

# Solitons in charge-density-wave crystals

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(Submitted 20 July 1990)

Zh. Eksp. Teor. Fiz. **99**, 887–898 (March 1991)

A theory is derived for charge density waves (CDWs) in a crystalline order at low temperatures. The various types of solitons which arise from the self-trapping of electrons are described. The adaptation of the CDW medium to the formation of  $\pi$  and  $2\pi$  solitons is examined. A model-independent approach is proposed for describing the interaction of solitons with the Coulomb field and the phase deformation. Screening effects, self-screening effects, and commensurability effects are examined. The interactions of solitons with each other and with impurities are described. Cases are found in which an attraction of solitons causes them to cluster in microscopic phase-slippage centers.

## 1. INTRODUCTION

The electronic properties of quasi-one-dimensional conductors with a charge density wave (CDW) are distinctive for two reasons. The first stems from the translational degeneracy of the ground state of the CDW, which leads to Fröhlich conductivity.<sup>1,2</sup> The effect is seen in a giant dielectric constant and in nonlinear and time-varying effects.<sup>3–7</sup> The second reason is a strong interaction of the CDW deformation with above-gap electrons. This interaction leads to a rapid self-trapping of the electrons as they convert into various types of solitons (see the reviews in Refs. 8 and 9). There has been essentially no theoretical work on these phenomena. The extensive experimental research has been devoted to the Fröhlich conductivity (see the reviews by Jerome, Gill, Grüner, Ong, Fleming, Nagy, Schlenker *et al.* in Refs. 3–6), while the physics of solitons is studied in another object, polyacetylene (see the reviews in Refs. 10 and 11). In the latter case, with a twofold commensurability, there are no CDW slippage effects.

In recent years, the main themes of the experimental research on CDWs have shifted to low temperatures and/or to materials with a well-developed CDW crystal structure and a corresponding conversion of the electronic spectrum to that of an insulator. This includes the so-called blue bronzes and the tetrachalcogenides of transition metals (see the reviews in Refs. 3–6 and 12). In this connection, and also because of the “gap” in the theoretical papers which we mentioned earlier, it is worthwhile to reexamine the microscopic picture of the conversion of normal carriers into solitons and of the evolution of solitons into a CDW slippage. It is particularly important to determine how the electrons injected at a contact ultimately evolve into an electron-free deformation of the CDW in the volume. For an isolated one-dimensional chain of CDWs, this process would be clear in principle. Each electron (or hole) with an energy  $E$  near the edge  $\pm \Delta_0$  of a gap  $2\Delta_0$  evolves spontaneously into an entity which is nearly an amplitude soliton.<sup>8,9,13–15</sup> The original electron is trapped at a local level near the center of gap, at  $E = 0$ . In this process, which plays out over times  $\omega_{\text{ph}}^{-1} \sim 10^{-11}$  s, where  $\omega_{\text{ph}}$  is the frequency of the phonons on the CDW wave vector  $Q$ , an energy  $\approx 0.3\Delta_0$  is liberated. Later, over long times (in the collision scale), pairs of amplitude solitons convert into  $2\pi$  phase slippages, in a process accompanied by the disappearance of a pair of electrons in

an expanded continuum below the gap. As a result, the rest of the original energy  $\Delta_0$  of the particle is liberated. Even in a quasi-one-dimensional system of weakly linked chains with a three-dimensional-ordering temperature  $T_c \ll \Delta_0$ , however, the picture is complicated by the fact that at  $T < T_c$  the very existence of topological solitons is questionable.<sup>8,9,14,16–18</sup>

In this paper we examine effects which stem from the long-range structural deformations and Coulomb fields which arise as a crystalline CDW medium adapts to various solitons created in the course of the conversion of electrons. Some of these results have been reported briefly elsewhere.<sup>9</sup>

We examine the static deformations in a CDW medium with a three-dimensional order and point solitons. We examine the interactions of solitons with each other and with impurity centers. We consider the screening by other carriers and the self-screening in the gas of solitons. The results of this study suggest a microscopic picture of the successive stages of the conversion of a normal current into a Fröhlich CDW slippage current. This picture is drawn in the Conclusion.

## 2. SOLITONS IN A QUASI-ONE-DIMENSIONAL MODEL OF A CDW CRYSTAL

A quasi-one-dimensional CDW crystal is characterized by a wave number  $Q \approx 2k_F$ , a gap  $2\Delta_0$  in its electronic spectrum, and a length  $\xi_0 = v/\Delta_0$ , where  $k_F$  and  $v$  are the Fermi momentum and velocity (we assume  $\hbar = 1$  everywhere). The deformation of the CDW is

$$\eta_n(x) = \text{Re } \Delta_n(x) \exp(iQx),$$

$$\Delta_n(x) = |\Delta_n(x)| \exp(i\varphi_n(x)),$$

where  $|\Delta_n(x)|$  and  $\varphi_n(x)$  are the amplitudes and phases on chains  $n$ , and the dependence on the coordinate  $x$  along the chain corresponds to a perturbed state. In the ground state we have  $\Delta_n \equiv \Delta$  and  $\varphi \equiv 0$ . To simplify the notation here and below, we assume that all the  $\varphi_n$  are equal at equilibrium, i.e., that the CDW wave vector is  $\mathbf{Q} = (Q, 0, 0)$ . As we will see in Sec. 3, the general results are model-independent.

In a system of weakly coupled chains, with  $T_c \ll \Delta_0$ , the self-trapping of electrons at an energy scale  $\Delta_0$  and a length scale  $\xi_0$  occurs independently on each chain. The topological solitons which form, however, are incompatible with the de-

definition of long-range order. As a result, adaptational deformations develop and equalize the values of the order parameter on all the chains. These deformations are characterized by an energy  $T_c \ll \Delta_0$  and a length  $l \sim v/T_c \gg \xi_0$ ; i.e., they can be described in terms of the phases  $\varphi_n$  for given amplitudes  $|\Delta_n| \equiv \Delta_0$ . The presence on chain  $n = j$  of a  $\pm 2\pi$  soliton, which corresponds to a self-trapping of  $\nu$  electrons (+) or holes (-), is taken into account by the boundary conditions

$$n=j: \varphi_j(+\infty) - \varphi_j(-\infty) = \pm \nu\pi; \quad n \neq j: \varphi_n(+\infty) = \varphi_n(-\infty) \quad (1)$$

with  $\nu = \pm 2$ . The presence of an amplitude soliton at the point  $x_j$  which corresponds to a self-trapping of one electron (+) or one hole (-) is taken into by the cut condition<sup>14</sup>

$$\varphi_j(x_j+0) - \varphi_j(x_j-0) = \pm \pi, \quad \varphi_j(\pm\infty) = \varphi_n(\pm\infty) = 0,$$

which is equivalent to condition (1) in the case  $\nu = \pm 1$  (Refs. 9 and 14). These conditions show that the electric charges are equal to  $\nu e$ .

