the metallic phase. Allowance for the Coulomb interaction should lift the degeneracy of the energy W_s with respect to the charge e_s. To first order

$$W_s(e_s) = \frac{2}{\pi}\Delta_0\left[1 + C\frac{e_s^2}{v_F}\right].$$

The determination of the coefficient $C \sim 1$ is difficult because of the necessity to take into account the dispersion (2) of the permittivity.

One may conclude that the electro-neutrality ($\nu_0 = 1$) of a soliton in a non-commensurable system was the only consequence of the condition of equilibrium under variations of the phase of the function $\Delta(x)$. The other properties are the consequence of the condition of equilibrium under variations of the modulus of $\Delta(x)$, and are the same for non-commensurable and two-fold commensurable systems.

The results of this subsection correspond to the model considered in Ref. 6, and the preceding study to the model of a chiral field considered in Ref. 7.

3. EFFECT OF PERTURBATIONS ON THE LOCAL CHARGE OF A SOLITON

1. We showed in the preceding section in the framework of the one-dimensional Peierls–Fröhlich model that the charge and energy of the system remain uniform when there is a soliton present. Because of this the solitons need not contribute to the electrical and thermal conductivity of the system. Their only kinetic manifestations could be spin diffusion.

In actual systems one might expect an appreciable change in the local soliton properties. In particular, it is important to take into account the electron-electron interaction which is usually not weak. Moreover, it is necessary to study the effects of the coupling between the chains, the effect of phonon dispersion, of commensurability, and also of the soliton motion. The delocalization of the energy is an accidental property of the simple model and must disappear when we take the correlation energy into account. The delocalization of the charge was connected with the electron-hole degeneracy of the solution and may be conserved also for a more complicated system. In the present section we consider the problem of the local charge of a self-trapped excitation for a rather general model of a quasi-one-dimensional system of electrons on a deformed lattice. This special study can be carried out by analogy with the special case (26) on the basis of the equations of motion without having at our disposal the explicit form of the solution for the complicated model.

2. We consider a quasi-one-dimensional system of conducting filaments with transverse coordinates $\mathbf{R}_n$. We shall assume that there are no electron transitions between the filaments. Let the electrons on the same filament and on different filaments interact through long-wavelength phonon fields $\Phi_{in} = \Phi_i(x, \mathbf{R}_n, t)$, including the Coulomb potential $\Phi_c(x, \mathbf{R}_n)$, and through short-wavelength fields

$$B_\alpha(x, \mathbf{R}_n, t)\exp(i2p_F x) + B_\alpha^+(x, \mathbf{R}_n, t)\exp(-i2p_F x).$$

These fields are characterized by parameters for the interaction with the electrons $g_{mn}^{(i,\alpha)}(x_m, x_n)$ and by the bare Green functions

$$D_{m,n}^{(i,\alpha)}(x_m - x_n) = \sum_{k,\mathbf{k}_\perp} \frac{\bar{\omega}_\lambda^2}{\omega^2 - \omega_\lambda^2(k, \mathbf{k}_\perp)} \exp\{i[k(x_m - x_n) + \mathbf{k}_\perp(\mathbf{R}_m - \mathbf{R}_n)]\}. \quad (29)$$

To fix the ideas we shall put

$$\omega_\alpha^2(\mathbf{k}, \mathbf{k}_\perp) = \omega_\alpha^2(k) + \Omega_\alpha^2(\mathbf{k}_\perp), \quad \omega_\alpha^2(k) \approx \bar{\omega}_\alpha^2 + 2\bar{\omega}_\alpha \bar{s}_\alpha k, \quad (29a)$$

$$\Omega_\alpha^2(\mathbf{k}_\perp) = \sum_m I_{mn}^{(\alpha)} \exp\{i\mathbf{k}_\perp(\mathbf{R}_m - \mathbf{R}_n)\}.$$

We introduce operators for the creation $\psi_n^+(x)$, the annihilation $\psi_n(x)$, the density $\rho_n(x)$, and the current $j_n(x)$ of particles on the chain n, and also operators of the CDW components $\eta_n(x)$ and $\eta_n^+(x)$:

$$\rho_n(x) = \psi_n^+ \hat{I}\psi_n, \quad j_n(x) = \psi_n^+ \hat{\sigma}_z \psi_n, \quad \eta_n(x) = \psi_n^+ \hat{\sigma}_- \psi_n, \quad \eta_n^+(x) = \psi_n^+ \hat{\sigma}_+ \psi_n,$$

where $\hat{\sigma}_z$, $\hat{\sigma}_\pm = \frac{1}{2}(\hat{\sigma}_x \pm i\hat{\sigma}_y)$ and $\hat{I}$ are the Pauli matrices and the unit matrix. In these variables the system which we are describing is characterized by the Lagrangian

$$\mathcal{L} = \sum_{m,n,i,\alpha} \int dx \Big\{ \Big[\frac{1}{2} \Phi_{im} (D_{mn}^{(i)})^{-1} \Phi_{in} + B_{\alpha m}^+ (D_{mn}^{(\alpha)})^{-1} B_{\alpha m} \Big]$$
$$- [\Phi_{im} g_{mn}^{(i)} \rho_n + \Phi_{im} \tilde{g}_{mn}^{(i)} j_n + \Delta_n \eta_n^+ + \Delta_n^+ \eta_n] + \psi_n^+ \Big(i\hat{I}\frac{\partial}{\partial t} + i\hat{\sigma}_z \frac{\partial}{\partial x} \Big) \psi_n \Big\}, \quad (30)$$

where

$$\Delta_n(x, t) = \sum_{m,\alpha} g_{nm}^{(\alpha)} B_{\alpha m}(x, t) \quad (30a)$$

is the field which is conjugate to the CDW density $\eta_n(x)$. In the zeroth approximation for the Peierls-Fröhlich model the operator $\Delta_n(x, t)$ changes to the classical gap function $\Delta_n(x)$.

