[2)] At the same time, estimates show that the photoresponse associated with conductivity due to hopping between excited levels is quite negligible for two reasons: 1) the probability for jumps between impurities during the time τ_{ph} (even between excited levels of those impurities) under conditions in which the average distance between the impurities is two orders of magnitude greater than the radius of the excited state, is negligible; and 2) with this mechanism the lifetime of a photocarrier would be the intraimpurity relaxation time τ_{ph}, which in pure materials is shorter than the lifetime of band carriers.

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Spin states in the Peierls model, and finite-band potentials

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Doubly periodic solutions are constructed in the one-dimensional Peierls continuum model with arbitrary number ρ of electrons per atom. The energy of the ground state of the system is obtained as a function of the concentration of the total number of particles and of the spin angular momentum. The dependence of the magnetic moment m on the external field h is investigated. This dependence is characterized by a critical value $h_c \neq 0$ such that a spontaneous moment is produced in the system at $h > h_c$. As $m \to 0$, solitons that carry out localized spin states are considered against the background of the periodic structure. These solitons correspond to single-particle states of a system with one extra particle. The triplet and electron-hole excitations are each a sum of two single-particle states. The soliton charge q_s, in contrast to the spin, is partially screened at $\rho \neq 1$, so that in the Frohlich model, at $|\rho - 1| \gg \Delta/\varepsilon_F$, the local charge vanishes like $q_s \sim e\Delta/\varepsilon_F|\rho - 1|$, where Δ is the gap on the Fermi surface, ε_F is the Fermi energy at $\rho = 1$, and e is the electron charge.

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1. INTRODUCTION

Most quasi-one-dimensional conductors reveal lattice superstructures that lead to the appearance of a gap E_g on the Fermi surface of the electrons. The theory of this phenomenon is frequently based on the Peierls model.[1] In this model, the direct interaction between the electrons is left out, but account is taken of the lattice-deformation potential $\Phi(x)$. In addition, it is assumed[2] that the frequency ω_{ph} corresponding to the deformation mode is small compared with $E_g : \omega_{ph} \ll E_g$. This condition makes it possible to consider lattice deformations as static and to disregard quantum effects.[2] As a result, the Peierls model is compatible with a correct investigation on the basis of the self-consistent-field approximation. The adiabaticity conditions are well satisfied in quasi-one-dimensional compounds of the KCP family and in polyacetylene, where $E_g/\omega_{ph} \sim 10$. It is important that the same compounds are distinguished by a large width of the electron band $t \gg E_g$, as a result of which the neglect of the repulsion of the electrons at one site is justified, whereas the Coulomb long-range action is effectively screened.

The properties of the Peierls model depend essentially on the number and degree of filling of the electron bands in the metallic phase. Investigations of the continuum models for one electron band[2-4] show that the wave vector $2\pi/l$ of the superstructure $\Phi(x)$ coincides, accurate to the wave vector $2\pi/a$ of the reciprocal lattice of the main structure, with the diameter $2k_F$ of the Fermi surface in the metallic phase. Such a superstructure can be regarded as singly periodic.

At the same time, many physical problems call for the investigation of quasiperiodic lattice deformations, which are characterized by incommensurate wave numbers $Q_i = 2\pi/l_i$. In the ground state of the system, different periods l_i could appear if the metallic phase contained several groups of electrons characterized by different Fermi momenta $k_F^{(i)}$. Such a problem arises, obviously, for a system in a strong magnetic field, when $k_{F\uparrow} \neq k_{F\downarrow}$ for different spin projections $\sigma_z = \uparrow\downarrow$.

Another possibility can be realized in organic conductors with complex molecules that contain usually large numbers (M) of π electrons. In these systems, the appearance of several unfilled bands can occur at $M \gtrsim T/t_{\parallel}$, where T and $t_{\parallel}$ are the hopping integrals between neighboring atoms in the molecule and between neighboring molecules in the conducting chain, respectively. Typically, $T \lesssim 10$ eV, $t_{\parallel} \sim 0.5$–1 eV and $M \sim 5$–15, i.e., the condition that many bands are present can actually be satisfied.

Quasiperiodic solutions are likewise a convenient means of finding solitons against the background of periodic structure, by going to the limit of infinite periods $l_i \to \infty$, $i > 1$ at a fixed fundamental period of the superstructure l_1. Investigations of the solitons are necessary to determine the electronic excitations in the system (see the review[5]). From along the known periodic solutions,[3,4] this limiting transition was used to obtain spinless charge excitations at $\rho = 1$ (domain walls[3]) and at $\rho = 0$ (polarons[4]). To determine the spectrum of spin excitations at arbitrary ρ it is already necessary to use doubly periodic structures.

The most interesting changes in the properties of a system occur in the concentration region $|\rho - 1| \ll 1$ adjacent to the limit of the half-filled band $\rho = 1$. This region corresponds to the experimental parameters of the intensively investigated doped polyacetylene[6,7] trans-$(CH)_x$. At $\rho \approx 1$ the essential wave vectors of the lattice deformations lie near the boundary of the Brillouin zone $\pm\pi/a$, as a result of which it is necessary to take exact account in the electron-phonon interaction the umklapp process of lowest (second) order.[8] At the same time, one can neglect the umklapp processes of higher order $k > 2$ which arise at $\rho \neq 1$ and whose amplitudes have a relative smallness[8,9]

$$(E_g/t)^{k-2} \ll 1, \quad k > 2.$$

As a result we arrive at a continuum model[8] that contains a real deformation field $\Delta(x)$

$$\Phi(x) \sim \Delta(x) \cos(\pi x/a), \quad \Delta(x)|_{\rho=1} = \Delta_1 = \text{const}, \tag{1}$$

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where the function $\Delta(x)$ varies slowly over distances of the order of the interatomic distance a.

At a large value of the concentration

$$n=|\rho-1|/a\gg\Delta_1/v_F, \quad |\rho-1|\gg\Delta_1/t, \tag{2}$$

where v_F is the Fermi velocity of the center of the band of the metal, the Fröhlich limit is reached,[10] at which the influence of the fundamental lattice becomes insignificant. In this limit it is possible[2,7] to describe the system by a complex field $\tilde{\Delta}(x)$:

$$\Phi(x)\sim \mathrm{Re}\,\tilde{\Delta}(x)\exp(2ik_Fx), \tag{3}$$

where $\tilde{\Delta}(x)$ varies slowly over distances of the order of

$$l=2\pi/Q, \quad Q=|2k_F-\pi/a|=|\rho-1|\pi/a.$$

The transition between the two limits takes place[3] continuously by development of the superstructure $\Delta(x)$ in (1) from a soliton lattice to an almost sinusoidal deformation (3).