In the semiclassical approximation, the energy functional of the system of chains is

$$H = \int dx \left\{ \left[ \sum_n \frac{v}{4\pi} \left( \frac{\partial \varphi}{\partial x} \right)^2 + \sum_{n,m} J_{nm} \cos(\varphi_n - \varphi_m) \right] + \frac{1}{\pi} \frac{\partial \varphi_n}{\partial x} \Phi_n - \int \frac{(\nabla \Phi)^2}{8\pi e^2} dr_{\perp}^2 \right\}, \quad (2)$$

where  $e\Phi = e\Phi(\mathbf{r})$  is the electric potential,  $\mathbf{r} = (x, \mathbf{r}_{\perp})$ ,  $J_{nm}$  is the matrix of transitions between chains  $n$  and  $m$ ,  $\Phi_n = \Phi_n(x, \mathbf{r}_{\perp n})$ , and  $\mathbf{r}_{\perp n}$  is the coordinate of chain  $n$ . We assume everywhere below that  $\Phi(n)$  is only a weak function of  $n$ . The presence of a soliton on chain  $j$  is reflected in (1).

When the electric field is ignored, Eqs. (1) yield the conservation law

$$\sum_n \frac{\partial \varphi_n}{\partial x} = 0. \quad (3)$$

When the Coulomb field  $\Phi$  is taken into account, we find the following conservation laws from (2):

$$\Phi'' - \kappa^2 \Phi = \text{const}, \quad (4)$$

$$\frac{v}{2\pi} \sum_n \frac{\partial \varphi_n}{\partial x} + \Phi = \text{const},$$

where

$$\kappa^2 = 8e^2 / \nu s_{\perp} = r_D^{-2}, \quad \Phi = \int \Phi d^2 r_{\perp} / s_{\perp},$$

$s_{\perp}$  is the cross-sectional area per chain, and  $r_D$  is the screening length in the metallic phase (without the CDW).

Let us examine a model which can be used to study the entire distance range  $|x| \gg \xi_0$  for arbitrary  $n$ . We assume that the matrix  $J_{mn}$  in (2) couples a large number  $Z \gg 1$  of chains. We can then assume that all the phases  $\varphi_n$  with  $n \neq j$  are approximately the same, and we can go over to a continuum description by making the substitutions

$$\sum_n \rightarrow \frac{1}{s_{\perp}} \int d^2 r_{\perp}, \quad \varphi_n(x) \rightarrow \varphi(\mathbf{r}), \quad \Phi_n \rightarrow \Phi(\mathbf{r}).$$

Taking the interaction with the electric field into account,

we find the following expression for the energy functional:

$$H = \int \frac{dr^3}{s_{\perp}} \left\{ \frac{v}{4\pi} \left[ \left( \frac{\partial \varphi}{\partial x} \right)^2 + \alpha \left( \frac{\partial \varphi}{\partial \mathbf{r}_{\perp}} \right)^2 \right] + \frac{\Phi}{\pi} \frac{\partial \varphi}{\partial x} + \sum_j s_{\perp} \delta(\mathbf{r}_{\perp} - \mathbf{r}_{\perp j}) \times \left[ \frac{v}{4\pi} \left( \frac{\partial \varphi}{\partial x} \right)^2 - J \cos(\varphi_j - \varphi) + \frac{\Phi}{\pi} \frac{\partial \varphi_n}{\partial x} \right] - \frac{s_{\perp}}{8\pi e^2} (\nabla \Phi)^2 \right\}, \quad (5)$$

where  $J \equiv J_n = \sum_m J_{nm} \sim T_c^2 / \nu$ , and  $\alpha = 2\pi J / \nu s_{\perp}$ . The summation in (5) is over the chains which contain solitons.

Varying the energy functional in (5) with respect to  $\varphi = \varphi(\mathbf{r})$ ,  $\varphi_j = \varphi_j(x)$ , and  $\Phi(\mathbf{r})$ , we find the conditions for an equilibrium of the system with solitons:

$$-\frac{v}{2} \hat{\Delta} \varphi - \frac{\partial \Phi}{\partial x} - J s_{\perp} \delta(\mathbf{r}_{\perp} - \mathbf{r}_{\perp j}) \sin(\varphi_j - \varphi) = 0, \quad (6)$$

$$\delta(\mathbf{r}_{\perp} - \mathbf{r}_{\perp j}) \left\{ -\frac{v}{2} \varphi_j'' + \pi J \sin(\varphi_j - \varphi) - \frac{\partial \Phi}{\partial x} \right\} = 0, \quad (7)$$

$$2 \frac{\Delta \Phi}{\nu \kappa^2} + \frac{\partial \Phi}{\partial x} + s_{\perp} \delta(\mathbf{r}_{\perp} - \mathbf{r}_{\perp j}) \frac{\partial \varphi_j}{\partial x} = 0. \quad (8)$$

We consider the case of one soliton on a chain:  $j = 0$ ,  $\mathbf{r}_{\perp j} = 0$ . If we ignore the electric field  $\Phi$ , Eqs. (6)–(8) become

$$-\hat{\Delta} \varphi - \varphi_0'' s_{\perp} \delta(\mathbf{r}_{\perp} - \mathbf{r}_{\perp j}) = 0, \quad \hat{\Delta} = \partial^2 / \partial x^2 + \alpha \partial^2 / \partial \mathbf{r}_{\perp}^2, \quad (9)$$

$$-l^2 \varphi_0'' + \sin(\varphi_0 - \varphi(0)) = 0, \quad l^2 = s_{\perp} / \alpha. \quad (10)$$

From (9) we find a self-consistency condition:

$$\varphi(0, x) = \frac{l^2}{4\pi} \int \frac{\varphi_j''(y) dy}{[|x-y|^2 + l^2]^{3/2}}. \quad (11)$$