We assume that in the model considered, as in the particular Peierls-Fröhlich case, there exist self-trapping stationary excited states. The adiabatic approximation developed in section 2, which corresponds to the strong coupling polaron theory, means in the general case that at least some of the modes B_α have frequencies $\bar{\omega}_\alpha$ which are small compared to the soliton binding energy. On the other hand, it will become clear in what follows that only modes with a considerable dispersion, $\bar{s}$, I_{mn}, will turn out to affect the charge of the soliton appreciably. Both conditions lead us practically to one and the same mode—phonons of the acoustic branch $\alpha = a$. In the main adiabatic approximation we may assume the $B_a^{(x)}$ to be classical local deformations. We need the other modes in the quantum-mechanical averaging $\langle \ldots \rangle_a$ for given $B_a^{(x)}$. In the Feynman formulation this means that the functional integration is performed by the saddle-point method over the fields $B_a(x, t)$ while the integration over the other fields $B_\alpha(x, t)$ with $\alpha \neq a$ is assumed exact.

3. Let there be an isolated moving self-trapped excited state of the system in the neighborhood of the chain $n = 0$. Since the energy and charge of the excitation must be finite, the characteristic perturbations of the

quantities $\rho_n(x)$, $j_n(x)$, $\Delta_n(x)$ must decrease sufficiently rapidly with increasing chain number n. We can therefore determine the total perturbations

$$\rho(x,t)=\sum_n\langle\rho_n(x,t)\rangle_a,\quad J(x,t)=\sum_n\langle j_n(x,t)\rangle_a.$$

We determine also the effective gap parameter

$$\Delta(x,t)=|\Delta(x,t)|\exp[i\chi(x,t)],\quad |\Delta(x,t)|\to\Delta_0,\quad x\to\pm\infty$$

according to the formulae

$$\frac{d}{dx}\sum_n\langle\Delta_n^+\Delta_n\rangle_a=\frac{d}{dx}|\Delta(x,t)|^2,$$

$$\frac{1}{2i}\sum_n\left\langle\Delta_n^+\frac{d}{dt}\Delta_n-\Delta_n\frac{d}{dt}\Delta_n^+\right\rangle_a=|\Delta(x,t)|^2\frac{d\chi(x,t)}{dt}. \tag{31}$$

The function $\Delta(x,t)$ changes to the solution

$$\Delta(x)=\Delta_0\,\mathrm{th}(x/\xi_0)$$

for a fixed soliton in the model considered in section 2.

We use the equations of motion derived in Appendix I, which connect the operators ρ_n, j_n, and Δ_n. We average Eq. (A.I.12) at fixed perturbations of $B_a(x,t)$ and substitute Eqs. (31). We get and equation connecting the perturbed distributions $\rho(x,t)$, $J(x,t)$, and $\Delta(x,t)$:

$$\frac{d}{dt}\left[J-\frac{v}{2\pi}\frac{1}{u^2}\left|\frac{\Delta}{\Delta_0}\right|^2\frac{d\chi}{dt}\right]+\left[\frac{d\rho}{dx}-\frac{\omega_p^2}{v_F^2}\int_0^x\rho(y)\,dy+\sum_i\frac{a\hat{k}^2}{\omega^2/s_i^2-\hat{k}^2}\frac{d\rho}{dx}\right]+\bar{s}\bar{\omega}\frac{d}{dx}\frac{|\Delta|^2}{\Delta_0^2}, \tag{32}$$

where

$$u^2/v_F^2=\lambda\bar{\omega}^2/4\Delta_0^2,\quad \lambda=vg^2/2\pi v_F,$$

g^2 is defined by (A.I.8a).

We consider a perturbation moving with a constant velocity $v\neq s_i$. We then have from (A.I.5a) $J=v\rho$ and $d/dt=-v\,d/dx$. We get from (32)

$$\frac{d\rho}{dx}-\varkappa^2\int_0^x\rho(y)\,dy=\frac{df}{dx}, \tag{33}$$

where

$$f(x,t)=\frac{\bar{s}\bar{\omega}}{bv_F^2}\frac{|\Delta|^2-\Delta_0^2}{\Delta_0^2}+\frac{v}{2\pi b}\frac{v_F^2}{u^2}\frac{|\Delta|^2}{\Delta_0^2}\frac{d\chi}{dx},\qquad b=1-\frac{v^2}{v_F^2}-\sum_i\frac{a}{1-(v/s_i)^2},\quad \varkappa=\frac{1}{b^{1/2}}\frac{\omega_p^2}{v_F^2}. \tag{33a}$$

It follows from (33) that

$$\rho(x)=\frac{1}{2\varkappa}\int f''(y)\exp\{-\varkappa|x-y|\}\,dy \tag{34a}$$

or

$$\rho(x)=f(x)+\frac{\varkappa}{2}\int f(y)\exp\{-\varkappa|x-y|\}\,dy. \tag{34b}$$

In view of the fact that in reality $\omega_p\gg\Delta_0$ while $f(y)$ changes over a length not less than $\xi_0=v_F/\Delta_0\gg1/\varkappa$, we find from (34a) $\rho(x)\approx(1/\varkappa^2)f''(x)$.

Since $f(y)\to0$ as $y\to\pm\infty$ we find from (34a) the exact result that the soliton charge Q and dipole moment P_1 are equal to zero while the second and higher moments are finite:

$$Q=0,\quad P_1=0,\quad P_2=e\int\rho(x)x^2dx=\frac{2e}{\varkappa^2}\int f(y)\,dy. \tag{35}$$

We introduce a characteristic soliton length ξ and gap deformation amplitude δ. We then have from (33) to (35)

$$\rho(x)\sim\frac{\bar{s}}{v_F}\frac{\bar{\omega}}{\varepsilon_F}\frac{\varepsilon_F^2}{\omega_p^2}\frac{\delta}{\Delta_0}\frac{1}{p_F\xi^2},\quad P_2\sim e\frac{\bar{s}}{v_F}\frac{\bar{\omega}}{\varepsilon_F}\frac{\varepsilon_F^2}{\omega_p^2}\frac{\delta}{\Delta_0}\frac{\xi}{p_F}. \tag{36}$$

For the model considered in section 2 we have exactly

$$f=\frac{\bar{s}\bar{\omega}}{\omega_p^2}\frac{\varkappa^2}{\mathrm{ch}^2(x/\xi_0)},\quad P_2=4e\frac{\bar{s}\bar{\omega}}{\omega_p^2},\quad \rho(x)\approx\frac{\bar{s}\bar{\omega}}{\omega_p^2}\frac{2}{\xi_0^2}\frac{3\,\mathrm{th}^2(x/\xi_0)-1}{\mathrm{ch}^2(x/\xi_0)}. \tag{37}$$

We see that the local charges are small both in the adiabatic parameter $p_F\bar{s}/\omega_p$ and in the atomic parameter Δ_0/ε_F.