The elementary electronic excitations cannot be band states in the potential of the superstructure $\Delta(x)$ of the ground state, because of the strong self-localization effect[11] (see the review[5]). At $\rho=1$ there are[12-14] spinless ($s=0$) excitations with charge $q=\pm e$, or else uncharged excitations ($q=0$) with spin $s=1/2$ of the domain-wall type

$$\Delta_s(x)=\Delta_1\,\mathrm{th}\frac{x}{\xi_1}, \quad \xi_1=\frac{v_F}{\Delta_1}, \quad E_s=\frac{2\Delta_1}{\pi}, \tag{4}$$

with energy $E_s<\Delta_i$, as well as symmetrical polarons[15-17] (bound states of an electron and two walls), which carry both a charge $\pm e$ and a spin 1/2, with energy E_p:

$$\Delta_p(x)=\Delta_1\left\{1-\frac{\sqrt{2}}{\mathrm{ch}(x\sqrt{2}/\xi_1)+\sqrt{2}}\right\}, \quad E_p=2^{3/2}\Delta_1/\pi. \tag{5}$$

We note that

$$E_s<E_p<\Delta_1.$$

In the limit of the Fröhlich model (2), (3) there are electronic excitations of only one type[11,13,18] which carry a spin but are not charged:

$$s=1/2, \quad q=0, \quad \tilde{\Delta}(x)=\Delta_\rho e^{i\varphi}\,\mathrm{th}\frac{(x-x_0)}{\xi}, \quad \xi=\frac{v_F}{\Delta_\rho}, E_s=\frac{2\Delta_\rho}{\pi}, \tag{6}$$

where E_s is the excitation (soliton) energy, and φ and x_0 are arbitrary constants.

Thus, the question arises of the change of the excitation spectrum with changing ρ. It is seen from the preceding paper[3] that at $\rho\neq1$ the charged walls (4) with $q=\pm e$, $s=0$ cannot be regarded as excitations of the system, since they make up the periodic superstructure of the ground state of $\Delta(x)$. It follows from our results[15] that the wall (4) with $q=0$, $s=1/2$ cannot be stable in the presence of another wall with $q=\pm e$, $s=0$. Two walls of the type (4) with $s=0$ and $s=1/2$ should coalesce into a polaron (5), with an energy gain

$$\delta E=2E_s-E_p=4\Delta_1/\pi-2^{3/2}\Delta_1/\pi>0.$$

It is therefore natural to assume that with increasing ρ the character of the single-electron excitations

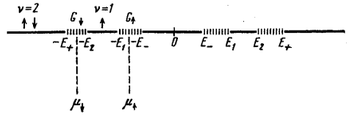

FIG. 1.

changes gradually from type (5) at $n\ll\Delta_1/v_F$ to type (6) at $n\gg\Delta_1/v_F$.

A solution of this problem will enable us to determine the change of the system energy $W(N)$ when the number N of the electrons is changed by unity, i.e., to find the chemical potential

$$\mu=W(N+1)-W(N).$$

We shall obtain simultaneously the triplet excited spin states of the system.

We construct in this paper doubly periodic solutions in the Peierls one-dimensional continuum model with the number ρ of the electrons per atom satisfying the condition $|\rho-1|\ll1$. We obtain the energy of the ground state of this system $W(n,m)$ as a function of the concentration of the total number of particles $n=n_+ + n_-=|\rho-1|/a$ and of the spin moment $m=n_+-n_-$, where n_+ and n_- are the concentrations of the electrons with different spin projections on the direction of the magnetic field H. We investigate the function $m(H)$, which is characterized by a critical value $H=H_c$ such that at $H>H_c$ a spontaneous moment $m\neq0$ is produced. At $m\neq0$ the superstructure of the lattice becomes doubly periodic, and an additional allowed and additional forbidden band appear in the vicinity of the Fermi level (Fig. 1).

We consider, as $m\to0$, solitons against the background of a singly periodic superstructure, which carry localized spin states. We investigate the soliton-charge screening, which turns out to be negligible at $n\ll\xi_1^{-1}$ and almost complete at $n\gg\xi_1^{-1}$ in accordance with (4) and (6).

2. GENERAL RELATIONS

We write down the electron wave functions $\psi(x)$ in the form

$$\psi(x)=2^{1/2}\left[u(x)\cos\frac{\pi x}{2a}+iv(x)\sin\frac{\pi x}{2a}\right]. \tag{7}$$

The components of the spinor $\overline{\psi}=(u,v)$ and the potential $\Delta(x)$ from (1) are connected by an equation for the eigenvalues of the energy E of the electrons:

$$u_E'-\Delta u_E=iEv_E, \quad v_E'+\Delta v_E=iEu_E \tag{8}$$

(the prime denotes the differentiation with respect to x). Here and elsewhere the Fermi velocity is equal to unity. From (8) we obtain the equivalent equations

$$u_E''+(E^2-p)u_E=0, \quad p=\Delta^2+\Delta'; \tag{9}$$

$$v_E''+(E^2-q)v_E=0, \quad q=\Delta^2-\Delta'.$$

The energy functional W of the system is of the form

$$W\{\Delta(x),f_\sigma(E)\}=\sum_{E,\sigma}f_\sigma(E)E+\int\frac{\Delta^2(x)}{g^2}dx, \tag{10}$$

where $f_\sigma(E)$ are the occupation numbers of the states with energy E and spin σ, and take on the values $f_\sigma(E)=0.1$, while g is the electron-phonon interaction constant. The stationary state of the system is determined from the condition that the functional (10) be an extremum with respect to the field $\Delta(x)$ for specified total numbers of the particles $N_\sigma=n_\sigma L$, where L is the length of the system.

We introduce the Fermi levels μ_σ and the thermodynamic potential $\tilde{W}(\mu_\sigma)$ that depend on them:

$$\frac{\delta\tilde{W}}{\delta\Delta(x)}\Big|_{\mu_\sigma}=0, \quad \tilde{W}(\mu_\sigma)=W-\sum_\sigma\mu_\sigma N_\sigma, \tag{11}$$

$$\mu_\sigma=\mu\pm h, \quad h=\mu_B H,$$

where μ and H are the total chemical potential and the external magnetic field, while μ_B is the Bohr magneton. The variation in (11) must be carried out with specified distribution functions $f_\sigma(E)$. These functions are determined further from the condition that the free energy of the system $\tilde{F}=\tilde{W}-TS$ be a minimum, where T is the temperature and S the entropy of the system. Confining ourselves only to the limit $T=0$, we must assume that

$$f_\sigma(E)=\begin{cases}1, & E<\mu_\sigma\\ 0, & E>\mu_\sigma\end{cases}.$$

For the variation of (10) with respect to $\Delta(x)$, we note that in accordance with (9)

$$\frac{\delta q(x)}{\delta\Delta(y)}=\delta(x-y)\left[2\Delta(x)+\frac{d}{dx}\right], \quad \frac{\delta E^2}{\delta q(x)}=2v^*(x)v(x). \tag{12}$$

Account is taken here of a fact that can be derived from (8), namely that the components $u(x)$ and $v(x)$ are independently normalizable:

$$\int u^*(x)u(x)dx=\int v^*(x)v(x)dx=\frac{1}{2}. \tag{13}$$

With the aid of (12) we obtain from (10) and (11)

$$\frac{\delta\tilde{W}}{\delta\Delta(x)}=\frac{2}{g^2}\Delta(x)+\sum_{E,\sigma}E^{-1}f_\sigma(E)\left[2\Delta+\frac{d}{dx}\right]v_E^*(x)v_E(x)=0. \tag{14}$$