Equations (10) and (11) determine in a self-consistent way the functions  $\varphi_0(x)$  and  $\varphi(0, x)$ , which describe the phases on the central chain and on the chains closest to it. We then find the phase  $\varphi(x, \mathbf{r}_{\perp})$  throughout the volume from Eq. (9). It is easy to see that Eqs. (10) and (11) do indeed have solutions which correspond to a topological soliton with a length scale  $l$  and which satisfy conditions (1). In contrast with the ordinary sine-Gordon equation, however, the asymptotic behavior at  $|x| \gg l$  is a power law rather than an exponential. The integral in Eq. (11) is dominated by the region  $|y| \leq l$  and  $x \approx y$ . Integrating by parts, using (1), we find, for  $|x| \gg l$ ,

$$\varphi_j(x) \approx \varphi(0, x) \approx -\frac{l^2}{4x^2} + \frac{3l^2 \ln(x/l)}{8\alpha x^4}. \quad (12)$$

The second term is a correction from the region  $y \sim l$ . When the Coulomb interaction is taken into account, we find, similarly,

$$\varphi_0(x) \approx \varphi(0, x) \propto 1/x. \quad (13)$$

The fields at large distances will be analyzed exhaustively in the following sections of this paper by a model-independent approach.

### 3. INTERACTION OF SOLITONS AT LARGE DISTANCES

If we are interested in only the distribution of the fields  $\varphi$  and  $\Phi$  far from the solitons, at distance  $r \gg l$ , we can take

the presence of solitons on selected chains into account in an approximate way, making use of asymptotic conditions (1), which can be written

$$\int_{|x-x_j| \gg \xi_0} \frac{1}{\pi} \frac{\partial \varphi_j}{\partial x} dx = 1. \quad (14)$$

The integral in (14) is dominated by the soliton region  $|x-x_j| \leq l$ . At large distances  $|x-x_j| \gg l$ , condition (14) can thus be written in the form

$$\frac{1}{\pi} \frac{\partial \varphi_j}{\partial x} = \delta(x-x_j). \quad (15)$$

We find the corresponding expression for an antisoliton in a similar way; the result differs from (15) in that there is a minus sign on the right side.

To find the distributions of the phase  $\varphi$  and the electric potential  $\Phi$  at distances large in comparison with the length of a soliton,  $r \gg l$ , we examine instead of Hamiltonian (5) a model-independent Hamiltonian. This model-independent Hamiltonian leads to the correct self-consistency conditions and becomes the same as (5) at  $r \gg l$  in the continuous limit:

$$H = \int \frac{dr^3}{s_{\perp}} \left\{ \frac{v}{4\pi} \left[ \left( \frac{\partial \varphi}{\partial x} \right)^2 + \alpha \left( \frac{\partial \varphi}{\partial \mathbf{r}_{\perp}} \right)^2 \right] + \frac{\Phi}{\pi} \frac{\partial \varphi}{\partial x} + \sum_j s_{\perp} \delta(\mathbf{r}-\mathbf{r}_j) \right. \\ \left. \times \left[ \frac{v}{2} \frac{\partial \varphi}{\partial x} + \Phi \right] - \frac{1}{\pi v \kappa^2} (\nabla \Phi)^2 \right\}. \quad (16)$$

Varying functional (16) with respect to  $\varphi$  and  $\Phi$ , we find the equations

$$-v \hat{\Delta} \varphi - 2 \frac{\partial \Phi}{\partial x} - \pi s_{\perp} v \frac{\partial}{\partial x} \delta(\mathbf{r}-\mathbf{r}_j) = 0, \quad (17)$$

$$\frac{2\Delta \Phi}{v \kappa^2} + \frac{\partial \varphi}{\partial x} + \pi s_{\perp} \delta(\mathbf{r}-\mathbf{r}_j) = 0, \quad (18)$$

where  $\hat{\Delta} = \partial^2 / \partial x^2 + \alpha \partial^2 / \partial \mathbf{r}_{\perp}^2$ . Integrating Eqs. (17) and (18) over the transverse plane, we find equations for the average values  $\bar{\Phi}$  and  $\bar{\varphi} = \int d\mathbf{r}_{\perp}^2 \varphi / s_{\perp}$  over the cross section:

$$\bar{\Phi}'' + \frac{e^2}{\pi} \bar{\varphi}'(x) + e^2 \delta(x-x_j) = 0, \quad \bar{\Phi}''(x) - \kappa^2 \bar{\Phi}(x) = \text{const}. \quad (19)$$

From these results we find  $\bar{\Phi} = \text{const}$  (we have discarded some solutions which grow exponentially, and we have ignored solutions which decay exponentially at the atomic scale,  $\kappa^{-1}$ ). Equations (19) are exact and were derived for discrete model (1). This result is further evidence in favor of the validity of Hamiltonian (16).

We first consider a system without a Coulomb field  $\Phi(x)$ . The solution of Eqs. (17) and (18) is

$$\varphi(\mathbf{r}) = -\frac{s_{\perp}}{4\alpha} \frac{x-x_j}{[(x-x_j)^2 + (\mathbf{r}_{\perp}-\mathbf{r}_{\perp j})^2/\alpha]^{3/2}}. \quad (20)$$

It is easy to see that (20) yields

$$\bar{\varphi}(x) = \frac{\pi}{2} \text{sgn}(x-x_j),$$

so that condition (19) is satisfied. The distribution of the charge density in the medium is determined by the equation

$$\rho(\mathbf{r}) = e \delta(\mathbf{r}-\mathbf{r}_j) + \frac{e}{\pi} \frac{1}{s_{\perp}} \frac{\partial \varphi}{\partial x} \\ = e \delta(\mathbf{r}-\mathbf{r}_j) + \frac{e}{4\pi\alpha} \left[ \frac{1}{|\hat{\mathbf{r}}|^3} - \frac{3x^2}{|\hat{\mathbf{r}}|^5} \right], \quad (21)$$

where

$$\hat{r}^2 = (x-x_j)^2 + (\mathbf{r}_{\perp}-\mathbf{r}_{\perp j})^2/\alpha.$$

We see from (21) that the charge on any chain  $\mathbf{r}_{\perp} \neq \mathbf{r}_{\perp j}$  is zero, i.e., that the charge of the soliton of the central chain ( $\mathbf{r}_{\perp} = \mathbf{r}_{\perp j}$ ) is not canceled by the interaction with the local field. In this sense the soliton has a charge  $\pm e$ .