4. The exact compensation established above for the charge Q and the dipole moment P_1 occurs thanks to the long-range three-dimensional Coulomb field. At large distances and for a weak coupling between the chains the screening occurs with the participation of a large number of chains. However, in kinetic phenomena local charges are important, in particular, on the central chain $n=0$, where the localized electron is situated.

We consider Eq. (A.I.9) neglecting all effects of the coupling between the chains, i.e., $I_{mn}=0$. For j_0 and ρ_0 we get Eqs. (32), (33) with $\varkappa=0$, $\omega_p=0$. The solution of (33) is, according to (34b) $\rho_0(x)=f(x)$. As a result the charge Q and the even moments will be non-vanishing

$$Q\infty\frac{e}{b}\frac{\bar{s}}{v_F}\frac{\bar{\omega}}{\varepsilon_F}\frac{\delta}{\Delta_0}p_F\xi. \tag{38}$$

Substituting the solution found in section 2 into (33) we find to first order in the dispersion $\bar{s}/v_F$:

$$\rho(x)=\frac{1}{b}\frac{\bar{s}\bar{\omega}}{v_F^2}\frac{1}{\mathrm{ch}^2(x/\xi_0)},\quad Q=2\frac{e}{b}\frac{\bar{s}}{v_F}\frac{\bar{\omega}}{\Delta_0}. \tag{38a}$$

For a moving soliton it is necessary to consider the second term in Eq. (33) for $f(x)$. When substituting the zeroth solution it vanishes, since $\Delta(x)$ changes in the complex plane along a straight line through the origin. When dispersion is taken into account the motion, in general, deforms the soliton. However, one can show that the general nature of the solution does not change likewise in the next perturbation theory order in $(v/u)^2$. We cannot exclude the possibility that $Q(v)-Q(0)\propto(v/u)^{2n}$ with $n\geq3$.

4. SOLITONS IN THE ORDERED PHASE AND STATISTICAL EFFECTS

1. We consider the quasi-one-dimensional Peierls-Fröhlich model, characterized by an equilibrium gap

Δ_0 and a low three-dimensional ordering temperature $T_c \ll \Delta_0$. The binding energy of the soliton is

$$W_b = \Delta_0 - W_s = \Delta_0(1-2/\pi) \approx 0{,}36\Delta_0,$$

i.e., $W_b \gg T_c$, so that its formation (electron self-trapping) proceeds mainly independently of the surrounding chains. As a result, however, there occurs on the central chain $n=0$ a change in sign of the parameter $\Delta(x)$ when one passes through the soliton region with center at the point x_0. Since the chains in the ordered phase must be correlated, the change in sign of $\Delta(x)$ far from the soliton will be smoothed out and this must be reflected in the soliton properties. If the perturbation of the surrounding chains decreases rapidly with increasing n, it is sufficient for a description of the effect to take into account the chain $n=0$, which carries the soliton, and Z of its nearest neighbors. Since the smoothing out will take place over distances $l \sim v_F/T_c \gg \xi_0$ we can use a quasi-classical description in terms of the phase χ_n on the chains, assuming $|\Delta_n(x)| \equiv \Delta_0$. In that case the presence of the soliton is taken into account by a jump in the phase $\chi_0(x)$:

$$\chi_0(x_0+0) - \chi_0(x_0-0) = \pi \tag{39}$$

while the phases $\chi_n(x)$, $n \neq 0$, are continuous.

2. The model described here is characterized by the energy functional

$$\mathcal{H}\{\chi\} = \sum_n \int \frac{v_F\,dx}{4\pi}\left[(\chi_n')^2 - \frac{1}{(Z+1)l^2}\cos(\chi_n - \chi_0)\right], \tag{40}$$

where the region $|x| \lesssim \xi_0$ is excluded from the integral.

The equilibrium state of the system is described by the extrema of (40) with the additional condition (39). We define for $n \neq 0$: $\chi_n(x) = \chi_0(x) + \psi(x)$. The functions χ_0 and ψ satisfy the equations

$$\begin{aligned} &(Z+1)\chi_0'' + Z\psi'' = 0, \\ &(Z+1)\psi'' + (Z+1)\chi_0'' - l^{-2}\sin\psi = 0 \end{aligned} \tag{41}$$

and the boundry conditions[6)]

$$\text{as } x \to \pm\infty\text{: } \psi(x),\ \psi'(x),\ \chi_0'(x) \to 0, \tag{42a}$$

$$\text{as } x \to x_0\text{: } \chi_0(x) = -\psi(x) = {}^1/_2\pi\,\mathrm{sgn}(x-x_0). \tag{42b}$$

From (41), (42) we get the following solution:

$$\psi(x) = -4\,\mathrm{arctg}\left\{\exp\left[\frac{l_0 - |x-x_0|}{l}\right]\right\}\mathrm{sgn}(x-x_0), \tag{43}$$

$$\chi_0(x) = \frac{1}{Z+1}\left[\frac{\pi}{2}\mathrm{sgn}\,x - Z\psi(x)\right], \quad \chi_n(x) = \frac{1}{Z+1}\left[\frac{\pi}{2}\mathrm{sgn}\,x + \psi(x)\right],$$

where $l_0 = l\ln(\tan\pi/8)$.

The functions $\chi_0(x)$ and $\chi_n(x)$ are shown in Fig. 3, and $\theta_z = \pi/2(Z+1)$.

