Solitons in a Peierls system with a commensurability of three

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A one-dimensional model is used in the continuum approximation to investigate soliton states in a Peierls system with a commensurability close to three. The equations used in this investigation allow for the commensurability effects. These effects violate the exact integrability of the problem and a self-consistent solution is obtained using perturbation theory. It is shown that four types of amplitude-phase solitons are possible in such a system and the formation of these solitons does not require that the charge excess or deficiency, relative to a state which is filled exactly to one-third, should be an integer. Each soliton carries a single filled localized state.

1. The properties of a Peierls system depend strongly on the number of electrons ρ in a unit cell in the normal metal phase. The value of ρ $(0<\rho<2)$ is known to have both rational and irrational values. The nature of the resultant state, regarded as a function of the parameter ρ, is governed by the relationship between two factors: the effects of elastic deformation, tending to couple the structure to a wave vector $Q=2k_F=\pi\rho/a$, which in principle may be incommensurable, and umklapp processes or commensurability effects which favor a commensurable phase with a wave vector Q_0 somewhat different from Q. Among the many rational values of $\rho=m/n$, where m and n are integers, the greatest interest lies in those which are characterized by the smallest value of n for a given m, for example, $\rho=1$, 2/3, 1/2, etc., which correspond, respectively, to a doubly commensurate case, triply commensurate case, etc. In such cases the commensurability effects are strongest and these values stand out from the rest.

In this connection we have to consider the problem of singularities of a Peierls state in the vicinity of some specific value of ρ. This problem has been discussed in greatest detail for values of ρ close to unity. It should be pointed out that a commensurability of two is exceptional: the order parameter $\Delta(x)$ is real if the commensurability effects are not demonstrated explicitly (both direct and first-order umklapp processes are equally important). Numerical calculations of linear chains[1] and analytic solutions of the corresponding continuous[2,3] and discrete[4] models have establshed the important role played in the determination of the nature of the ground state and excitation spectrum by particle-like entities of the soliton type, which have a definite charge and spin, and they have shown that in the range $|\rho-1|\ll 1$ there is a spatially inhomogeneous state formed by solitons of this type. In the case of a commensurability of three, numerical calculations of linear chains have also been made[5,6] and have shown that one-soliton states with definite charge and spin ratios are possible. Attempts to solve this problem analytically in the continuum approximation[7] have not given correct results, as pointed out in Ref. 6. The case of triple commensurability is somewhat special. It is shown in Ref. 8 that for rational values of $\rho\neq 1$ a Peierls state exhibits not only displacements corresponding to the wave vector Q_0, but also displacements corresponding to the vectors $2Q_0$, $3Q_0$, etc. These displacements corresponding to multiple harmonics make a contribution of the same order as the commensurability effects,[8] which complicates the problem greatly. When $\rho=2/3$ (4/3) there are no multiple harmonic displacements and the commensurability effects seem to appear in their "pure" form.

We shall use the continuum approximation to investigate the characteristics of a Peierls system with commensurability close to three. The equations obtained allow correctly for commensurability effects. In contrast to the case when $|\rho-1|\ll 1$, our equations are not exactly soluble, since the commensurability effects violate the exact integrability of the problem. Therefore, these effects will be allowed for using perturbation theory. It is shown that four types of amplitude-phase solitons are possible in this system. The results obtained are in agreement with those deduced by numerical calculations.

2. We shall consider specifically the case of ρ close to $\rho_0=2/3$. The state in the range $|\rho-\rho_0|\ll 1$ will be described as the result of spatial modulation of a triply commensurate phase. The complete system of equations describing this state and allowing for the commensurability effects was obtained in Ref. 8 and in the representation of the crystal quasimomentum k it has the following form (we shall assume that $\hbar=1$):

$$(\lambda-E_1)\Psi_1=\Delta\Psi_2+\Delta^*\Psi_3,\quad (\lambda-E_2)\Psi_2=\Delta\Psi_3+\Delta^*\Psi_1,\quad (\lambda-E_3)\Psi_3=\Delta\Psi_1+\Delta^*\Psi_2, \tag{1}$$

where

$$E_l=\varepsilon(k+(l-1)Q_0),\quad \varepsilon(k)=-t_0\cos ka+t_0\cos k_F^0 a,$$