The energy of the interaction of two solitons can be found easily from (16)–(20):

$$W(\mathbf{r}) = \mp \frac{v}{2} \frac{\partial \varphi}{\partial x} = \mp \frac{v s_{\perp}}{4\alpha} \left[ \frac{1}{|\hat{\mathbf{r}}|^3} - \frac{3x^2}{|\hat{\mathbf{r}}|^5} \right]. \quad (22)$$

The  $\mp$  correspond to solitons which have the same sign or opposite signs. The interaction changes sign on the cone  $|x|/|\mathbf{r}| = (\alpha/2)^{1/2}$ .

Equations (17) and (18) also have an exact solution when the Coulomb interaction is taken into account. For the functions  $\Phi(\mathbf{r})$  and  $\varphi(\mathbf{r})$  we easily find the equations

$$\hat{K} \Phi_0(\mathbf{r}) = \pi s_{\perp} (\kappa^2 - \Delta) \frac{\partial}{\partial x} \delta(\mathbf{r}), \quad (23)$$

$$\hat{K} \Phi_0(\mathbf{r}) = -4\pi e \alpha \Delta_{\perp} \delta(\mathbf{r}), \quad \Delta_{\perp} = \partial^2 / \partial \mathbf{r}_{\perp}^2 \quad (24)$$

where

$$\hat{K} = \hat{\Delta} \Delta - \kappa^2 \frac{\partial^2}{\partial x^2}, \quad \varphi(\mathbf{r}) = \sum \varphi_0(\mathbf{r}-\mathbf{r}_j),$$

$$\Phi(\mathbf{r}) = \sum \Phi_0(\mathbf{r}-\mathbf{r}_j), \quad \Delta_{\perp} = \frac{\partial^2}{\partial \mathbf{r}_{\perp}^2}.$$

Taking Fourier components, we find

$$\Phi_k = \frac{4\pi e \alpha k_{\perp}^2}{k^2 \bar{k}^2 + \kappa^2 k_{\parallel}^2}, \quad (23')$$

$$\varphi_k = \frac{i k_{\parallel} (\kappa^2 + k^2) \Phi_k}{4e^2 \alpha k_{\perp}^2}, \quad (24')$$

where  $\bar{k}^2 = k_{\parallel}^2 + \alpha k_{\perp}^2$ . Taking Fourier transforms of the functions (23') and (24'), we find expressions for the potentials  $\Phi$  and  $\varphi$ . With  $\alpha = 1$ , the integrals can be evaluated exactly:

$$\Phi_0(\mathbf{r}) = \frac{e^2 \kappa}{4} \left[ \text{ch } \tilde{x} \frac{\exp(-\tilde{r})}{\tilde{r}} + \text{sh } x \frac{\tilde{x}}{\tilde{r}^3} (1+\tilde{r}) \exp(-\tilde{r}) \right], \\ \alpha = 1, \quad (25)$$

$$\Phi_0(\mathbf{r}) \approx \alpha^{1/2} \Phi_0(x \alpha^{1/2}, \mathbf{r}_{\perp}), \quad \alpha \ll 1,$$

$$\varphi_0(\mathbf{r}) = -\frac{\kappa^2 s_{\perp}}{16} \left[ \text{sh } \tilde{x} \frac{\exp(-\tilde{r})}{\tilde{r}} + \text{ch } x \frac{\tilde{x}}{\tilde{r}^3} (1+\tilde{r}) \exp(-\tilde{r}) \right],$$

$$\alpha = 1,$$

$$\varphi_0(\mathbf{r}) \approx \varphi_0(x \alpha^{1/2}, \mathbf{r}_{\perp}), \quad \alpha \ll 1, \quad (26)$$

where  $\tilde{x} = \kappa r/2$  and  $\tilde{r} = \kappa r/2$ .

Since  $\kappa^2 \sim k_F^2$ , the functions  $\Phi$  and  $\varphi$  fall off rapidly in the perpendicular direction, with a screening length on the order of the distance between chains. Along the direction of the chains, in the limit of large  $x$  ( $\alpha^{1/2}x \gg r_1$ ), we find from (25) and (26)

$$\Phi_0(\mathbf{r}) \approx \frac{e^2}{2|x|} \exp\left(-\frac{r_\perp^2}{d}\right), \quad d = \frac{4\alpha^{1/2}}{\kappa}, \quad (25')$$

$$\varphi_0(\mathbf{r}) \approx \frac{s_\perp \kappa}{8\alpha^{1/2}} \frac{1}{x} \exp\left(-\frac{r_\perp^2}{d|x|}\right). \quad (26')$$

In the transverse sector we have  $r_1 > \alpha^{1/2}x$ . At  $r_1 \gg d$  the quantities  $\varphi_0$  and  $\Phi_0$  fall exponentially:  $\varphi_0, \Phi_0 \propto \exp(-r/d)$ . The quantities  $\varphi_0$  and  $\Phi_0$  are not exponentially small, so an interaction can arise in the region  $\alpha^{1/2}\kappa r < 1$ . This region is realized in the case of a weak Coulomb interaction and a relatively strong coupling of chains:  $d^2 \gg l^2 = s_\perp/\alpha$ , i.e.,  $\alpha^2 \gg e^2/v\epsilon_\infty$  at short distances  $l < r < d$ .

We calculate now the energy of the interaction of two solitons, with indices  $\nu_1$  and  $\nu_2$ , which are separated by a distance  $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ . Integrating the energy functional (16) by parts, and using Eqs. (17) and (18), we find

$$W(\mathbf{r}) = \Phi_0(\mathbf{r}) + \frac{v}{2} \frac{\partial \varphi_0(\mathbf{r})}{\partial x}. \quad (27)$$

Substituting the obtained solutions (25) and (26) into (27), we finally get

$$W(\mathbf{r}) = \frac{e^2 \kappa}{8} \exp(-\tilde{r}) \left[ 2\tilde{x} \left( \frac{1}{\tilde{r}^2} + \frac{1}{\tilde{r}^3} \right) \text{sh } \tilde{x} + \left( \frac{1}{\tilde{r}} - \frac{1}{\tilde{r}^2} - \frac{1}{\tilde{r}^3} + \frac{\tilde{x}^2}{\tilde{r}^3} + \frac{3\tilde{x}^2}{\tilde{r}^4} + \frac{3\tilde{x}^2}{\tilde{r}^5} \right) \text{ch } \tilde{x} \right]. \quad (28)$$

The asymptotic form of (28) at  $\tilde{r} \gg 1$  is

$$W(\mathbf{r}) = \frac{e^2 \kappa}{8} \exp(-\tilde{r}) \left[ \frac{2\tilde{x}}{\tilde{r}^2} \text{sh } \tilde{x} + \left( \frac{1}{\tilde{r}} + \frac{\tilde{x}^2}{\tilde{r}^3} \right) \text{ch } \tilde{x} \right]. \quad (28')$$