3. Although the core of the soliton is uncharged, in the region where the phase is smoothed out $\xi_0 \ll |x-x_0| \lesssim l$ there appear charges q_n with a density $\rho_n(x) = e_n\chi_n'(x)/\pi$. From (42) we have

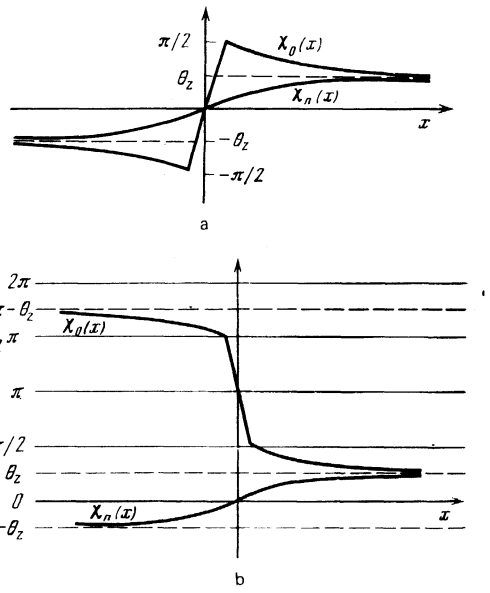

FIG. 3.

$$q_0 = 2\frac{e_0}{\pi}[\chi_0(\infty) - \chi_0(0)] = -\frac{e_0 Z}{Z+1},$$

$$q_n = \frac{e_n}{\pi}[\chi_n(+\infty) - \chi_n(-\infty)] = \frac{e_n}{Z+1}, \quad n \neq 0.$$

For a soliton with the opposite change in amplitude all charges q_0 and q_n change in sign. The total charge q of the system depends on the signs of the carrier charges e_n:

a) all chains are charged identically:

$$e_n = e_0,\ q = q_0 + Zq_n = 0$$

in agreement with the results of section 3;

b) the surrounding chains are charged opposite to the central one:

$$e_n = -e_0,\quad q = q_0 - Zq_n = -\frac{2Z}{Z+1}e_0,$$

as $Z \to \infty$ we have $q \to -2e$, i.e., the charge is doubled;

c) the charges of the chains alternate:

$$\sum_{n\neq 0} e_n = 0,\quad q = q_0 = -\frac{Z}{Z+1}e,$$

$q \to e$, as $Z \to \infty$—the system has a single charge. Case a) corresponds to systems with total charge transfer, for instance, KCP, while case c) corresponds to systems with partial transfer, for instance, from the TTF-TCNQ series. In KCP the solitons thus remain uncharged, while in TTF-TCNQ they have a charge $\sim -e$ localized in a region $l \sim v_F/T_c$.

4. The presence of coupling between the chains also leads to a more appreciable interaction between the solitons. As shown above, the change in $\Delta(x)$ for an isolated soliton occurs along a well defined diameter which is perpendicular to the direction of ordering $\Delta(+\infty) = \Delta(-\infty)$. We can therefore speak of solitons with two signs: corresponding to $\psi(x) \approx \pm\frac{1}{2}\pi\ \mathrm{sgn}(x - x_i)$ as $x \to x_i$.

We obtain in Appendix II a solution of Eqs. (41) for two solitons positioned at a distance $d \gg \xi_0$. The calcu-

lation of the energy $\mathcal{H}$ of (40) and of the interaction force $\mathcal{F} = -\partial\mathcal{H}/\partial d$ shows that solitons of opposite sign on the same filament and of the same sign on neighboring filaments attract one another, $\mathcal{F}_{\perp\perp} < 0$, while solitons with the same sign on the same filament and of opposite sign on neighboring filaments repel one another, $\mathcal{F}_{\perp\perp}$, $\mathcal{F}_{\perp\perp} > 0$. According to (A.II.3, 6, 11) we have for $d \lesssim l$

$$|\mathcal{F}| \sim v_F/e^2 \approx T_c^2/v_F, \tag{44a}$$

and for $d \gg l$

$$|\mathcal{F}| \sim (v_F/e^2)\exp\{-2d/l\}. \tag{44b}$$

At a finite temperature $T \ll T_c$, attracting solitons will be in a region $d \lesssim l_T$ where the thermal length l_T is determined from the relation $\mathcal{F} l_T \propto T$ under the condition that $l_T \ll l$. We get

$$l_T \sim v_F T/T_c^2, \quad l_T/l \sim T/T_c \ll 1.$$

When $T < T_c^2/\Delta_0 \ll T_c$, we have $l_T \sim \xi_0$. In that case bound solitons on a single filament must annihilate.

Quantum oscillations of a pair of solitons at distances $\xi_0 < |x| < l$ can be described by the Hamiltonain

$$\hat{\mathcal{H}} = -\frac{1}{2M_s}\frac{\partial^2}{\partial x^2} + \frac{v_F}{l^2}|x|, \tag{45}$$

where M_s is given by Eq. (28). From (45) we can estimate the amplitude of the zero-point oscillations $d_0 = \langle |x| \rangle$:

$$\frac{d_0}{l} \sim \left(\frac{u}{v_F}\right)^{2/3}\left(\frac{T_c}{\Delta_0}\right)^{1/3}. \tag{46}$$

For typical parameters $u/v_F \sim T_c/\Delta_0 \sim 10^{-1}$ we have $d_0/l \sim 10^{-1}$. The estimates given here are valid if $d_0 \gg \xi_0$. In reality, however,

$$d_0/\xi_0 \sim \left(\frac{u}{v_F}\frac{\Delta_0}{T_c}\right)^{2/3} \sim 1.$$

The Hamiltonian (45) also possesses a large number

$$N \sim \frac{v_F}{u}\left(\frac{\Delta_0}{T_c}\right)^{1/2} \sim 10^2$$

of quasi-classical levels

$$\varepsilon_n \sim T_c(n/N)^{2/3}.$$

In the states with $n \gg 1$ the average distance between the solitons $|x| \gg \xi_0$.