$$k_F^0=\pi\rho_0/2a,$$

Ψ_i $(i=1,2,3)$ are the wave functions of electrons, and λ are the eigenvalues. The quantity Δ is related to static displacements $u(x)$ by

$$u(x)=[\Delta(x)\exp(iQ_0x)+\text{c.c.}]/v_0. \tag{2}$$

In Eq. (2) v_0 is the matrix element of the electron-phonon interaction operator. The system (1) is supplemented by the self-consistency condition

$$\Delta=-\frac{v_0^2}{\omega_0}\sum_{\lambda}{}'[\Psi_{1\lambda}^*\Psi_{3\lambda}+\Psi_{2\lambda}^*\Psi_{1\lambda}+\Psi_{3\lambda}^*\Psi_{2\lambda}]. \tag{3}$$

The summation in Eq. (3) is over all the occupied states and ω_0 is the frequency of a phonon with a wave vector Q_0. The energy levels λ are measured from the position of the Fermi

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level of the initial metal phase. Linearization of $E_l(k)$ near the point $k = k_F^0$ and introduction of the momentum operator in the continuum limit yields the following system obtained from (1):

$$-iv_F\Psi_1'+\Delta\Psi_2+\Delta^*\Psi_3=\lambda\Psi_1, \quad iv_F\Psi_2'+\Delta^*\Psi_1+\Delta\Psi_3=\lambda\Psi_2,$$
$$(\lambda-\varepsilon_0)\Psi_3=\Delta\Psi_1+\Delta^*\Psi_2. \tag{4}$$

Here, $v_F = t_0 a \sin k_F^0 a$, $\varepsilon_0 = 3/2t_0$, and $\Psi_i' = d\Psi_i/dx$. Expressing Ψ_3 in Eqs. (3) and (4) in terms of Ψ_1 and Ψ_2, we finally obtain the following equations in the continuum approximation (we shall assume that $v_F = 1$):

$$-i\Psi_1'+\left(\Delta-\frac{\Delta^{*2}}{\varepsilon_0}\right)\Psi_2-\frac{|\Delta|^2}{\varepsilon_0}\Psi_1=\lambda\Psi_1,$$
$$i\Psi_2'+\left(\Delta^*-\frac{\Delta^2}{\varepsilon_0}\right)\Psi_1-\frac{|\Delta|^2}{\varepsilon_0}\Psi_2=\lambda\Psi_2, \tag{5}$$

$$\Delta=-\frac{v_0^2}{\omega_0}\sum_\lambda{}'\left[\Psi_{2\lambda}^*\Psi_{1\lambda}-\frac{\Delta}{\varepsilon_0}(\Psi_{1\lambda}^*\Psi_{1\lambda}+\Psi_{2\lambda}^*\Psi_{2\lambda})\right.$$
$$\left.-\frac{2\Delta^*}{\varepsilon_0}\Psi_{1\lambda}^*\Psi_{2\lambda}\right]. \tag{6}$$

In going over from the system (4) to the system (5), we have dropped terms of the order of $\lambda/\varepsilon_0 \ll 1$, since this condition is satisfied throughout the range of energies that we are investigating. The systems (5) and (6) are identical with those obtained by a different method in Ref. 7. We shall supplement the systems (5) and (6) by the condition that the number of electrons be constant,

$$N_{el}=N_0\rho=\text{const}, \tag{7}$$

where N_0 is the number of atoms in a chain of length $L = N_0 a$. In this problem the order parameter is complex:

$$\Delta(x)=f(x)\exp(i\varphi(x)), \tag{8}$$

and it is necessary to consider the spatial changes not only in the ampliude $f(x)$, but also in the phase $\varphi(x)$. The terms proportional to $\Delta^{*2}/\varepsilon_0 \ll 1$, and $\Delta^2/\varepsilon_0 \ll 1$ in the system (5) describe the contribution of the commensurability effects. The diagonal terms of the $|\Delta|^2/\varepsilon_0$ type in the system (5) describe the general shift of the energy and play no significant role in the problem under discussion. We can readily see from the systems (1) and (5) that if $\rho = \rho_0$, then the ground state is homogeneous and triply degenerate in the initial phase φ_0^0. It is convenient to identify a small parameter $\gamma_0 = |\Delta_0^0|/\varepsilon_0$, where Δ_0^0 denotes the value of Δ corresponding to $\rho = \rho_0$.