Let us analyze the function  $W(x, r_1)$ . Since the diffusion coefficient of the solitons is highly anisotropic along and across the chains, we should begin with the functional dependence  $W_\parallel(x) = W(x, r_1 = \text{const})$ . We have a positive derivative  $\partial W_\parallel / \partial x > 0$  at  $x < x_0 \sim r_1^2/2$ , a vanishing derivative  $\partial W_\parallel / \partial x = 0$  at  $x = x_0$ , and a negative derivative  $\partial W_\parallel / \partial x < 0$  at  $x > x_0$  [ $W_\parallel(x_0) \sim e^2 \kappa / \tilde{r}_1^2$ ]. The function  $W_\parallel(x)$  has a minimum at  $x = 0$ ; this minimum value is

$$W_\parallel(0) = \frac{e^2 \kappa}{8} \exp(-\tilde{r}_\perp) \left( \frac{1}{\tilde{r}_\perp} - \frac{1}{\tilde{r}_\perp^2} - \frac{1}{\tilde{r}_\perp^3} \right),$$

$$W_\parallel(0) < 0, \quad \tilde{r}_\perp \leq 1.$$

The minimum is isolated by a potential barrier of size  $W_\parallel(x_0)$ . The depth of the minimum and the height of the barrier increase with decreasing  $r_1$ . At  $r_1 = 0$ , there are no extrema, and the situation is dominated by a repulsion of the type of an unscreened Coulomb interaction.

Let us analyze the functional dependence  $W_\perp(r_1) = W(x = \text{const}, r_1)$ . At  $\tilde{r} \gg 1$ , we have a derivative  $\partial W_\perp / \partial r_1 < 0$ , which indicates a repulsion in the direction perpendicular to the chains. The maximum of  $W_\perp(r_1)$  at  $\tilde{r} \gg 1$  is reached at  $r_1 = 0$ ; this maximum value is

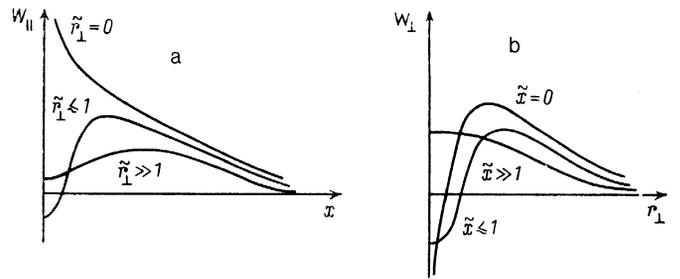


FIG. 1. Energy of the interaction of two solitons. a— $W_\parallel(x) = W(x, r_1 = \text{const})$ ; b— $W_\perp(r_1) = W(x = \text{const}, r_1)$ .

$W_\perp(0) \approx e^2 \kappa / 4 |\tilde{x}| > 0$ . The attraction and the minimum of  $W_\perp(r_1 = 0)$  are realized in the region  $\tilde{r} \lesssim 1$ . In particular, for  $x = 0$ , the potential

$$W_\perp(x=0, r_\perp) = W_\parallel(0)$$

has an infinitely deep minimum at  $r_1 = 0$  and a barrier at  $r_1 \sim 1$ . Figure 1 shows  $W_\parallel(x)$  and  $W_\perp(r_1)$ .

Solitons of equal sign thus attract each other in the narrow region  $\tilde{r} \lesssim 1$ . As we have already mentioned, this region is realized if the Coulomb interaction is weak,  $e^2/v \ll 1$ , in which case the Coulomb screening length  $1/\kappa$  is greater than the soliton length  $l \sim s_\perp^{1/2}$ .

#### 4. SCREENING OF THE COULOMB POTENTIAL

1. Two screening mechanisms can operate in real systems. One stems from the presence of a charge in the system of free carriers. An example of this situation is a compound which has an unfilled band of electrons which are not participating in the formation of a charge density wave (CDW), i.e., which are not interacting with  $\partial \varphi / \partial x$ . It is easy to see that incorporating screening reduces to the substitution  $k^2 \rightarrow k^2 + \lambda^2$  in Eqs. (17) and (18), where  $\lambda^2 = 4\pi e^2 N_F$ , and  $N_F$  is the density of states at the Fermi level of the free electrons.

Along with the screening, we (simultaneously) consider the effects which stem from the commensurability of the periods of the CDW and the lattice. In Hamiltonian (16), we consider the term  $A \cos N\varphi$ , where  $N$ , a natural number, is the commensurability factor. At small values of  $\varphi$ , commensurability effects can thus be dealt with by making the substitution  $\hat{\Delta} \rightarrow \hat{\Delta} - \varepsilon^2$  in Eqs. (17) and (18). Equations (23') and (24') become

$$\Phi_{\mathbf{k}} = \frac{4\pi e (\alpha k_\perp^2 + \varepsilon^2)}{(k^2 + \lambda^2) (\tilde{k}^2 + \varepsilon^2) + \kappa^2 k_\parallel^2}, \quad (29)$$

$$\varphi_{\mathbf{k}} = \frac{ik_\parallel (\kappa^2 + k^2 + \lambda^2) \Phi_{\mathbf{k}}}{4e^2 (\alpha k_\perp^2 + \varepsilon^2)}.$$

We find exact expressions for  $\varphi(\mathbf{r})$  and  $\Phi(\mathbf{r})$  for  $\alpha = 1$ , and  $\lambda = \varepsilon$  which are analogous to Eqs. (23)–(25):

$$\Phi_0(\mathbf{r}) = \frac{e\kappa}{8} \left[ \text{ch } \tilde{x} \frac{\exp(-\tilde{r}\mu)}{\tilde{r}} + \text{sh } x \frac{\tilde{x}}{\tilde{r}^3} (1 + \tilde{r}\mu) \exp(-\tilde{r}\mu) \right],$$

$$\varphi_0(\mathbf{r}) = -\frac{\kappa^2 s_\perp}{16} \left[ \text{sh } \tilde{x} \frac{\exp(-\tilde{r}\mu)}{\tilde{r}} + \text{ch } x \frac{\tilde{x}}{\tilde{r}^3} (1 + \tilde{r}\mu) \exp(-\tilde{r}\mu) \right], \quad (30)$$

where  $\mu = (1 + 4\lambda^2/\kappa^2)^{1/2}$ .