5. From the estimates given above it follows that as the result of thermal motion when $T \ll T_c$ solitons on the same chain must attract and annihilate one another, but on neighboring chains they must form quasi-classical bound states, when $l_T > \alpha_0$, or quantum states when $l_T < \alpha_0$. The linear concentration of solitons c has the form

$$c = (\overline{M}_s T/2\pi)^{1/2}\exp\{-W_s/T\},$$

in reality

$$cl \sim 100(T/W_s)^{1/2}\exp\{-W_s/T\},$$

whence for $T < T_c < W_s/4$ we have $cl \ll 1$.

We find that when $T < T_c$ separate solitons and bound complexes are on average far from one another and pratically do not interact. Due to the rare collisions there may occur a coupling of solitons of the same sign on a large number of neighboring filaments so that planes are formed with a simultaneous change in sign of all $\Delta_n(x)$. An analogous coupling may occur between solitons and microscopic defects.

6. The interaction of the CDW with the main structure at odd-order commensurability leads qualitatively to the same effects as the described interaction of the chains. In practice only the case of three-fold commensurability is important. The jump in phase must proceed from $\chi(x_0 - 0) = -\pi/6$ to $\chi(x_0 + 0) = 5\pi/6$ with a corresponding smoothing out of the phase to $\chi(-\infty) = 0$, $\chi(+\infty) = 2\pi/3$. Hence, the soliton charge $q_s = 2e/3$.

5. CONCLUSION

1. In the present paper and in an earlier one[5] we have shown that in the quasi-one-dimensional Peierls-Fröhlich system a particularly strong interaction is realized between the electron and phonon degrees of freedom of the excited states. As a result purely electron or hole excitations with wavevector k and energy $\varepsilon_k = [\Delta_0^2 + (v_F k)^2]^{1/2}$ go over into self-trapped states of size $\sim \xi_0$. The deformation of the Peierls superstructure [gap parameter $\Delta(x)$] has the form of a domain wall $\Delta(x) = \Delta_0 \tanh(x/\xi_0)$. This deformation produces one bound state which must be occupied by one electron, $\nu_0 = 1$. As a result of the polarization of the vacuum states of the continuous spectrum, the local charge density turns out to be exactly compensated $\rho_s(x) = 0$. As a result the soliton turns out to be electrically non-active, $e_s = 0$. However, it carries a localized spin $\frac{1}{2}$. A special case is a system with commensurability 1:2 (doubling of the period). In that case bound states can have any multiplicity of occupation, $\nu_0 = 0, 1, 2$, and correspondingly $e_s = -e,\ 0,\ e$; $s = 0,\ \frac{1}{2},\ 0$.

The energy, and also the charge, of the soliton turn out to be delocalized. The soliton mass $M_s \sim \Delta_0/u^2$, where u is the CDW phase velocity. It is larger than the electron effective mass, as follows

$$\frac{M_s}{m^*} \sim \frac{v_F^2}{u^2} \sim \frac{M}{m} \sim 10^2.$$

These results were given in section 2.

The property of electro-neutrality of the stationary self-trapped state is conserved also for systems with electron-electron interactions. It is subject to a weak influence of the initial phonon dispersion in the Kohn anomaly region $\omega(2p_F + q) \approx \bar{\omega} + \bar{s}q$. As a result there appears a local soliton charge $e_\varepsilon \propto \Delta_0/\varepsilon_F$. These problems were considered in section 3.

The effects of coupling between the chains and of even-order commensurability lead to the smoothing out of the jump in the phase of the function $\Delta(x)$ in the region $\sim\xi_0$. The smoothing out occurs at distances $l \sim v_F/T_c$

and v_F/T_p, where T_c and T_p are the three-dimensional ordering and pinning temperatures. As a result the soliton may acquire a charge $e_s \sim e$, localized in a region $\sim l$ without a change in the spin. This problem was studied in section 4.

The same effects are responsible for the attraction of solitons of opposite sign on the same chain or the same sign on neighboring ones. As a result there appears a system of bound states with a large number of levels. This effect is considered in section 4.

2. The self-trapped states considered here must manifest themselves in spin diffusion effects and in photo-electric effects. They may be discovered in absorption or luminescence at the frequency Δ_0. The experimental effects will be considered in detail in a separate publication. The polaron effect must, in principle, affect the semi-conducting properties of systems such as a Peierls dielectric.

The principal role must be played by the fast build-up of solitons with increasing temperature in view of their large mass $M_s \gg m^*$ and lowered energy $W_s < \Delta_0$. The result may become a phase transition into an intermediate state at a temperature $T^* < \Delta_0$ when the soliton density becomes of the order of ξ_0^{-1}.

Soliton states are of great importance for systems close to two-fold commensurability when

$$n = \pi^{-1}|2p_F - \pi/a| < \xi_0^{-1}, \tag{47}$$

where a is the period of the undeformed lattice. Such a situation can be realized accidentally when there is incomplete charge transfer or when there is alloying as in polyacetylene.[13]

It was shown in Ref. 14 that when condition (47) is satisfied a superstructure will be formed with a wave-vector $Q = \pi/a \neq 2p_F$. For a uniform deformation $\Delta(x)$ = const states above the gap (electron or hole states for $2p_F \gtrless Q$ might be occupied with a density n. From the results of the present paper and of Ref. 5 it is clear that as the result of the polaron effect a system is formed of charged, $e_s = e$, spinless, $s = 0$, solitons with a density n, carrying a two-fold occupied ($\nu_0 = 2$) local level. When $n < \xi_0^{-1}$ the interaction between the solitons is unimportant. Similar conclusions were reached by Su, Schrieffer, and Heeger[15] as a result of numerical calculations of soliton states on a chain of finite length with a Peierls dimerization. The qualitative conclusions and quantitative results of Ref. 15 agree with the results of the analytical study given in section 2 of the present paper when applied to a system with two-fold commensurability (subsection 9). The results of Ref. 15 agree quantitatively with the data about the activation energies in alloyed polyacetylene.[13] It is especially important that an explanation is obtained for the absence in this substance of spin paramagnetism of the current carriers. The Peierls nature of the dimerization in $(CH)_x$ is thus confirmed and also the self-trapping of the current carriers[5] in a one-dimensional Peierls system. We note that there is in polyacetylene a well defined adiabatic parameter $M/m = \pi M_s/m^*$. According to Ref. 15 $M_s = 7m_e$ and $m^*/m_e \approx \Delta_0/\varepsilon_F \approx 10$ (m_e is the free electron mass, $m_e \approx m$). Hence, $M/m \sim 10^2$.