It follows from the system (4) that in this approximation we allow for the interaction of the two branches of the spectrum closest to k_F^0, $E_1(k)$ and $E_2(k)$, so that even in the homogeneous case the initial three-band structure can be approximated by a two-band scheme. Some of the states then lie within the continuous spectrum; this aspect will be considered later.

3. If terms of order γ_0 are ignored, the system of equations (5)–(6) is known to be exactly solvable and belongs to a class of finite-band potentials. The terms responsible for the commensurability effects violate the exact integrability of the problem but the nonintegrable corrections can be regarded as a small perturbation which acts on a given finite-band solution. This makes it possible to allow for the commensurability effects using perturbation theory. It should be pointed out that, as can be seen from the structure of the system of equations (5), perturbation theory can describe only the "amplitude" solitons which are affected mainly by spatial changes in the amplitude $f(x)$. In describing "phase" solitons, when the main role is played by spatial radiations of the phase, we have to go outside the perturbation theory framework because the nontrivial dependence on the phase is now governed by terms of order γ_0.

The perturbation theory of finite-band solutions has been considered in Refs. 9 and 10 and we shall follow them in future. Moreover, a discrete analog of the Peierls model in its most general form was used in Ref. 10 to investigate the commensurability effects and, in particular, the limit of a half-filled band. As already pointed out, since the system of equations (5) and (6), strictly speaking, is valid to within terms of order γ_0^2, we shall confine ourselves to the first order of perturbation theory. We solve the problem employing the usual self-consistency procedure: we initially determine the potential $\Delta_0(x)$ and the function Ψ_{i0} of the unperturbed problem and then we use them to find from Eq. (6) the first-approximation (iteration) potential to within terms of order γ_0 inclusive; this is followed by finding the first-approximation functions, etc., until the self-consistency condition is satisfied in a given order.

We shall consider the unperturbed problem described by the reduced equations (5) and (6). These equations have been used earlier to describe, for example, the range $|\rho - 1| \ll 1$ (Refs. 2 and 3), in which case the field $\Delta(x)$ is real, and an incommensurate system,[2] in which case this field is complex. We can show that in the reached system of equations in the class of finite-band complex potentials of interest to us the two-band potential corresponds to the extremal state. Solitons in an incommensurate system are described in Ref. 2 using a particular solution of the reduced equations corresponding to the symmetric positions of the band edges relative to a selected reference system. A similar solution was also used in Ref. 7 to describe a triply commensurate system and, as pointed out above, it gave an incorrect result. The correct boundary conditions can be satisfied only when the degeneracy of a discrete level is not an integer. Solutions of this type are valid if a system is characterized by an electron-hole symmetry and in this case the self-trapping of an electron or a hole gives the same result. In the problem under discussion the energy spectrum does not have this

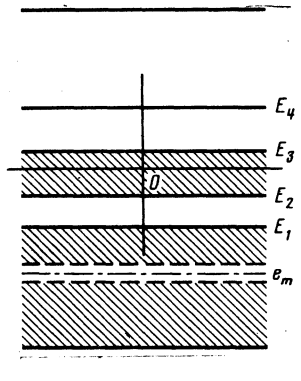

FIG. 1.

symmetry and it is necessary to employ a general solution of the reduced system of equations.

The general solution of this system is given in Ref. 11. According to Ref. 11, the three-band state of interest to us (Fig. 1) is described by six parameters: the edges of the energy bands E_i $(i = 1,...,4)$, an initial phase φ_0^0, and a quantity V_0 governing the position of the soliton lattice. The function $\Delta_0(x)$ is given by[11]

$$\Delta_0(x)=i|A|\exp\{i(\varphi_0^0+\beta x)\}\frac{\theta_2(iv+i\eta-2w)}{\theta_2(iv+i\eta)}. \qquad (9)$$