From (8) it follows that

$$\Delta(x)=-v_0'(x)/v_0(x), \quad q(x)=v_0''(x)/v_0(x),$$
$$v_0(x)=v(x)\,|_{E=0}. \tag{15}$$

Using (15), we can write Eq. (14) in the form

$$\frac{d}{dx}v_0^{-2}(x)\left[\sum_{E,\sigma}E^{-1}f_\sigma(E)\,|v_E(x)|^2+g^{-2}\right]=0. \tag{16}$$

Equation (16) can be integrated and the integration constant can be determined from the normalization condition (13). We obtain

$$\sum_{E,\sigma}E^{-1}f_\sigma(E)\left[|v_E(x)|^2-v_0^2(x)\right]+\frac{1}{g^2}(1-2Lv_0^2(x))=0. \tag{17}$$

All we lose on going from (14) to (17) are the self-consistency conditions on the particular case of the homogeneous solution

$$|v_E(x)|=(2L)^{-1/2},$$

corresponding to $\rho=1$.

Substituting (15) in the second equation of (9), we obtain

$$\frac{v_E''}{v_E}-\frac{v_0''}{v_0}+E^2=0, \quad \frac{v_0''}{v_0}=q(x). \tag{18}$$

The system (18) and (16) or (17), with allowance for the normalization condition (13), determines the sought set of wave functions. We shall show that this system has solutions in the class of finite-band potentials $q(x)$. The Schrödinger equations (18), whose spectrum has only a finite number of forbidden bands, have been investigated in detail (see the reviews[19,20]) in connection with solutions of the Korteweg-de Vries (KdV) equations with respect to $q(x)$. Our problem calls for additional account of the functional connection (16), (17) between the solutions $v_E(x)$. It turns out that for finite-band potentials Eqs. (17) reduces to an algebraic equation.

We shall consider specifically the case of interest to us, that of a spectrum with two forbidden bands $G_{1,2}$, but the derivation presented below can be generalized in elementary fashion to the case of an arbitrary number of forbidden bands. We define the boundaries of the spectrum $E_\alpha=(E_-,E_1,E_2,E_+)$ as shown in Fig. 1, where the forbidden bands $G_{1,2}$ are hatched:

$$G_1: \quad E_-^2<E^2<E_1^2, \quad G_2: \quad E_2^2<E^2<E_+^2.$$

According to Novikov *et al.*[19-21] the two-band potential $q(x)$, its eigenfunctions $v_E(x)$, and the state density $dN(E^2)/dE^2$ are expressed in terms of two (in accord with the number of forbidden bands) functions $\gamma_{1,2}(x)$ which are defined in the regions of the forbidden bands $G_{1,2}$:

$$E_-^2\leqslant\gamma_1(x)\leqslant E_1^2, \quad E_2^2\leqslant\gamma_2(x)\leqslant E_+^2,$$

namely

$$v_E(x)=\left[\frac{(E^2-\gamma_1(x))(E^2-\gamma_2(x))}{2LA(E)}\right]^{1/2}\exp\left\{\pm i\int\frac{R^{1/2}(E^2)dx}{(E^2-\gamma_1(x))(E^2-\gamma_2(x))}\right\}, \tag{19}$$

$$R(\varepsilon)=\varepsilon(\varepsilon-E_-^2)(\varepsilon-E_1^2)(\varepsilon-E_2^2)(\varepsilon-E_+^2).$$

The normalization coefficient $A(E)$ in (19) is equal to

$$A(E)=\langle|(E^2-\gamma_1(x))(E^2-\gamma_2(x))|\rangle, \tag{20}$$

Here and below $\langle\ldots\rangle_L$ denotes averaging over the length of the system:

$$\langle F(x)\rangle=\frac{1}{L}\int_0^L F(x)dx.$$

For the potentials we have

$$q(x)=E_+^2+E_-^2+E_1^2+E_2^2-2(\gamma_1(x)+\gamma_2(x)),$$
$$\Delta(x)=-\frac{1}{2}\frac{d}{dx}\ln[\gamma_1(x)\gamma_2(x)]. \tag{21}$$

The number of states dN in the interval dE^2 is

$$dN=\frac{Ldp}{2\pi}=\frac{LdE^2}{2R^{1/2}(E^2)}\langle|(E^2-\gamma_1(x))(E^2-\gamma_2(x))|\rangle, \tag{22}$$

where

$$p(E^2\{=\pm R^{1/2}(E^2)\langle\{E^2-\gamma_1(x))(E^2-\gamma_2(x))\}^{-1}\rangle \tag{23}$$

is the wave vector of the function (19). With the aid of (20) we can rewrite (22) in the form

$$\frac{dN}{dE^2}=\frac{LA(E)}{4R^{1/2}(E^2)}. \tag{24}$$

The following important additional conditions also apply[19,20]

$$\int_{a_i} dN(E^2)=0. \tag{25}$$

Equations (25) ensure uniqueness of the momentum $p(E^2)$ continued from the intervals of the forbidden bands to the Riemann surface $y^2=R(E^2)$.

We present also for completeness differential equations that determine the family of functions

$$\gamma_j'=\pm 2iR^{1/2}(\gamma_j)/(\gamma_2-\gamma_1).$$

In this case $q(x)$ satisfies the second KdV equation

$$q^{(IV)}-5(q')^2-10qq'+10q^3+C_1q=C_2.$$

It is remarkable that in the subsequent calculations no use is made of the coordinate dependences or of the equations for the functions $\gamma_{1,2}(x)$.

We substitute (19) in (16) and (17). We then obtain from (17)

$$\frac{1}{L}\sum_{E,\sigma}\frac{f_\sigma(E)}{E}\left[\frac{|E^2-\gamma_1(x)|\,|E^2-\gamma_2(x)|}{A(E)}-\frac{\gamma_1(x)\gamma_2(x)}{A(0)}\right] +\frac{1}{g^2}\left[1-\frac{\gamma_1(x)\gamma_2(x)}{A(0)}\right]=0. \tag{26}$$

Equation (26) is of the form

$$B_1+B_2(\gamma_1(x)+\gamma_2(x))+B_3\gamma_1(x)\gamma_2(x)=0, \tag{27}$$

where B_1, B_2, B_3 are constants. In analogy with (16) we obtain

$$\frac{d}{dx}[B_1\gamma_1^{-1}\gamma_2^{-1}+B_2(\gamma_1^{-1}+\gamma_2^{-1})]=0,$$

whence, with allowance for (21),

$$B_1\Delta'+B_2(\Delta'''-6\Delta^2\Delta')=0. \tag{28}$$

The solution of Eq. (28), which is of the form of a modified KdV equation, can be only a singly periodic potential[3] with one forbidden band $E_-^2<E^2<E_+^2$. To obtain a potential with two forbidden bands it is necessary to require $B_1=B_2=B_3=0$. As a result we obtain from (26) three self-consistency conditions:

$$B_1=\frac{1}{\sigma^2}+\frac{1}{L}\sum_{E,\sigma}f_\sigma(E)\frac{E^2}{A(E)}\operatorname{sign}[R(E^2)]=0, \tag{29}$$

$$B_2=\frac{1}{L}\sum_{E,\sigma}f_\sigma(E)\frac{E}{A(E)}\operatorname{sign}[R(E^2)]=0, \tag{30}$$

$$B_3=-\frac{1}{g^2A(0)}+\frac{1}{L}\sum_{E,\sigma}\frac{f_\sigma(E)}{E}\left[\frac{\operatorname{sign}[R(E^2)]}{A(E)}-\frac{1}{A(0)}\right]=0. \tag{31}$$

Using the relations (19), we find that Eqs. (29)–(31) are linearly dependent. We shall use therefore hereafter only two of them.