In conclusion we emphasize that the self-localized states described here exist only for a sufficiently weak coupling between the superstructures on neighboring chains. For non-commensurable systems the necessary restriction is expressed by the inequality $T_c \ll \Delta$. For a system with a two-fold commensurability a condition must be satisfied by the anisotropy parameter of the phonon spectrum $\alpha = \Omega^2/\omega^2(2k_F) : \alpha \gg \lambda$, where $\lambda = g^2/\pi v_F$.

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APPENDIX I

We consider the system described in section 3 and determined by the Lagrangian (30) and Eqs. (29), (29a), (30a). We formulate the equations of motion for the operators $\rho_n(x,t)$ and $j_n(x,t)$, using the commutation relations

$$[\rho_n(x), \eta_m(y)] = 0, \quad [\rho_n(x), \eta_m^+(y)] = 0,$$
$$[\rho_n(x), j_m(y)] = i2\pi \frac{\partial}{\partial x}\delta(x-y)\delta_{mn}, \tag{A.I.1}$$
$$[j_n(x), \eta_m(y)] = 2\eta(x)\delta(x-y)\delta_{mn}, \quad [j_n(x), \eta_m^+(y)] = -2\eta^+(x)\delta(x-y)\delta_{mn}.$$

These relations follow from the corresponding boson representations,[16] valid for electrons in the vicinity of the Fermi level. They also require refinements of the interatomic radius when there are interactions present. However, one usually assumes that these effects lead only to a change in the numerical coefficients in the equations which follow below. For us the coefficient of $d\rho_n/dx$ in (A.I.3) is important and it will in what follows be renormalized as the compressibility of the system. We get

$$\frac{d\rho_n}{dt} + \frac{dj_n}{dx} = -2\pi \sum_{m,i} \tilde{g}_{mn}^{(i)} \Phi_{im}, \tag{A.I.2}$$

$$\frac{dj_n}{dt} + \frac{d\rho_n}{dx} = -2\pi \sum_{m,i} g_{mn}^{(i)} \frac{d}{dx} \Phi_{in} + \frac{2}{i}(\Delta_n \eta_n^+ - \Delta_n^+ \eta_n). \tag{A.I.3}$$

Varying (30) with respect to Φ_{in}, $B_{\alpha n}$, and $B_{\alpha n}^+$ we get

$$\Phi_{im} = \sum_{l,n} D_{ml}^{(i)} [g_{ln}^{(i)} \rho_n + \tilde{g}_{ln}^{(i)} j_n], \quad B_{\alpha m} = \sum_{l,n} D_{ml}^{(\alpha)} g_{ln}^{(\alpha)} \eta_n. \tag{A.I.4}$$

We substitute (A.I.4) in (A.I.3) and put $\tilde{g}^{(i)} = 0$, which corresponds to neglecting relativistic interactions. We obtain

$$\frac{d\rho_n}{dt} + \frac{dj_n}{dx} = 0, \tag{A.I.5}$$

$$\frac{dj_n}{dt} + \frac{d}{dx} \sum_m \left[\delta_{mn} + 2\pi \sum_{i,m,l} g_{nl}^{(i)} D_{lm}^{(i)} \right] \rho_m = h_n, \tag{A.I.6a}$$

where

$$h_n = \frac{2}{i} \sum_m (\eta_n^+ R_{nm} \eta_m - \eta_m^+ R_{nm}^* \eta_n),$$

or

$$h_n = \frac{2}{i} \sum_m (\Delta_n^+ R_{nm}^{-1} \Delta_m - \Delta_m^+ R_{nm}^{*-1} \Delta_n), \tag{A.I.6b}$$

$$R_{nm} = \sum_{k,l,\alpha} g_{nl}^{(\alpha)} D_{lk}^{(\alpha)} g_{km}^{(\alpha)}. \tag{A.I.7}$$

For small ω, k we write

$$R_{nm}^{-1}(k)=\frac{1}{g^2}\left[\left(1+\frac{\bar{s}}{\bar{\omega}}k-\frac{\omega^2}{\bar{\omega}^2}\right)\delta_{mn}+I_{mn}\right], \tag{A.I.8}$$

where

$$g^2=\sum_{\alpha,m}(g_{mn}^{(\alpha)})^2. \tag{A.I.8a}$$

If the coupling constants do not have dispersion $g_{mn}^{(\alpha)}=g_\alpha\delta_{mn}$, the quantities $\bar{s}/\bar{\omega}$, $\bar{\omega}^{-2}$ and I_{mn} in (A.I.8) are averages over α of the corresponding quantities in (30), with weight g_α^2/g^2. Substituting (A.I.8) in (A.I.5) we get

$$\frac{d}{dt}\left[j_n+\frac{2i}{\sigma^2\bar{\omega}^2}\left(\Delta_n^+\frac{d\Delta_n}{dt}-\frac{d\Delta_n^+}{dt}\Delta_n\right)\right]+\frac{d}{dx}\left\{\sum_m\left[\delta_{mn}+2\pi\sum_{i,l}(g_{ml}^{(i)})^2D_{ln}^{(i)}\right]\rho_m+\frac{4}{g^2}\frac{\bar{s}}{\bar{\omega}}\Delta_n^+\Delta_n\right\}$$
$$=\frac{4i}{g^2\bar{\omega}^2}\sum_m I_{mn}(\Delta_n^+\Delta_m-\Delta_m^+\Delta_n). \tag{A.I.9}$$