The following notation is used in Eq. (9):

$$|A|=\frac{(E_4+E_3-E_2-E_1)\theta_4}{2\theta_4(2w)}, \quad v=\frac{[(E_4-E_2)(E_3-E_1)]^{1/2}x}{2K(k')},$$
$$\eta=\frac{V_0}{2K(k')},$$
$$k'^2=\frac{(E_4-E_1)(E_3-E_2)}{(E_4-E_2)(E_3-E_1)}, \quad w=\frac{F(\varkappa,k')}{2K(k')}, \qquad (10)$$
$$\sin\varkappa=\frac{(E_3-E_1)^{1/2}}{(E_4-E_1)^{1/2}},$$
$$\beta=(E_4-E_3+E_2+E_1)+2[(E_4-E_2)(E_3-E_1)]^{1/2}Z(\varkappa,k'),$$

where $\theta_i(v)$ is the Jacobi theta function; $\theta_i=\theta_i(0)$; $K(k')$ and $F(\varkappa,k')$ are, respectively, complete and incomplete elliptic integrals of the first kind; and $Z(\varkappa,k')$ is the Jacobi zeta function.[12] It is convenient to use normalized functions Ψ_{10} and Ψ_{20}, which are given by

$$\Psi_{10}=\left[\frac{(E_4-E_2)(E_3-E_1)n_0}{2LD}\right]^{1/2}\exp\left\{-i\left(\omega-\frac{\beta}{2}\right)x\right\}$$
$$\times\frac{\theta_4\theta_2\theta_2(iv+i\eta-u_0-w)}{\theta_3\theta_1(u_0+w)\theta_2(iv+i\eta)},$$
$$\Psi_{20}=\left[\frac{(E_4-E_2)(E_3-E_1)n_0}{2LD}\right]^{1/2}\exp\left\{-i\left(\omega+\frac{\beta}{2}\right)x+i\varphi_0^0\right\} \qquad (11)$$
$$\times\frac{\theta_4\theta_2\theta_2(iv+i\eta-u_0+w)}{\theta_3\theta_1(u_0-w)\theta_2(iv+i\eta)}.$$

Here,

$$D=2\lambda^2-\varepsilon_1\lambda+E_1E_4+E_2E_3+(E_4-E_2)(E_3-E_1)\left[1-\frac{E(k)}{K(k)}\right],$$
$$\varepsilon_1=E_4+E_3+E_2+E_1, \quad k^2=1-k'^2=$$
$$(E_4-E_3)(E_2-E_1)/(E_4-E_2)(E_3-E_1), \qquad (12)$$
$$n_0=1-\theta_1^2(u_0+w)\theta_1^2(i\eta)/\theta_2^2(u_0+w)\theta_2^2(i\eta), \; u_0(\lambda)=-U(\lambda),$$

where $E(k)$ is a complete elliptic integral of the second kind. In Eqs. (11) and (12)

$$U(\lambda)=\int_{E_4}^{\lambda}\frac{c_1\,d\lambda}{(P_0(\lambda))^{1/2}}, \quad P_0(\lambda)=\prod_{i=1}^{4}(\lambda-E_i) \qquad (13)$$

is an Abel integral of the first kind normalized by the condition

$$\int_{a_1}dU=1,$$

where a_1 is an a cycle defined in the usual way,[11] and

$$\omega(\lambda)=\int_{E_4}^{\lambda}\frac{\lambda^2-{}^1/_2\varepsilon_1\lambda+c}{(P_0(\lambda))^{1/2}}d\lambda, \quad \int_{a_1}d\omega=0 \qquad (14)$$

is an Abel integral of the second kind.

Equation (9) is not quite convenient, because it does not allow us to separate explicitly the phase $\varphi_0(x)$, so that we shall use an alternative form for $\Delta_0(x)$ representing the solution of the following differential equation[11]:

$$\Delta_0''-2|\Delta_0|^2\Delta_0+2\varepsilon_2\Delta_0-i\varepsilon_1\Delta_0=0,$$
$$\varepsilon_2={}^1/_4\varepsilon_1^2-\sum_{i<j}E_iE_j. \qquad (15)$$

We find from Eq. (15) that

$$f_0^2(x)=z_3+(z_2-z_3)\,\mathrm{sn}^2(u+V_0;\,k), \qquad (16)$$
$$\varphi_0(x)=\varphi_0^0+{}^1/_2\varepsilon_1x+\left[\frac{z_1z_2}{z_3(z_2-z_3)}\right]^{1/2}\Pi(\delta,\alpha^2,k). \qquad (17)$$

In Eqs. (16) and (17) the notation is as follows:

$$u=(z_1-z_3)^{1/2}x, \quad \sin\delta=\mathrm{sn}(u+V_0;\,k), \quad \alpha^2=(z_3-z_2)/z_3,$$