The investigated state of the system is characterized by six parameters: $\mu_\sigma, \sigma=\uparrow\downarrow$ and $E_i(i=1,2,+,-)$. Equations (30) and (31) and the conservation laws for the number of particles with each spin projection

$$N_\sigma=Ln_\sigma=\sum_E f_\sigma \tag{32}$$

imposes for constraints on these parameters, which define, say, E_i in terms of μ_σ. The remaining two parameters are determined from the condition that the total energy of the system (10) on the class of two-band potentials be a minimum, or else from the extremum condition on a larger class of potentials.

We assume in this paper that the Fermi levels μ_σ pass through the forbidden bands of the potential. This assumption is sufficient for the investigation of the single-electron states, when we must consider remote solitons with a local level E_0:

$$E_1\to E_2\to E_0.$$

In this case

$$E_+^2>\mu_\uparrow^2>E_0^2, \quad E_0^2>\mu_\downarrow^2>E_-^2.$$

This assumption is natural also in strong fields $h\gg\Delta_1, m\gg\Delta_1/v_F$. In this limit the deformations $2k_F\uparrow$ and $2k_F\downarrow$, and accordingly the gaps $G_\uparrow=\{E_+^2, E_2^2\}$ and $G_\downarrow=\{E_1^2, E_-^2\}$ on the Fermi levels and should be approximately independent.

We shall assume hereafter that $\rho<1$, i.e., that the electron band is on the whole less than half filled (the case $\rho>1$ differs only in that the electrons are replaced by holes). This means that the bands $E>E_+$ and $E_-<E<-E_-$ are not filled: $n_\sigma(E)=0$ at $E>-E_-$. Next, the band $E<-E_+$ is always filled for both spin components: $n_\sigma(E)=1, E<-E_+, \sigma=\uparrow\downarrow$, i.e., each band state is doubly filled. The filling of the additional band $-E_1>E>-E_2$ should be different, depending on the locations of the levels μ_σ. For the state-filling multiplicity of this band $\nu=n_\uparrow(E)+n_\downarrow(E)$, $-E_1>E>-E_2$ we have

$$\nu=\begin{cases} 0, & -E_2>\mu_{\uparrow\downarrow}>-E_+ & \text{(33a)}\\ 2, & -E_-<\mu_{\uparrow\downarrow}<-E_1. & \text{(33b)}\\ 1, & -E_-<\mu_\uparrow<-E_1, \quad -E_2>\mu_\downarrow>-E_+. & \text{(33c)}\end{cases}$$

We consider now the self-consistency condition (30) at an arbitrary value of ν. Changing from summation over E to integration, we obtain with the aid of (24)

$$-2\int_{E_-^2}^{\infty}\bar R^{-1/2}(\varepsilon)\,d\varepsilon+\nu\int_{E_1^2}^{E_2^2}\bar R^{-1/2}(\varepsilon)\,d\varepsilon=0, \tag{34}$$

$$\bar R(\varepsilon)=(\varepsilon-E_+^2)(\varepsilon-E_-^2)(\varepsilon-E_1^2)(\varepsilon-E_2^2). \tag{34a}$$

Calculating the integrals in (34), we obtain

$$\frac{E_2^2-E_-^2}{E_+^2-E_-^2}=\operatorname{sn}^2\left(\frac{\nu}{2}K(p);p\right), \quad p^2=\frac{(E_2^2-E_1^2)(E_+^2-E_-^2)}{(E_+^2-E_1^2)(E_2^2-E_-^2)}. \tag{35}$$

Here $K(p)$ is an elliptic integral of the first kind. From (35) we obtain the following results:

a) $\nu=0$: $E_2^2=E_-^2$, i.e., the empty additional band $\{-E_1, -E_2\}$ is clamped and attached to the empty band $\{E_-, -E_-\}$ above it;

b) $\nu=2$: $E_2^2=E_+^2$, i.e., the completely filled additional band is attached, retaining the finite width corresponding to the particle number, to the completely filled band $\{E<-E_+\}$ below it;

c) $\nu=1$: it follows from (35) that

$$E_+^2+E_-^2=E_1^2+E_2^2=2E_0^2, \tag{36}$$

i.e., the bands have a common center designated E_0^2 in (36).

The results of items a) and b) show that in a single-band ($m=0$) Peierls state the Fermi level $\mu_\sigma=\mu_\sigma$ can pass only through the forbidden band. In the opposite case the system is absolutely unstable with respect to a difference between the state densities on the Fermi level, with subsequent joining together of equally filled bands. These results agree with the conclusion arrived at earlier[11,13] in the Fröhlich limit $|\rho-1|\sim 1$, that there are no activation charge excitations, despite the presence of a gap in the state spectrum of the rigid potential. We note that the usual picture of degenerate semiconductors would correspond precisely to location of the Fermi level in an allowed band.

We consider now the self-consistency condition (29) or (31). We subtract from (29) Eq. (30) multiplied by E_0^2, and change from summation to integration with the aid of (13). We obtain

$$\frac{1}{g^2}-\int_{-E_m}^{-E_+}dE\frac{E^2(E^2-E_0^2)}{\pi R^{1/2}(E^2)}+\frac{1}{2}\int_{-E_2}^{-E_1}\frac{E^2(E^2-E_0^2)}{\pi R^{1/2}(E^2)}dE=0. \tag{37}$$

When account is taken of relations (36), it is easy to find that the last term in (37) vanishes. The logarithmic dependence on the cutoff energy E_m is eliminated if one subtracts from (37) the same equation at $\rho=1$, when $E_1=E_2=E_-=0, E_+=\Delta_1$. As a result we obtain from (37), subject to the condition (36), a second relation

$$(E_+^2-E_-^2)^2-(E_2^2-E_1^2)^2=\Delta_1^4. \tag{38}$$

It shows that the interval (E_+^2, E_2^2), which stems from the forbidden band of the single-band potential, broadens when an additional allowed band (E_1^2, E_2^2) is included. At $E_1=E_2$ Eq. (38) goes over into the relation $E_+^2-E_-^2=\Delta_1^2$, which is equivalent to the result of the earlier paper.[3]

Relations (36) and (38) impose two constraints on the four parameters $E_i, i=+,-,1,2$. The free parameters of the band structure can be connected with the particle densities n_σ or with the limiting momenta of the bands p_+ and p_- (Fig. 2):

$$n=n_\uparrow+n_\downarrow=\pi^{-1}(2p_-+p_+-p_-)=\pi^{-1}(p_++p_-),$$
$$m=n_\uparrow-n_\downarrow=(p_+-p_-)/\pi, \tag{39}$$

where

$$p_-=\int_0^{E_-^2}\frac{dp}{dE^2}dE^2, \quad p_+-p_-=\int_{E_1^2}^{E_2^2}\frac{dp}{dE^2}dE^2. \tag{40}$$

We introduce the notation

$$z=E^2-E_0^2, \quad 2a=E_+^2-E_-^2, \quad 2b=E_2^2-E_1^2 \tag{41}$$

[from (38) we have $a^2-b^2=\Delta_1^2/4$] and use the relation

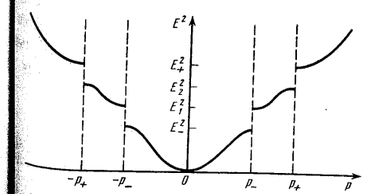

FIG. 2.