3. We introduce the total charge density $\rho(x)$ and current $J(x)$ along the chains:

$$\rho(x)=\sum_n\rho_n(x),\quad J(x)=\sum_n j_n(x). \tag{A.I.10}$$

If we sum (A.I.9) over n, the right-hand side vanishes and on the left-hand side we can write for the Fourier representation

$$2\pi\sum_{i,l,m}g_{ml}^{(i)}D_{lk}^{(i)}g_{kn}^{(i)}=\sum_{i\neq e}\frac{a_ik^2}{(\omega/s_i)^2-k^2}+\frac{4\pi e^2}{\varepsilon_\infty S_\perp k^2}, \tag{A.I.11}$$

where $a_i\sim 1, \Sigma a_i=a$ is the relative correction to the compressibility of the system, s_i are the sound velocities, ε_∞ is the permittivity of the structure, and $S_\perp$ is the cross section per filament. We get

$$\frac{d}{dt}\left[J+\frac{4i}{g^2\bar{\omega}^2}\sum_n(\dot{\Delta}_n\Delta_n^+-\dot{\Delta}_n^+\Delta_n)\right]+\frac{d}{dx}\left\{\left[1-a+\sum_i\frac{a_i\hat{\omega}^2}{\omega^2-s_i^2\hat{k}^2}+\frac{\omega_p^2}{v_F^2\hat{k}^2}\right]\rho(x)+\bar{s}\bar{\omega}\sum_n\Delta_n^+\Delta_n\right\}=0, \tag{A.I.12}$$

where

$$\omega=i\partial/\partial t,\quad \hat{k}=-i\partial/\partial x,\quad \omega_p^2=4\pi e^2v_F/\varepsilon_\infty S_\perp.$$

APPENDIX II

1. We consider two solitons of the same sign positioned at the points $\pm d/2$. The boundary condition (42b) is generalized in accordance with Fig. 4a

$$\psi\left(-\frac{d}{2}-0\right)=\pi+\psi\left(-\frac{d}{2}+0\right)=\psi_-,$$
$$\psi\left(\frac{d}{2}+0\right)=-\pi+\psi\left(\frac{d}{2}-0\right)=\psi_+. \tag{A.II.1}$$

The solutions of Eqs. (41) outside the discontinuity points $x=\pm d/2$ are characterized by the first integral H or k:

$$^1/_2l^2\psi'^2-(1-\cos\psi)=H,\quad H=2/k^2-2. \tag{A.II.2}$$

It follows from (42a) that when $|x|>d/2$ we have $H=0$, $k=1$. When $|x|<d/2$ the quantity $H=H(d)$ is, according to the principle of least action for the functional (40), proportional to the force of the interaction between solitons $\mathcal{F}$:

$$\mathcal{F}=-\frac{\partial\mathcal{H}}{\partial d}=\frac{Z}{Z+1}\frac{v_FH}{2\pi l^2}. \tag{A.II.2a}$$

The quantity (40) is at the extrema of (A.II.2) equal to

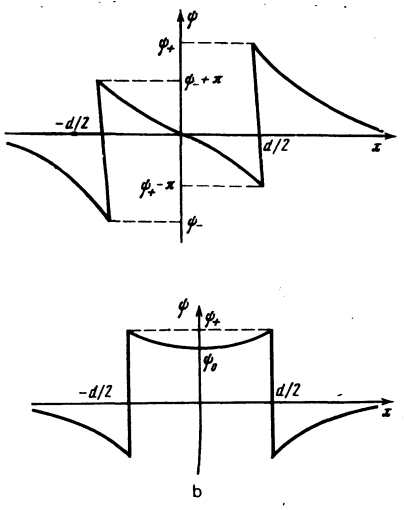

FIG. 4.

$$\frac{2\pi}{v_F}l^2\frac{Z+1}{Z}\mathcal{H}=\int_{\psi_-}^{\psi_+}\left(2H+4\sin^2\frac{\psi}{2}\right)^{1/2}d\psi+\int_{\psi_+-\pi}^{\pi+\psi_-}2\left|\sin\frac{\psi}{2}\right|d\psi-Hd. \tag{A.II.3}$$

Varying (A.II.3) with respect to ψ_+, ψ_- for given H we get $\psi_+=-\psi_-$, i.e., the solution is antisymmetric and

$$\cos\frac{\psi_\pm}{2}=\frac{1}{2^{1/2}k},\quad \frac{1}{2^{1/2}}\leqslant k\leqslant 1. \tag{A.II.4}$$

The solution of (A.II.2) can be written in the form

$$\cos\frac{\psi}{2}=\mathrm{sn}\left(\mathrm{K}(k)-\frac{x}{kl},k\right), \tag{A.II.5}$$

where $\mathrm{K}(k)$ is the complete elliptical integral of the first kind. The quantity k is, according to (A.II.1, 4, 5) determined from the equation

$$\mathrm{sn}\left(\mathrm{K}(k)-\frac{d}{2kl},k\right)=\frac{1}{2^{1/2}k}. \tag{A.II.6}$$

When $d\gg l$ we have $k\to 1$, $\psi_\pm\to\pi/2$ and $H=[32/(2^{1/2}+1)^2]e^{-d}$. We found in particular that for an isolated soliton the smoothing out of the phase occurs antisymmetrically (see footnote 6).

When $d\ll l$ we have $k\to 2^{-1/2}$, $\psi_\pm\to 0$ and $H\to 2$, i.e., the repulsive force is finite.

2. We consider the case of solitons of opposite sign. Instead of (A.II.1) we have in correspondence with Fig. 4b

$$\psi\left(-\frac{d}{2}+0\right)=\psi\left(\frac{d}{2}-0\right)=\psi_+,\quad \psi\left(-\frac{d}{2}-0\right)=\psi\left(\frac{d}{2}+0\right)=\pi-\psi_+. \tag{A.II.7}$$

Since $\psi'(0)=0$ and $\psi(0)\neq 0$, now $H<0$ in (A.II.2), i.e., there is an attraction. Instead of (A.II.3) we have

$$\frac{2\pi}{v_F}l^2\frac{Z+1}{Z}\mathcal{H}=2\int_{\psi_0}^{\psi_+}\left(2H+4\sin^2\frac{\psi}{2}\right)^{1/2}d\psi+4\int_{\psi_+-\pi}^{0}\sin^2\frac{\psi}{2}d\psi-Hd. \tag{A.II.8}$$

Varying (A.II.8) with respect to ψ_0 and ψ_+ we get

$$\cos\psi_+=-\sin^2\frac{\psi_0}{2},\quad H=-2\sin^2\frac{\psi_0}{2}. \tag{A.II.9}$$