$\mathrm{sn}(u;k)$ is an elliptic sine, $\Pi(\delta,\alpha^2,k)$ is an ellipitc integral of the third kind, and the parameters z_1, z_2, and z_3 are given by

$$z_1=\frac{(E_4+E_3-E_2-E_1)^2}{4}, \quad z_2=\frac{(E_4-E_3+E_2-E_1)^2}{4},$$
$$z_3=\frac{(E_4-E_3-E_2+E_1)^2}{4}. \qquad (18)$$

Equation (9) describes in general a quasiperiodic function. A periodic function with a period

$$l_0=2K(k)/(z_1-z_3)^{1/2} \qquad (19)$$

is defined by the modulus of $f_0(x)$. Nevertheless, the parameter l_0 is singled out and for the functions Ψ_{10} and Ψ_{20} there is an analog of the Floquet theorem in which the role of the quasimomentum $p_0(\lambda)$ is played by the quantity $p_0(\lambda)=\omega(\lambda)+(2\pi/l_0)U(\lambda)$, so that the differential of the quasimomentum is defined uniquely. It follows from Eqs. (9), (16), and (17) that the function $\Delta_0(x)$ describes a lattice of amplitude-phase solitons with a constant phase shift $\Delta\varphi_0$ in one period l_0. The quantity $\Delta\varphi_0$ is given by

$$\Delta\varphi_0=\beta l_0+4\pi\omega=[{}^1/_2\varepsilon_1+(z_1z_3/z_2)^{1/2}l_0+\pi(1-\Lambda_0(\delta_1;\,k))], \qquad (20)$$

where $\sin\delta_1=(z_3/z_2)^{1/2}$ and $\Lambda_0(\delta_1;\,k)$ is the Heuman lamda function. It should be noted that the solution $\Delta_0(x)$ is degenerate with respect to the initial case φ_0^0 and the parameter V_0.

Using the functions Ψ_{i0} and $\Delta_0(x)$, we find from Eq. (6), to within terms of order γ_0 inclusive, the first approximation to the potential $\Delta_1(x)$. The summation of the occupied states in Eq. (6) is carried out in the usual manner[13] and the states in the ground band $(\lambda\leqslant E_1)$ have a population multiplicity $\nu=2$ if the spin degeneracy is allowed for and the states in the "soliton" band $(E_2\leqslant\lambda\leqslant E_3)$ will be ascribed temporarily an arbitrary occupation multiplicity ν_0 $(0\leqslant\nu_0\leqslant2)$. Since the number of electrons in a system is fixed, we shall truncate the width of the ground band at the value E_0: $|E_0|\gg|E_i|$. We shall determine the parameter E_0 using the condition (7), which in the case of an unperturbed system becomes

$$N_{el}=\nu_0\frac{L}{l_0}+\frac{2L}{\pi}\left\{\left[\frac{(E_4-E_0)(E_3-E_0)(E_1-E_0)}{E_2-E_0}\right]^{1/2}\right.$$
$$\left.-\frac{\pi}{l_0}\Lambda_0(\varkappa_1;k)\right\}, \qquad (21)$$

where

$$\sin \varkappa_1=[(E_4-E_2)(E_1-E_0)/(E_4-E_1)(E_2-E_0)]^{1/2}.$$

Substituting Ψ_{i0} and $\Delta_0(x)$ into Eq. (6) and summing over λ, we obtain

$$\Delta_1(x)=\Delta_0(x)(1-g_0y_0/\varepsilon_0)-2\Delta_0^{*2}(x)/\varepsilon_0. \tag{22}$$

Equation (22) is valid subject to the following conditions:

$$\nu F(\varkappa_1;\ k)=\nu_0 K(k), \quad E_4+E_3-E_2-E_1=2|\Delta_0^0|/k'. \tag{23}$$

The following quantities are introduced in Eq. (22): $g_0=v_0^2/\pi a\omega_0$ is a dimensionless coupling constant which in the continuum limit obeys the inequality $g_0\ll 1$; $y_0=N_{el}/L$ is the electron density. Terms of order $g_0\gamma_0$ will be ignored. It follows from the first condition in Eq. (23) that the case $\nu_0=1$ is nontrivial, i.e., the formation of one soliton gives rise to a singly filled discrete level formed from a state split off from the continuous spectrum.