(36). Equation (24) then takes the form

$$\frac{dp}{dz}=\frac{z^2+\langle q\rangle z/2-A_0}{2Q^{1/2}(z)}, \quad Q(z)=(z+E_0^2)(z^2-a^2)(z^2-b^2). \tag{42}$$

The quantities q and $A_0=A(E_0)$ are defined in (11) and in (10a). The coefficients $\langle q\rangle$ and A_0 in (42) can be obtained from the conditions (25).

We define the family of hyperelliptic integrals

$$I_n^\pm(z_1,z_2)=\int_{z_1}^{z_2}\frac{z^n\,dz}{|(E_0^2\pm z)(z^2-a^2)(z^2-b^2)|^{1/2}} \tag{43}$$

and introduce the abbreviated notation

$$I_n^\pm(b,a)=I_n^\pm, \quad I_n^\pm(-b,b)=J_n^\pm, \quad I_n^\pm(a,e_0)=\mathcal{J}_n^\pm \tag{43a}$$

for the integrals over the forbidden ($I_n^\pm$) and allowed ($J_n^\pm, \tilde J_n^\pm$) bands. Substituting (25) in (42) we obtain

$$A_0=-\langle(E_0^2-\gamma_1)(E_0^2-\gamma_2)\rangle=\frac{I_2^-I_1^++I_2^+I_1^-}{I_0^-I_1^++I_0^+I_1^-}, \tag{44}$$

$$\langle q\rangle=\langle\Delta^2\rangle=2[2E_0^2-\langle\gamma_1+\gamma_2\rangle]=2\frac{I_2^-I_0^+-I_2^+I_0^-}{I_0^-I_1^++I_0^+I_1^-}. \tag{45}$$

Substituting (42) in (40) we obtain

$$p_+-p_-=\tfrac{1}{2}(J_2^++\tfrac{1}{2}\langle q\rangle J_1^++A_0J_0^+), \tag{46}$$

$$p_-=\tfrac{1}{2}(J_2^-+\tfrac{1}{2}J_2^-\langle q\rangle+A_0J_0^-). \tag{47}$$

Equations (46) and (47), with allowance for (44), (45), and (39), jointly with the constraints (36) and (38), determine completely the limits of the bands E_0 given the particle numbers $n_\uparrow$ and $n_\downarrow$.

We introduce now general relations for the densities of the energy $w(x)$, of the charge $\rho(x)$, and of the spin $\sigma(x)$. By definition

$$w(x)=\frac{\Delta^2(x)}{g^2}+\sum_{E,\sigma}f_\sigma(E)\bar\psi_{E^*}(x)\bar\psi_E(x), \quad \langle w(x)\rangle=W/L. \tag{48}$$

Using (8), (19), and (29), we transform (48) into

$$w(x)=L^{-1}\sum_E A^{-1}(E)E^3[E^2-(E_1^2+E_2^2+E_+^2+E_-^2)/2]. \tag{49}$$

We find that, as in the case of a single-band potential[3] and in the limit of an isolated soliton,[13] the total energy of the system is delocalized, i.e.,

$$w(x)=W/L=\text{const}.$$

The summation in (49) diverges rapidly far from the Fermi levels. We can regularize it by subtracting from (49) the energy density w_1 of the Peierls dielectric at $\rho=1$, when

$$E_1=E_2=E_-=0, \quad E_+=\Delta_1, \quad p_+=p_-=0, \quad w_1=w_{\text{met}}-\Delta_1^2/2\pi.$$

Here w_{met} is the energy density of a metal with $\rho=1$ without lattice deformation. Since the sum over E converges for $w-w_1$, we can calculate w and w_1 separately, introducing the arbitrary limiting momentum $p_m\gg p_+, p_-$. The value of p_m must be fixed, in order for the changes of the particle densities n_σ to be connected with the momenta $p_\pm$ by the relations (39). The quantity p_m is connected with the energy E_m corresponding to this state by relation (23). Since $E_m\gg E_i$, we have from (13)

$$p_m \approx E_m\left[1-\frac{\langle q\rangle}{2E_m^2}+O\left(\frac{E_1^2}{E_m^2}\right)\right]. \tag{50}$$

The condition $p_m = \text{const}$ can be rewritten approximately in accordance with (50) as

$$E_m^2 - \langle q\rangle = \text{const} + O(\gamma_{1,2}/E_m^2). \tag{51}$$

This result is in fact not connected with the form of the potential $q(x)$, but follows directly from (9) at $E_m^2 \gg \langle q\rangle$.

For the case (33c) of interest to us we have $\nu = 1$, and expression (49) reduces, when account is taken of (24) and (36), to

$$w = \int_{E_1^2}^{E_2^2} dE^2 \frac{E^3(E^2-E_0^2)}{2\pi R^{1/2}(E^2)} - \int_{E_2^2}^{E_m^2} dE^2 \frac{E^3(E^2-E_0^2)}{\pi R^{1/2}(E^2)}.$$

Calculating the integrals, we obtain

$$w = w(n,m) = \frac{E_0^2-E_m^2}{\pi} = \frac{E_0^2-\langle q\rangle}{\pi} + \text{const}, \tag{52}$$

whence

$$w(n,m) - w(0,0) = \frac{E_+^2+E_-^2+\Delta_1^2-2\langle\Delta^2\rangle}{2\pi}, \quad w(0,0) = w_1. \tag{53}$$

The quantity $\langle\Delta^2\rangle$ as a function of E_i is determined by (45).

Equation (53) yields a simpler form of the energy for the single-band potential than the form given earlier,[3] since the energy in (3) was reckoned from the energy of a metal with a given number of particles. In place of (53) we obtain the expression

$$w(n,m) - w_{\text{met}}(n,m) = \frac{E_+^2+E_-^2-p_+^2-p_-^2-2\langle\Delta^2\rangle}{2\pi}$$

which goes over into the result of the preceding paper[3] at $m = 0$, $p_+ = p_- = \pi n/2$.