The solution of (A.II.2) now is

$$\cos\frac{\psi}{2}=\cos\frac{\psi_0}{2}\,\mathrm{sn}\left[\mathrm{K}\left(\cos\frac{\psi_0}{2}\right)-\frac{x}{l},\cos\frac{\psi_0}{2}\right]. \tag{A.II.10}$$

According to (A.II.8, 9, 10) the quantity ψ_0 is deter-

mined from the equation

$$\operatorname{sn}\left[K\left(\cos\frac{\psi_0}{2}\right)-\frac{d}{2l},\ \cos\frac{\psi_0}{2}\right]=\frac{1}{2^{1/2}}. \qquad \text{(A.II.11)}$$

The solution of (A.II.11) has a continuous singularity at the point $d/l=\pi/2, \psi_0=\pi$. When $d\gg l$ we have $\psi_0\to 0$, $\psi_+\to\pi/2$.

$$H\approx-[32/(2^{1/2}+1)^2]e^{-d}.$$

When $d\leq(\pi/2)l$ we have $\psi_0\equiv\psi_+\equiv\pi, H\equiv 2$. In this region there is a finite attractive force (A.II.2a) for $H=2$ which is independent of distance.

Note added in proof (27 December 1979). Correction: the last terms in Eqs. (A.I.12) and (32), the first term in the definition (33a) and the right-hand sides of Eqs. (36), (37), (38), and (38a) must be multiplied by the coefficient $v_F\Delta_0^2/g^2\overline{\omega^2}=\nu v_F^2/2\pi u^2$. As a result the local charges turn out to be small in the parameter Δ_0/ε_F, but not in $\bar{s}/v_F$.

The uniform change (25a) of the phonon charge when there is a soliton present is in fact compensated by a decrease by one of the number of states in the occupied band: the local level $\mu=0$ is formed from detached states of the continuous spectrum (remark by J. R. Schrieffer).

For the compound K(*def*)TCP the situation turns out to be more complicated than was assumed in section 2.9 in view of the fact that the two-fold commensurability occurs only when we take into account the weak potential of the K^+ ions and the energy for fixing the phase may be small compared to Δ_0. The theory of this compound will be given separately.

The exact solution for a system with a two-fold commensurability which is equivalent to the results of subsection 2.9 was found recently by Takayama, Lin-Lin, and Maki (1979 preprint).

The authors express their deep gratitude to J. R. Schrieffer for interesting discussions of the theory of quasi-one-dimensional systems and of the physics of poly-acetylene.

[1)]In related three-dimensional systems of the exciton insulator type and in superconductors there is a weak coupling parameter $(\Delta/\varepsilon_F)^2\ll 1$.

[2)]In what follows $v_F=1$ in all intermediate formulae. Also $\hbar=1$ everywhere.

[3)]In the cited papers they found also stationary soliton-antisoliton pairs with a fixed distance l, which depended on ν_0/ν. However, when $\nu=1$ these solutions are not present, while for $\nu=2$ we have $l=\infty$, i.e., only isolated solitons are stationary.

[4)]The arguments given here allow us to avoid the more laborious direct calculation of the energy $W(\theta)$, given in Refs. 6, 7.

[5)]In that case, however, the so-called spin-Peierls dimerization may occur[11] where analogous effects again arise. For the easy plane kind of anisotropy the spin-lattice system will in general be isomorphic to the Peierls-Fröhlich electron model.

[6)]Condition (42b) assumes in addition to (39) that we have chosen an extremum (39) which is anti-symmetric with respect to x_0. One can show that such a choice corresponds to an absolute minimum of $\mathcal{H}$ (see Appendix II).

[1]L. N. Bulaevskiĭ, Usp. Fiz. Nauk **115**, 263 (1975) [Sov. Phys. Usp. **18**, 131 (1975)].
[2]J. J. Andre, A. Bieber, and F. Gautier, Ann. Phys. (Paris) **1**, 145 (1976).
[3]G. A. Toombs, Phys. Rep. **40**, 183 (1978).
[4]S. A. Brazovskiĭ and I. E. Dzyaloshinskiĭ, Zh. Eksp. Teor. Fiz. **71**, 2338 (1976) [Sov. Phys. JETP **44**, 1233 (1976)].
[5]S. A. Brazovskiĭ, Pis'ma Zh. Eksp. Teor. Fiz. **28**, 656 (1978) [JETP Lett. **28**, 606 (1978)].
[6]G. R. Dashen, B. Hasslacher, and A. Neveu, Phys. Rev. **D12**, 2443 (1975).
[7]S. S. Shei, Phys. Rev. **D14**, 535 (1976).
[8]V. A. Fateev, A. S. Shvarts, and Yu. S. Tyupkin, Lebedev, Phys. Inst., Akad. Nauk SSSR, Preprint No. 155, 1976.
[9]É. I. Rashba, Opt. Spektrosk. **2**, 88 (1957).
[10]V. I. Mel'nikov, Zh. Eksp. Teor. Fiz. **72**, 2345 (1977) [Sov. Phys. JETP **45**, 1233 (1977)].
[11]E. Pytte, Phys. Rev. **B10**, 4637 (1977).
[12]K. Carneiro, J. W. Williams, and C. S. Jacobsen, Proc. Internat. Conf. on Quasi-One-Dimensional Conductors, Lecture Notes in Physics, Springer, 1979.
[13]A. J. Heeger, and A. G. MacDiarmid, Proc. Internat. Conf. on Quasi-One-Dimensional Conductors, Lecture Notes in Physics, Springer, 1979.
[14]S. A. Brazovskiĭ, I. A. Dzyaloshinskiĭ, and S. G. Obukhov, Zh. Eksp. Teor. Fiz. **72**, 1550 (1977) [Sov. Phys. JETP **45**, 184 (1977)].
[15]W. P. Su, J. R. Schrieffer, and A. J. Heeger, Preprint, Univ. Pennsylvania, 1979.
[16]A. Luther and I. Peschel, Phys. Rev. **B9**, 2911 (1974).

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