For  $\lambda \neq \varepsilon$  and  $\alpha \neq 1$  it is a simple matter to find the asymptotic behavior at  $x \gg (\kappa^2 + \varepsilon^2 + \alpha\lambda^2)^{1/2}/\alpha$  ( $\alpha\lambda^2 + \varepsilon^2$ ),  $r_{\perp} \gg \alpha^{1/2}/(\varepsilon^2 + \alpha\lambda^2)^{1/2}$ :

$$\varphi = \frac{s_{\perp}(\kappa^2 - \Delta - \lambda^2)}{4(\kappa^2 + \varepsilon^2 + \alpha\lambda^2)^{1/2}(\varepsilon^2 + \alpha\lambda^2)} \frac{\partial}{\partial x} f(r),$$

$$\Phi = \frac{e(\alpha\Delta_{\perp} - \varepsilon^2)}{(\kappa^2 + \varepsilon^2 + \alpha\lambda^2)^{1/2}(\varepsilon^2 + \alpha\lambda^2)} f(r), \quad (31)$$

where

$$f(r) = \frac{\exp\{-\varepsilon\lambda[x^2/(\kappa^2 + \varepsilon^2 + \alpha\lambda^2) + r_{\perp}^2/(\varepsilon^2 + \alpha\lambda^2)]^{1/2}\}}{[x^2/(\kappa^2 + \varepsilon^2 + \alpha\lambda^2) + r_{\perp}^2/(\varepsilon^2 + \alpha\lambda^2)]^{1/2}}.$$

If there is no pinning ( $\varepsilon = 0$ ) we find approximate expressions from a solution of Eqs. (17) and (18):

$$\Phi_{\mathbf{k}} = \frac{4\pi e \alpha k_{\perp}^2}{(k^2 + \lambda^2) \tilde{\kappa}^2 + \kappa^2 k_{\parallel}^2} \approx \frac{4\pi e \alpha k_{\perp}^2}{\alpha(k_{\perp}^2 + \lambda^2)k_{\perp}^2 + \tilde{\kappa}^2 k_{\parallel}^2}, \quad (32)$$

$$\Phi(\mathbf{r}) = \frac{e^2}{\alpha^{1/2}} \frac{\partial^2}{\partial x^2} \int dk_{\perp} \frac{J_0(k_{\perp} r_{\perp}) \exp[-\alpha^{1/2} k_{\perp} |x| (\lambda^2 + k_{\perp}^2)^{1/2}/\kappa]}{(\lambda^2 + k_{\perp}^2)^{1/2}},$$

where  $\tilde{\kappa}^2 = \kappa^2 + \lambda^2$ .

In the limiting case of characteristic values  $|k_{\parallel}|, |k_{\perp}| \ll \lambda_0$ , the integral can be evaluated exactly:

$$\Phi(\mathbf{r}) = \frac{e^2 \tilde{\kappa}}{\alpha^{1/2} \lambda^3} \frac{\partial^2}{\partial x^2} \left( r_{\perp}^2 + \frac{\alpha \lambda^2}{\tilde{\kappa}^2} x^2 \right)^{-1/2}. \quad (33)$$

Expression (33) is correct if the integral in (32) converges at  $k_{\perp} \sim \kappa/|x| \lambda_0 \alpha^{1/2} \ll \lambda$ . Hence

$$|x| \gg \tilde{\kappa}/\lambda^2 \alpha^{1/2}.$$

In the same limit we find the following expression for the phase  $\varphi$ :

$$\varphi(\mathbf{r}) = \frac{s_{\perp} \tilde{\kappa}}{4\alpha^{1/2} \lambda} \frac{\partial}{\partial x} \left( r_{\perp}^2 + \frac{\alpha \lambda^2}{\tilde{\kappa}^2} x^2 \right)^{-1/2}. \quad (34)$$

Substituting (33) and (34) into expression (27) for the interaction energy, we find

$$W(\mathbf{r}) = \frac{v s_{\perp}}{8\alpha} \left( \frac{\tilde{\kappa}}{\lambda} \right)^4 \frac{2x^2 - r_{\perp}^2 \tilde{\kappa}^2 / \alpha \lambda^2}{[x^2 + r_{\perp}^2 \tilde{\kappa}^2 / \alpha \lambda^2]^{3/2}}. \quad (35)$$

It follows from (35) that at large distances solitons of a common sign repel each other along the  $x$  axis and attract each other in the perpendicular direction.

**2. Case of self-screening.** Let us look at the case of a finite soliton concentration:  $n_c \ll l^{-3}$ . We focus on one soliton in this system and take an average over the others. We wish to determine how the fields  $\Phi$  and  $\varphi$  produced by the given soliton are screened. In Hamiltonian (16) we need to make the substitutions

$$\Phi \rightarrow \langle \Phi \rangle + \Phi, \quad \Sigma \delta(\mathbf{r} - \mathbf{r}_j) \rightarrow \delta(\mathbf{r} - \mathbf{r}_0) + n_c + \delta n(\mathbf{r}),$$

$$\frac{\partial \varphi}{\partial x} \rightarrow \left\langle \frac{\partial \varphi}{\partial x} \right\rangle + \frac{\partial \varphi}{\partial x} = -\pi s_{\perp} n_c x + \frac{\partial \varphi}{\partial x}. \quad (36)$$

The local change caused in the concentration of solitons by the perturbation by the external fields  $\Phi$  and  $\varphi$  is

$$\delta n(\mathbf{r}) = -\frac{\partial n}{\partial \mu} W(\mathbf{r}), \quad W(\mathbf{r}) = \left[ e\Phi(\mathbf{r}) + \frac{v}{2} \frac{\partial \varphi}{\partial x} \right], \quad (37)$$

where  $\mu$  is the chemical potential of the soliton gas, and  $W$  is

the energy of the interaction of a soliton at point  $r$  with the soliton on which we are focusing. Substituting expressions (36) and (37) into functional (16), we find (discarding some inconsequential terms)

$$H = \int \frac{d^3 r}{s_{\perp}} \left\{ \frac{v}{4\pi} (\hat{\partial} \varphi)^2 + \frac{\Phi}{\pi} \frac{\partial \varphi}{\partial x} - \frac{(\nabla \Phi)^2}{8\pi l^2} s_{\perp} \right. \\ \left. + \delta(\mathbf{r} - \mathbf{r}_0) \left( \Phi + \frac{\partial \varphi}{\partial x} \frac{v}{2} \right) - \frac{\partial n}{\partial \mu} s_{\perp} \left( \Phi + \frac{v}{2} \frac{\partial \varphi}{\partial x} \right)^2 \right\}, \quad \hat{\partial} = \left( \frac{\partial}{\partial x}, \alpha^{1/2} \frac{\partial}{\partial r_{\perp}} \right). \quad (38)$$