The particle-number density $n(x)$ in the system is by definition

$$n(x) = \sum_{E,\sigma} f_\sigma(E)\bar{\psi}_E^*(x)\bar{\psi}_E(x).$$

Using (8), (19), (30), and (42) we obtain

$$n(x) = C\Delta^2(x) + D[2(E_0^2-\gamma_1)(E_0^2-\gamma_2)^{-1} - {}^1/_4(4E_0^2\Delta' - 6\Delta^2\Delta' + \Delta''')], \tag{54}$$

$$C = [\nu J_1^+ - 2I_1^+(a,\infty)]/4\pi, \tag{54a}$$

$$D = [\nu J_0^+ - 2I_0^+(a,\infty)]/4\pi. \tag{54b}$$

The particle spin density is by definition

$$\sigma(x) = \frac{1}{2}\sum_E [f_\uparrow(E) - f_\downarrow(E)]\bar{\psi}_E^*(x)\bar{\psi}_E(x), \quad \langle\sigma(x)\rangle = \frac{m}{2}.$$

In analogy with (54) we obtain

$$\sigma(x) = {}^1/_2\tilde{C}\Delta^2 + {}^1/_2\tilde{D}[2(E_0^2-\gamma_1)(E_2^2-\gamma_2)^{-1} - {}^1/_4(4E_0^2\Delta' - 6\Delta^2\Delta' + \Delta''')], \tag{55}$$

$$\tilde{C} = \nu J_1^+/4\pi, \quad \tilde{D} = \nu J_0^+/4\pi. \tag{55a}$$

Equations (36), (38), (39), (43), (46), (47), and (53)–(55) enable us to investigate the basic static properties of the Peierls model at zero temperature. Simpler relations can be obtained in the limit of large n and in the limit of small m.

3. FRÖHLICH LIMIT PHASE TRANSITION IN A MAGNETIC FIELD

We consider the general relations of the theory on going to the Fröhlich limit

$$n \gg \Delta_1, \quad E_0^2 \approx E_+^2 \approx E_-^2 \gg \Delta_1^2, \ a, \ b.$$

It is natural to express all the physical quantities in this limit in terms of the gap width $E_g = E_+ - E_-$ between the doubly filled and unfilled states and the width $E_b = 2\Delta_b = E_2 - E_1$ of the singly filled band $E_g \approx a/E_0$, $E_b \approx b/E_0$. The results should not depend explicitly on the value of E_0, which now determines only the general shift of the Fermi levels relative to the band center. The energy scale is defined by the quantity

$$\Delta_0 = \Delta|_{b=0} \approx \frac{\Delta_1^2}{4E_0}, \quad E_g = 2\Delta, \quad k = \frac{\Delta_0}{\Delta} < 1. \tag{56}$$

Expanding the integrals (43) up to terms $\sim E_0^{-3}$ inclusive, we obtain from (34) and (45)

$$\langle q\rangle = \langle\Delta^2\rangle \approx 2\Delta^2(2-k^2) + 4\Delta^2 E(k)/K(k), \tag{57}$$

$$A_0 = -\langle(E_0^2-\gamma_1)(E_0^2-\gamma_2)\rangle \approx 4E_0^2\Delta^2 E(k)/K(k), \tag{58}$$

$E(k)$ is a complete elliptic integral of the second kind. From (46), (47), (57), and (58) we obtain

$$m = (p_+ - p_-)/\pi \approx \Delta/K(k), \tag{59}$$

$$n = \frac{p_+ + p_-}{\pi} \approx \frac{2}{\pi}E_0\left[1 + \frac{\Delta^2}{E_0^2}\left(\frac{E(k)}{K(k)} - \frac{3}{2}\right) + \frac{3}{16}\frac{\Delta_0^2}{E_0^2}\right]. \tag{60}$$

From (60) we can determine E_0 and substitute, together with (57) and (58), into Eq. (53) for the energy. We obtain

$$w(n,m) - w(0,0) = \frac{\pi}{4}n^2 + \frac{\Delta_1^2}{2\pi} + \frac{\Delta_0^2}{2\pi} + \frac{\Delta^2}{\pi}\left(2\frac{E(k)}{K(k)} - 1\right),$$

where

$$w(n,m) - w(n,0) \approx \Delta_0^2 f(k)/\pi, \tag{61}$$

$$f(k) = 1 - k^{-2}[1 - 2E(k)/K(k)].$$

Equations (59) and (61) make it possible to determine the energy of the spin excitation in the Fröhlich limit. As $m \to 0$ we have according to (59) $k \to 1$ and $\Delta \to \Delta_0$, and from (61) we obtain

$$w(n,m) - w(n,0) \approx E_s m, \quad E_s = 2\Delta_0/\pi. \tag{62}$$

The quantity E_s coincides with the energy of the self-localized state[11,13,18] with spin $s = 1/2$ in the Peierls-Fröhlich model.

At high spin density $m \gg \Delta_0$ we have from (59) $k \to 0$, and from (61) we get

$$w(n,m) - w(n,0) = \pi m^2/4 - \Delta_0^2/\pi^2 m^2. \tag{63}$$

We have considered so far the properties of the system for given particle numbers $N_\uparrow, N_\downarrow$, i.e., for given n and m. We consider now the properties of the system in the case when only the total number of particles is specified

$$N_\uparrow + N_\downarrow = nL = \text{const}.$$

The spin density m should be determined from the condition that the free energy be a minimum

$$\tilde{w}(n,h) = w(n,m) - mh \tag{64}$$

at a given magnetic field h. An investigation of expression (64) at arbitrary n is quite difficult. We confine ourselves to the Fröhlich limit considered above $n \gg \Delta_1$. This region is of greatest interest, first because it includes practically all the quasi-one-dimensional substances with structural dielectric transitions. Second, with increasing n the value of the gap 2Δ decreases in accordance with (56) and (60) in proportion to n^{-1}, and can be compared with the attainable magnetic fields.

Substituting (59) and (61) in (64) we obtain

$$\tilde{w}(n,m) - \tilde{w}(n,0) = \frac{\Delta_0^2}{\pi}\left[1 + \frac{1}{k^2}\left(2\frac{E(k)}{K(k)} - 1\right) - \frac{2}{k}\frac{h}{E_s}\right] = \frac{\Delta_0^2}{\pi}\tilde{f}(k), \tag{65}$$

where $k = \Delta_0/\Delta$ according to (56). From (65) we have

$$\frac{d\tilde{f}}{dk} = \frac{2E(k)}{K^2(k)}\frac{hk/E_s - E(k)}{k^3(1-k^2)}, \tag{66}$$

where $E_s = 2\Delta_0/\pi$ in accordance with (62). It is seen from (66) that the function $\tilde{f}(k)$ has a minimum at $k = k_m < 1$ only at $h > h_c + E_s$:

$$E(k_m)/k_m = h/h_c. \tag{67}$$

Equations (67) and (59) determine the function $m(h)$. Plots of $\tilde{f}(k)$ at $h > h_c$ and of $m(k)$ are shown in Fig. 3. As $h \to h_c + 0$ we have

$$\frac{h}{h_c} \sim \frac{1-k^2}{2\ln(1-k^2)}, \quad \frac{m}{\Delta_0} \sim \frac{1}{\ln(1-k^2)},$$

whence

$$h \approx \frac{m}{\pi\Delta_0}\exp\left(-\frac{\Delta_0}{m}\right), \quad \frac{1}{\chi} = \frac{\partial h}{\partial m} \approx \frac{1}{\pi m}\exp\left(-\frac{\Delta_0}{m}\right). \tag{68}$$

At $h \gg h_c$ the modulus $k \to 0$ and we have

$$\frac{h}{h_c} \approx \frac{\pi}{2k}, \quad m \approx \frac{h_c}{k}, \quad h = \frac{\pi m}{2}, \quad \chi = \frac{2}{\pi} = \chi_P,$$

where χ_P is the Pauli susceptibility for the metal.