4. Substituting Eq. (22) in place of $\Delta(x)$ in the system (5), we obtain an equation for the determination of lowest-order functions. We shall select the perturbing potential $\phi(x)$ in the form

$$\Phi=\begin{pmatrix} v_1 & v_2^* \\ v_2 & v_1 \end{pmatrix}, \tag{24}$$

where $v_1=|\Delta_0(x)|^2/\varepsilon_0$, and $v_2=3\Delta_0^2(x)/\varepsilon_0$. In perturbation theory the problem reduces to finding first-order corrections with respect to the parameter γ_0 to the function Ψ_{i0} and to the potential $\Delta_1(x)$. We shall show later that the greatest interest lies in the case of a soliton lattice with large internal distances and obeying the condition

$$l_0/a\gg 1/\gamma_0\gg 1, \tag{25}$$

and we shall confine our attention to this case. The condition (25) means that the distance between solitons is much larger that the characteristic scale of the system, which is the coherence length $\xi_0=a/\pi\gamma_0$.

The spectrum of the operator of the unperturbed problem has two lacunae (forbidden bands) with edges at E_i, and also doubly degenerate points e_m (representing lacunae contracted to a point), the positions of which are given by the equation

$$\int_{E_4}^{e_m} d\mathbf{p}_0=\pi m/l_0, \quad m=2,3,\ldots . \tag{26}$$

The points e_m lie in the regions $\lambda<E_1$ and $\lambda>E_4$ (Fig. 1). The effect of perturbing Eq. (24) is generally a shift of the "old" band edges and the appearance at the points e_m of new lacunae of width Δe_m (Fig. 1). We can expect Δe_m to be of the order of γ_0. According to Ref. 9, the corrections of interest to us can be found by linearizing the solutions for the three-band potential in the vicinity of the two-band potential. The Appendix gives the expressions for the lowest-order functions $\Psi_i^{(1)}$ [Eq. (A.2)] and for the second-order potential $\Delta_2(x)$ [Eq. (A.6)]. These expressions include the "shifted" band edges, which should be regarded as new parameters of the problem. The self-consistent potential obtained in the first order of perturbation theory is given by Eq. (A.6). The quantities Δe_m can be determined using standard perturbation theory for a degenerate level. We then obtain

$$\Delta e_m=2\frac{|\langle v_2^*\Psi_{10}^2-v_2\Psi_{20}^2\rangle|}{|W(e_m)|}, \tag{27}$$

where $W(\lambda)=(P_0(\lambda))^{1/2}/LD$ and the angular brackets in the above equation denote averaging over a period. Using Eq. (25), we find that $k'^2\ll 1$, and in this limit Eq. (27) yields the following expression valid in the range $\lambda<E_1$:

$$\Delta e_m\approx\gamma_0|\Delta_0^0|/l_0(E_2-e_m). \tag{28}$$

In the same limit the quantity E_2-e_m is described by the following estimate obtained from Eq. (26):

$$E_2-e_m\approx(|\Delta_0^0|^2+(m-1)^2/l_0^2)^{1/2}.$$

As expected, the widths of the newly formed lacunae depend also on the oscillation period of the perturbing potential and the greatest contribution comes from the lacunae with low values of m ($m\ll l_0\gamma_0/a$). It follows from Eqs. (25) and (28) that the condition $\Delta e_m/|\Delta_0^0|<\gamma_0$, is satisfied, i.e., the corrections due to the overlap of the new lacunae include contributions of lower order than γ_0, since it is clear from Eq. (A.6) that the formation of each new lacunae gives rise to an additional phase shift which in one period amounts to $4\pi w_1\Delta e_m/|\Delta_0^0|$, where w_1 is defined by Eq. (A.5). In other words, in the case of a soliton lattice with large internal spacings the influence of the nonintegrable correction to the states in the ground bands can be ignored in the first order of perturbation theory. This conclusion agrees with the results of Ref. 10. The corrections due to opening up of new lacunae will be ignored in future, because they do not play a significant role. In this approximation the correction to the ground-state energy is governed by the average value of the perturbing potential of Eq. (24).