Varying functional (38) with respect to the fields  $\Phi$  and  $\varphi$ , we find self-consistency conditions analogous to conditions (17) and (18):

$$-\frac{v}{2\pi} \hat{\Delta} \varphi + \frac{\partial n}{\partial \mu} s_{\perp} \frac{v^2}{2} \varphi'' - \frac{1}{\pi} \Phi' \\ + \frac{\partial n}{\partial \mu} s_{\perp} v \Phi' - \frac{s_{\perp}}{2} v \delta'(\mathbf{r} - \mathbf{r}_0) = 0, \\ \frac{s_{\perp}}{4\pi l^2} \Delta \Phi - \frac{\partial n}{\partial \mu} s_{\perp} \Phi + \frac{1}{2\pi} \Phi' - \frac{\partial n}{\partial \mu} s_{\perp} e v \varphi' + s_{\perp} \delta(\mathbf{r} - \mathbf{r}_0) = 0. \quad (39)$$

For the Fourier components we easily find from (39)

$$\Phi_{\mathbf{k}} = \frac{4\pi \alpha k_{\perp}^2}{\alpha k_{\perp}^2 (k^2 + \lambda^2) + (1 - \lambda^2/\kappa^2) (\kappa^2 + k^2) k_{\parallel}^2}, \quad (40)$$

$$\varphi_{\mathbf{k}} = \frac{i k_{\parallel} \pi s_{\perp} (k^2 + \lambda^2)}{\alpha k_{\perp}^2 (k^2 + \lambda^2) + (1 - \lambda^2/\kappa^2) (\kappa^2 + k^2) k_{\parallel}^2},$$

where  $\lambda^2 = 8\pi e^2 \partial n / \partial \mu$ .

Using  $\lambda^2 \ll \kappa^2$ , and expanding (39) in  $\lambda^2/\kappa^2$ , we find that expressions (40) are the same as the corresponding expressions [(29)–(31)] for the case of screening by free charge carriers. The solutions for  $\Phi(\mathbf{r})$  and  $\varphi(\mathbf{r})$  and the energies of the interaction of two solitons are therefore given by (29)–(31), in which we should make the substitution  $\lambda^2 \rightarrow \lambda^2 + 8\pi e^2 \partial n / \partial \mu$ .

All the results derived above for  $\pi$  solitons can easily be generalized to the case of  $2\pi$  solitons by making the substitution  $e \rightarrow 2e$  in all the equations.

## 5. INTERACTION OF SOLITONS WITH IMPURITY CENTERS

Let us consider the interaction of solitons with defects which pin CDWs, e.g., dopant particles or structural defects. We consider an isolated defect at point  $\mathbf{r}_0$  with a minimum of the pinning energy at  $\varphi(\mathbf{r}_0) = \theta$ . We add to energy functional (16) a term to describe the interaction with the impurity centers:

$$\delta W = \int dx dr_{\perp} C [\varphi(\mathbf{r}) - \theta]^2 \delta(\mathbf{r} - \mathbf{r}_0) / 2, \quad (41)$$

where the interaction constant  $C$  is found at the atomic scale from the microscopic theory. Interaction (41) tends to fix the phase of the CDW at point  $\mathbf{r}_0$ ; in particular, as  $C \rightarrow \infty$  we find  $\varphi(\mathbf{r}_0) = \theta$ .

Varying functional (16) with the additional term in (41), we find equilibrium equations:

$$-\frac{v}{2\pi} \hat{\Delta} \varphi - \frac{1}{\pi} \frac{\partial \varphi}{\partial x} - \frac{s_{\perp} v}{2} \frac{\partial}{\partial x} \delta(\mathbf{r} - \mathbf{r}_j) + C s_{\perp} (\varphi - \theta) \delta(\mathbf{r} - \mathbf{r}_0) = 0, \quad (42)$$

$$\frac{2\Delta\Phi}{\pi v \kappa^2} + \frac{1}{\pi} \frac{\partial \varphi}{\partial x} + s_{\perp} \delta(\mathbf{r}-\mathbf{r}_j) = 0.$$

Equations (42) describe the interaction of a soliton localized at the point  $\mathbf{r}_j$  with an impurity center at the point  $\mathbf{r}_0$ . Working from (16) and (41), and using Eqs. (42), we find an expression for the interaction energy:

$$W = \frac{\Phi(\mathbf{r}_j)}{2} + \frac{v}{2} \frac{\partial}{\partial x} \varphi(\mathbf{r}_j) - \frac{C}{2} [\varphi(\mathbf{r}_0) - \theta]. \quad (43)$$

We first consider the interaction with an impurity center in the absence of a Coulomb field  $\Phi$ . From the first equation in (42) we find

$$\begin{aligned} \varphi(\mathbf{r}) &= -\frac{s_{\perp}}{4\alpha} \frac{x-x_j}{|\hat{\mathbf{r}}-\hat{\mathbf{r}}_j|^3} - \frac{Cs_{\perp}[\varphi(\mathbf{r}_0)-\theta]}{2\alpha v |\hat{\mathbf{r}}-\hat{\mathbf{r}}_0|} \\ &= \varphi_0(\mathbf{r}-\mathbf{r}_j) - \frac{Cs_{\perp}[\varphi(\mathbf{r}_0)-\theta]}{2\alpha v |\hat{\mathbf{r}}-\hat{\mathbf{r}}_0|}. \end{aligned} \quad (44)$$

The last term in (44) formally diverges as  $\hat{\mathbf{r}} \rightarrow \hat{\mathbf{r}}_0$ , since the continuum model is not valid on the atomic scale. To eliminate the divergence, we impose an additional condition, which places a limit on  $\varphi(\mathbf{r})$  as  $\hat{\mathbf{r}} \rightarrow \hat{\mathbf{r}}_0$ :

$$\varphi(\mathbf{r})|_{|\hat{\mathbf{r}}-\hat{\mathbf{r}}_0| \leq \varepsilon} = \varphi(\mathbf{r})|_{|\hat{\mathbf{r}}-\hat{\mathbf{r}}_0| = \varepsilon}, \quad (45)$$

where  $\varepsilon$  is of the order of the microscopic scale. Using condition (45), we find

$$\varphi(\mathbf{r}) = \varphi_0(\mathbf{r}-\mathbf{r}_j) - \frac{Cs_{\perp}[\varphi_0(\mathbf{r}_0-\mathbf{r}_j)-\theta]}{2\alpha v |\hat{\mathbf{r}}-\hat{\mathbf{r}}_0|}, \quad (46)$$

where

$$\bar{C} = \frac{C}{1+2Cs_{\perp}\alpha v \varepsilon}.$$

Substituting solution (46) into expression (43) for the energy, we find

$$W = \bar{C} [\varphi_0(\mathbf{r}_0-\mathbf{r}_j) - \theta]^2 / 2. \quad (47)$$

As expected, the minimum  $W = 0$  is reached at  $\varphi(\mathbf{r}_0) = \theta$ .