We have found that at $h < h_c$ the system does not have paramagnetic susceptibility: $m = 0$, $\chi = 0$. At $h > h_c$ the system becomes paramagnetic, and with a susceptibility χ that becomes infinite at $h \to h_c$. At $h \gg h_c$ the value of χ coincides with χ_P for a normal metal, despite the presence of gaps on the Fermi levels $\mu_\uparrow$ and $\mu_\downarrow$.

The results are applicable also to other systems with overlap of two bands, if the Fermi velocities can be regarded as close. The field h corresponds here to the difference between the Fermi momenta for two groups of electrons in the metallic phase, while $\pi m/2$ corresponds to the difference between the limiting momenta in the dielectric phase.

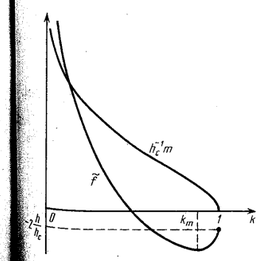

FIG. 3.

4. SINGLE-ELECTRON AND SPIN EXCITATIONS

We consider the limit of an infinitely small spin density, when the number of states and the number of particles in the band $\{-E_1, -E_2\}$, which is equal to the number of states, tends to zero. The band contracts then to a local level $-E_0$, and we have

$$m \to 0, \quad E_1 \to E_2 \to E_0, \quad b \to 0, \quad a \to \Delta_1^2/2, \quad m \sim \ln(\Delta_1^2/b).$$

To calculate the first-order effects in m, it suffices to separate in the integrals (43) the terms $\sim\ln(\Delta_1^2/b)$ and to neglect the corrections of higher powers of b.

Assume that a small spin density $m = M/L \ll n$ is produced in the system and that the total density is changed $n \to n + \delta n$, $\delta n \ll n$. The values of m and δn determine the width b and the shift of the spectrum $\delta(E_0^2)$ of the band $\{E_1^2, E_2^2\}$. From (46) and (47) we obtain in first order in m

$$n = \frac{\Delta_1}{rK(r)}, \quad m \approx \frac{\Delta_1 Z(\pi/4, r)}{r\ln(\Delta_1^2/b)}, \tag{69}$$

$$m + \delta n = \frac{rE(r)}{\Delta_1(1-r^2)K^2(r)}\delta(E_0^2) + mS(r), \tag{70}$$

where

$$S(r) = \frac{4}{\pi}K(r')\left[Z\left(\frac{\pi}{4}, r\right) - \frac{r^2}{2}\left(1 - \frac{r^2}{2}\right)^{-1/2}\right] + 2\Lambda_0(\varphi, r'),$$

$$r = \Delta/E_+, \quad r' = E_-/E_+, \quad r^2 + r'^2 = 1, \quad \operatorname{ctg}\varphi = r',$$

$$Z(\theta, r) = K^{-1}(r)[E(\theta, r)K(r) - F(\theta, r)E(r)],$$

$$\Lambda_0(\varphi, r') = \frac{2}{\pi}[K(r')E(\varphi, r) - \{K(r') - E(r')\}F(\varphi, r)],$$

$Z(\theta, r)$ is the Jacobi zeta function, $\Lambda_0(\varphi, r')$ is the Heymann lambda function, and $F(\theta, r)$, $E(\theta, r)$ are elliptic integrals of first and second kind respectively $[K(r) \equiv F(\pi/2, r)$, $E(r) \equiv E(\pi/2, r)]$.

We calculate $\delta\langle q\rangle$ from (45) and $\delta(E_0^2)$ from (70) and substitute in (53). We obtain the change in the system energy

$$\delta W = L[w(n+\delta n, m) - w(n, 0)] = \mu(\delta N - M) + E_s M,$$

$$\mu = \frac{\partial w(n,0)}{\partial n} = \frac{2\Delta_1}{\pi r}E(r), \quad E_s = \mu S(r), \quad \delta N = L\delta n, \quad M = Lm. \tag{71}$$

In the limiting cases, Eq. (71) takes the form

$$\delta W = \frac{2}{\pi}\Delta_1(\delta n - m) + \frac{2^{3/2}}{\pi}\Delta_1 m, \quad n \ll \Delta_1, \tag{72}$$

$$\delta W \approx E_+\,\delta n + \frac{2}{\pi}\Delta m, \quad 2\Delta = E_+ - E_-, \quad n \gg \Delta_1. \tag{73}$$

From (71) it follows that the change of the system energy upon addition of a singlet pair ($\delta N = 2$, $M = 0$) is $\delta W_s = 2\mu$, upon addition of a triplet pair ($\delta N = M = 2$) $-\delta W_t = 2E_s$, and on going from a singlet to a triplet state ($\delta N = 0$, $M = 2$) we have

$$W_t - W_s = 2(E_s - \mu) = 2E_a,$$

Upon addition of one particle ($\delta N = M = 1$)

$$\delta W_{+1} = \mu_+ = E_s,$$

Upon removal of one particle ($\delta N = -M = -1$)

$$\delta W_{-1} = \mu_- = 2\mu - E_a,$$

and upon excitation of an electron-hole pair

$$E_a^* = \mu_+ - \mu_- = 2(E_a - \mu) = 2E_a.$$

We note that the electron-hole and spin excitations have the same activation energy E_a, while the single-particle chemical potentials are equal to $\mu_\pm = \mu \pm E_a$. These facts, as well as the investigation of the corresponding coordinate dependences show that the two-particle state is simply an aggregate of two remote solitons, each carrying a single localized particle. At $n \gg \Delta_1$, it follows from (73) that $E_a \approx 2\Delta/\pi$, i.e., each soliton constitutes a domain wall (6).

At $n \ll \Delta_1$ it follows from (72) that

$$E_a = 2^{1/2}\pi^{-1}\Delta_1 - 2\pi^{-1}\Delta_1,$$

i.e., the activation is effected via a transition of spinless domain walls (4) into polarons (5).

We consider now the local properties of one soliton, namely the charge and the spin. To this end it is necessary to investigate the transition $m \to 0$ in Eqs. (54) and (55). Far from the soliton (as $x \to \pm\infty$) we have

$$\Delta(x) \to \Delta_{\pm\infty}(x),$$

where $\Delta_{\pm\infty}(x)$ satisfies Eq. (28) with $B_1/B_2 = 4E_0^2$, and

$$(E_0^2 - \gamma_1(x))(E_0^2 - \gamma_2(x)) = -A(E_0)\,|v_{E_0}(x)|^2 \to 0,$$

since $v_{E0}(x)$ degenerates into the wave function of the local level. Therefore the expression in the square brackets of (54) and(55) tends to zero as $x \to \pm\infty$.