We shall now give some relationships which will be required later. These relationships and the expressions given later are valid for a soliton lattice with large internal spacings, when the quantities occurring in the problem under consideration can be expanded in powers of $k'^2\ll 1$. The following relationship between the parameter E_0 and the Fermi energy of the normal metal $\varepsilon_F=\pi\rho/2a$ is obtained from Eq. (21) if an allowance is made for Eq. (23):

$$|E_0|\approx\varepsilon_F-\frac{E_4+E_3-E_2+E_1}{2}-\frac{(E_4-E_2)(E_4-E_3)}{2\varepsilon_F}+\frac{(1-k)K(k)}{l_0}. \tag{29}$$

The expressions in Eq. (23) give definite relationships between the parameters E_i which can be expressed in terms of the quantities z_i (i, 1, 2, 3):

$$z_1^{1/2}=|\Delta_0^0|/k', \quad z_2^{1/2}=|\Delta_0^0|k'^{1/2}, \quad z_3^{1/2}=|\Delta_0^0|^2/\varepsilon_F. \tag{30}$$

Averaging the perturbing potential of Eq. (24) over the functions Ψ_{i0}, we obtain (including the leading terms), the following expression for the correction $\delta\lambda$ to the eigenvalues of the unperturbed problem:

$$\delta\lambda = -\frac{(z_1-z_3)^2}{2\varepsilon_0 LD} m \sin(3\varphi_0{}^0-2\beta x_0)\left\{\frac{2(E_2-\lambda)}{(z_1-z_3)^{1/2}}\left[\frac{\cos\tilde\beta l_0}{\tilde\beta}-\frac{B}{\tilde\beta}+\frac{2B}{3\varepsilon_0}\right]\left(1+\frac{3}{4}k'^2\right)-\frac{2B}{3(z_1-z_3)^{1/2}}\left(1+\frac{1}{2}k'^2\right)\right\}$$
$$-\left[\frac{z_1-z_3}{\varepsilon_0}-\frac{2(z_1-z_3)^{3/2}}{3\varepsilon_0 LD}\right]\left(1+\frac{1}{2}k'^2\right), \qquad (31)$$

where $\overline{\beta}=3\beta/2$, $B=y/\mathrm{sh}\ y$, $y=\pi\overline{\beta}/(z_1-z_2)^{1/2}$, and $m=L/l_0$ is the number of solitons. The last term in Eq. (31) governs the contribution of the diagonal perturbation v_1; we can see that this term gives rise only to a general energy shift and can be omitted. In the first term of Eq. (31) we shall retain a contribution of the order of $O(\gamma_0^2)$, the role of which we shall discuss later.

5. We shall calculate the energy of the system F given by

$$F=\sum_\lambda{}' (\lambda+\delta\lambda)+\frac{\omega_0}{v_0{}^2}\int |\Delta(x)|^2\,dx. \qquad (32)$$

Substituting Eq. (22) into Eqs. (31) and (32), integrating with respect to x, and summing over λ we find that Eqs. (21), (23), and (29) yield the following expression for the change in the energy δF relative to the metal state with the same number of particles:

$$\delta F = -\frac{L}{\pi}\left\{[(z_1-z_3)^{1/2}(1-k)-(E_4+E_3-E_2+E_1)-2\delta\mu]\varepsilon_F-\frac{1}{4}(E_3-E_2)^2\right.$$
$$\left.\div\frac{1}{2}(E_4-E_2)(E_4-E_3)\right\}-\frac{(z_1-z_3)^{3/2}}{\pi g_0\varepsilon_0} m\sin(3\varphi_0{}^0-2\beta x_0)$$
$$\times\left[\frac{\cos\tilde\beta l_0}{\tilde\beta}-\frac{B}{\tilde\beta}+\frac{2B}{3\varepsilon_0}\right]\left(1+\frac{3}{4}k'^2\right), \qquad (33)$$

where $\delta\mu=\pi(\rho-\rho_0)/2a$ is the deviation of the chemical potential from the value corresponding to $\rho_0=2/3$. The last term in Eq. (33) depends on the parameters φ_0^0 and x_0 and it determines the energy of the commensurability of the system, the value of which is proportional to $1/g_0$. It follows from Eq. (33) that an extremal state corresponds to

$$x_0=0, \quad |\sin 3\varphi_0{}^0|=1, \quad \varphi_0{}^0=\pm\pi/6. \qquad (34)$$

Therefore, the addition of the commensurability energy gives a fixed value of the parameter x_0 and of the initial phase φ_0^0, i.e., it results in pinning of the soliton lattice.