We now examine Eqs. (42) with a Coulomb field. It is a simple matter to derive equations for the fields  $\Phi(\mathbf{r})$  and  $\varphi(\mathbf{r})$ :

$$\bar{K}\Phi = -4\pi e^2 \alpha \Delta_{\perp} \delta(\mathbf{r}-\mathbf{r}_j) - (8\pi e^2/v) C (\varphi-\theta) \frac{\partial}{\partial x} \delta(\mathbf{r}-\mathbf{r}_0), \quad (48)$$

$$\bar{K}\varphi = \pi s_{\perp} (\kappa^2 - \Delta) \frac{\partial}{\partial x} \delta(\mathbf{r}-\mathbf{r}_j) + (2\pi s_{\perp}/v) C (\varphi-\theta) \Delta \delta(\mathbf{r}-\mathbf{r}_0). \quad (49)$$

Solutions of Eqs. (48) and (49) are found with the help of (23) and (24). Comparing the right sides of Eqs. (48), (49) with (23), (24), we can express the solutions of Eqs. (48) and (49) in terms of  $\varphi_0$  and  $\Phi_0$ , i.e., in terms of the solutions of Eqs. (23) and (24) found with Coulomb forces but without impurity centers:

$$\begin{aligned} \Phi(\mathbf{r}) &= \Phi_0(\mathbf{r}-\mathbf{r}_j) - C [\varphi(\mathbf{r}_0) - \theta] \varphi_0(\mathbf{r}-\mathbf{r}_0), \\ \varphi(\mathbf{r}) &= \varphi_0(\mathbf{r}-\mathbf{r}_j) - (s_{\perp}/2\alpha v) C [\varphi(\mathbf{r}_0) - \theta] \Phi_0(\mathbf{r}-\mathbf{r}_0) \end{aligned} \quad (50)$$

$$+ (2/\kappa^2 v) C [\varphi(\mathbf{r}_0) - \theta] \frac{\partial}{\partial x} \varphi_0(\mathbf{r}-\mathbf{r}_0). \quad (51)$$

We can set  $\varphi(\mathbf{r}_0) = \varphi_0(\mathbf{r}_0)$  on the right of sides of expressions (51) and (52).

Let us calculate the interaction energy in (43). To avoid laborious calculations, we first find the potential  $V = e\Phi + (v/2)(\partial\varphi/\partial x)$  and  $\mathbf{r} = \mathbf{r}_j$ . Using Eqs. (48) and (49), we find an equation for  $V(\mathbf{r})$ :

$$\bar{K}V = -\pi s_{\perp} C \kappa^2 (\varphi-\theta) \frac{\partial}{\partial x} \delta(\mathbf{r}-\mathbf{r}_0). \quad (52)$$

Working from this equation, and using (23) and (24), we find

$$V = -C \varphi_0(\mathbf{r}_j-\mathbf{r}_0) [\varphi(\mathbf{r}_0-\mathbf{r}_j) - \theta].$$

Substituting solution (52) into expression (43) for the energy, and making use of the odd parity of  $\varphi_0(\mathbf{r})$ , we finally find

$$W = C' [\varphi_0(\mathbf{r}_0-\mathbf{r}_j) - \theta]^2 / 2, \quad (53)$$

where the constant  $C'$  is determined by the solution on microscopic scales, outside the range of applicability of the continuum model.

Let us examine the functional dependence  $W(x, \mathbf{r}_{\perp})$ . Because of the pronounced anisotropy, we naturally begin with  $W_{\parallel}(x) = W(x, \mathbf{r}_{\perp} = \text{const})$ . The function  $\varphi_0(x, \mathbf{r}_{\perp})$  is odd in  $x$  and has extrema at  $x = \pm x_m(\mathbf{r}_{\perp})$ . In the general case  $\theta \sim \pi$ , Eq. (53) describes an attraction toward  $x_m(\mathbf{r}_{\perp})$  from the region  $x_n < x < \infty$ . Perpendicular forces in the valley  $x = x_m(\mathbf{r}_{\perp})$  are directed toward the defect. At small values of  $\theta$  the absolute maximum is near the defect and is determined by the equation  $\varphi_0(\mathbf{r}-\mathbf{r}_0) = \theta$ . For the particular case  $\theta = 0$ , there is an attraction toward the  $x = 0$  plane from the region  $|x| < x_m$ , while there is a repulsion in the perpendicular direction. This situation may also arise in the special case of a mobile impurity (see Ref. 19 and the bibliography there).

At large distances the interactions of  $\pi$  and  $2\pi$  solitons with defects differ only in the coefficient  $\nu$  ( $\nu = 1$  and  $2$ ). Bound states at the defect, in contrast, are fundamentally different, since the  $\pi$  solitons contain a core at which the amplitude crosses zero, so the binding energy is on the order of  $\Delta$ .

There is the possibility that at low temperatures the impurity particles will form a neutral complex with a  $\pi$  soliton, which would play the role of the neutral defect discussed above. Bound states of charged impurity centers with solitons were recently studied by Barisic and Batistic.<sup>20</sup>

## 6. CONCLUSION

We have examined some questions concerning the conversion of a normal current into a Fröhlich current in CDW crystals. We have examined the formation of  $\pi$  and  $2\pi$  solitons, and we have constructed a model for describing the structure of solitons in systems with a crystalline order.

We have proposed a model-independent approach for describing the interaction of solitons with long-range Coulomb and deformation fields. We have taken this approach to study the interaction of solitons with each other and with impurity centers. We have also studied the combined effects of a weak commensurability and a screening or self-screening of the residual electrons or solitons. In all cases we have found the regions of attraction of the solitons.

The results indicate that solitons tend to cluster in complexes equivalent to dislocation loops.

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Translated by D. Parsons