According to Kuznetsov and Mikhaĭlov[22] the asymptotic singly periodic solutions $\Delta_{\pm\infty}(x)$ in the presence of one soliton differ exactly by half a period, from which we get in our case $\Delta_{+\infty}(x) = -\Delta_{-\infty}(x)$. Taking these remarks into account, we obtain from (54) the soliton charge q_s:

$$q_s = e\lim_{m\to 0}[\langle n(x) - n_\infty(x)\rangle/m] = e\lim_{m\to 0}\{[C\langle\Delta^2 - \Delta_\infty^2(x)\rangle + 2D\langle(E_0^2 - \gamma_1)(E_0^2 - \gamma_2)\rangle]/m\}. \quad (74)$$

Calculating the coefficients C and D in (54a) and (54b) as $b \to 0$, we obtain

$$C = -\frac{K(r')}{\pi E_+}, \quad D = \frac{1}{\Delta_1^2 E_0}\left[3 - 2\frac{F(\pi/4, r)}{K(r)} - \frac{4}{\pi}K(r')Z\left(\frac{\pi}{4}, r\right)\right]. \quad (75)$$

Calculating (44) and (45) as $b \to 0$, we obtain, with allowance for (69)

$$\langle\Delta^2(x)\rangle - \langle\Delta_\infty^2(x)\rangle \approx 4mE_+Z(\pi/4,\ r), \quad A_0 \approx \Delta_1^2 E_0 m. \quad (76)$$

Substituting (75) and (76) in (74) we obtain ultimately

$$q_s = e\left[1 - 2\frac{F(\pi/4, r)}{K(r)}\right] = e\begin{cases} 1 - \dfrac{n}{\Delta_1}\ln\dfrac{\sqrt{2}+1}{\sqrt{2}-1}, & n \ll \Delta_1 \\ \dfrac{2}{\pi^3}\dfrac{\Delta_1^2}{n^2}, & n \gg \Delta_1 \end{cases}. \quad (77)$$

Equation (77) shows that at $n \ll \Delta_1$ the soliton charge is close to the single-electron charge. With increasing n, partial screening of the charge is caused by the deformation of the periodic structure in the vicinity of the soliton.

In the Fröhlich limit $n \gg \Delta_1$, $r \ll 1$ we have $q_s \to 0$, i.e., the charge is completely screened in accordance with the earlier results.[11,13] The residual charge

$$q_s \sim e\frac{\Delta^2}{E_+^2} \sim \frac{\Delta_1^2}{n^2}e$$

is a weak effect of a remote commensurability point, which was lost in the previously employed[11,13] Fröhlich Hamiltonian based on the jellium model.

The calculation of the spin density in accordance with (55) and (55a) as $m \to 0$ leads to the obvious result

$$\sigma(x) = m|v_E(x)|^2.$$

The spin of one soliton is $s = 1/2$.

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Light scattering and the dispersion of susceptibilities in an incommensurate phase

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A consistent investigation of light scattering and the dispersion of the dielectric and elastic susceptibilities in the incommensurate phase is carried out. It is shown that the Goldstone excitation (phason) is always active in light scattering whether or not there is a change in the polarization. The intensity of the phason line vanishes at the symmetric–incommensurate phase transition point, and depends essentially on the direction of the scattering vector. In the scattering spectrum the phason line is a narrow central peak whose width is proportional to the square of the scattering vector. The phason also contributes always to the elastic susceptibility, but its contribution to the dielectric susceptibility is nonzero only if the crystal is piezoelectric in the symmetric phase. These contributions depend essentially on the direction of propagation of the elastic or electromagnetic waves, and manifest themselves only at very low frequencies (of the order of a hertz or a fraction of a hertz). The question of the appearance in the incommensurate phase of new spectral lines corresponding to non-Goldstone excitations is also considered. The selection rules are determined, and the intensities of the new lines and the scattering geometry in which they can be observed are discussed. The temperature dependence of the frequencies corresponding to these lines is also discussed. The analysis is carried out primarily for the case of a two-component order parameter, but the distinctive features that arise when the order parameter has a large number of components are analyzed also in the particular case of a four-component order parameter.

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The experimental investigations of light scattering and dielectric dispersion in incommensurate phases have greatly gained in scope (see, for example, Refs. 1–11). At the same time, the corresponding theory seems to us to be insufficiently developed. For example, the literature contains the most diverse opinions about the manifestation in such experiments of the characteristic excitation of the incommensurate phase, viz., the Goldstone phason mode. Thus, Cowley, actually asserts in his review article[12] that the phason mode is equivalent to an acoustic mode, and should similarly manifest itself in Mandel'shtam–Brillouin scattering. On the other hand, it is claimed in Refs. 13–15 that the Goldstone mode is inactive in light scattering and light absorption. The opinion also exists[3] that the phason is active in light scattering only if the crystal does not possess a center of inversion. The absence of a definite theory also leads to lack of coordination in the interpretation of experiment. Some experimenters have sought the manifestation of phasons in light scattering accompanied by a change in the polarization[1,4,6,7]; others, in light scattering not involving a change in the polarization.[2,3] Attempts have been made to detect the contribution of the phason to both the central peak[2,3] and the Mandel'shtam–Brillouin sideband components.[11]

The purpose of the present paper is to give a consistent and, as far as possible, exhaustive description of light scattering and the dispersion of the dielectric and elastic susceptibilities in the incommensurate phase on the basis of a phenomenological theory that goes back to the Landau theory of phase transitions. Let us emphasize that such an approach is standard, having been repeatedly used to investigate light scattering in the vicinity of phase-transition points.[14–16] As we shall see, the specific nature of the incommensurate phase manifests itself only in the necessity of the consideration of certain terms containing the spatial derivatives of the order parameter, which are usually neglected since they turn out to be insignificant in the analysis of commensurate phase transitions.

We note that in such an approach, as always in the Landau theory, we need consider only the symmetry of the high-temperature phase (which is the normal symmetry), the properties of the incommensurate phase being then determined automatically. In particular, it is not at all necessary to describe the symmetry of the incommensurate phase with the aid of the superspace groups that have been introduced in a number of papers (see, for example, Ref. 17).

1. MANIFESTATION OF THE PHASON IN THE CASE OF A TWO-COMPONENT ORDER PARAMETER

There are in the literature two equivalent methods of describing the transition into the incommensurate phase. In the unified description of the most frequently observed case of two transitions—from the high-temperature phase into the incommensurate phase, and from this phase into the low-temperature commensurate phase—the incommensurate phase is treated as a spatial modulation of the commensurate phase, and only the order parameter corresponding to the high-temperature—commensurate phase transition is introduced. The structure of the incommensurate phase is then described as an inhomogeneous structure with a "frozen-in" order-parameter wave, and a special role is played in the study of the transition into the incommensurate phase by the Lifshitz invariant, which is that term in the thermodynamic-potential density which contains the first derivatives of the order parameter.[18,19] The presence of the Lifshitz invariant makes a

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