We still do not know the parameter β and the quantity $\delta\mu$, which determines the excess (or deficiency)—compared with $\rho=\rho_0$—in the electron density necessary for the formation of solitons. In fact, the change in the phase over one period is not known either. In this approximation it follows from Eqs. (9) and (22) that the phase $\varphi(x)$ is given by

$$\varphi(x)=\varphi_0(x)+\frac{2f_0(x)}{\varepsilon_0}\sin 3\varphi_0(x), \qquad (35)$$

where the quantity $\varphi_0(x)$ is given by Eq. (17) which for $k=1$ (isolated soliton) becomes

$$\varphi_0(x)=\varphi_0{}^0+\beta x+\mathrm{arctg}\left[\left(\frac{z_2-z_3}{z_3}\right)^{1/2}\mathrm{th}\,u\right]. \qquad (36)$$

We can see that in the soliton region the phase changes rapidly by π. We shall introduce the average wave vector of the superstructure q, given by $q=\Delta\varphi/L$, where $\Delta\varphi=\varphi(L/2)-\varphi(-L/2)$ is the total change in the phase. Using Eqs. (20) and (35), we can transform Eq. (33) to

$$\delta F = -\frac{L}{\pi}\left\{\left(\frac{\pi}{l_0}-2\delta\mu-q\right)\varepsilon_F-\frac{2E(k)(E_4-E_2)}{l_0}\right.$$
$$\left.-\frac{1}{4}(E_3-E_2)^2+\frac{1}{2}(E_4-E_2)(E_4-E_3)+(E_4-E_2)(E_3-E_2)\right\}$$
$$-\frac{(z_1-z_3)^{3/2}}{\pi g_0\varepsilon_0} m\sin 3\varphi_0{}^0\left[\frac{2B_1}{3\varepsilon_0}-\frac{2B_1}{3(q-\pi/l_0)}-\frac{2\sin(3/2 ql_0)}{3(q-\pi/l_0)}\right]\left(1+\frac{3}{4}k'^2\right), \qquad (37)$$

where B_1 is found from B by the replacing β with $q-\pi/l_0$.

We now consider the case of isolated solitons with $k=1$, $E_3=E_2$, and $l_0=L$. We shall identify the contributions made to the leading term of Eq. (37). The contribution proportional to $2\delta\mu$ is responsible for the elastic deformation effects which favor a structure with the wave vector $Q=2k_F=Q_0+2\delta\mu$, whereas the umklapp processes tend to balance the linear increase in the phase by an abrupt change of the phase by an amount π. The value of the vector q is the result of a compromise between these two effects and, according to Eq. (37), it is given by

$$q=\frac{\pi}{L}-2\delta\mu=\frac{\pi}{L}(1-\delta\rho N_0). \qquad (38)$$

Therefore, the complete change in the phase depends on $\delta\rho=\rho-\rho_0$, which thus determines the so-called topological charges of the solitons. In the system under discussion, the ground state of which is triply degenerate, there can be three types of soliton for each sign of $\delta\rho$ and they differ in their topological charges, but (as already pointed out) within the framework of the approach adopted here, we can describe only amplitude-phase solitons. We shall determine the types of these solitons and the corresponding values of $\delta\rho$ by superimposing on the phase of the order parameter certain boundary conditions, which in the case of a triply commensurate system can be derived from Eq. (35):

$$\varphi\left(\frac{L}{2}\right)=\varphi\left(-\frac{L}{2}\right)+p, \quad p=0, \quad \frac{2\pi}{3}\ (\mathrm{mod}\,2\pi). \qquad (39)$$

This yields the following values of $\Delta\varphi$: $\Delta\varphi=0$, 2π, $2\pi/3$, $4\pi/3$. It follows from Eq. (38) that the corresponding values of the quantity $\delta n=N_0\delta\rho$ are $\delta n=\pm 1$, $\pm 1/3$. We can assume that the values of δn expressed in suitable units are equal to the topological charges of the solitons. Solitons with different values of δn are essentially different objects and the energies of formation of these objects are also different, as will be shown below. In all cases the formation of a soliton gives rise to a singly occupied discrete level, the position of which is described by the equation

$$E_3=E_2={}^1/_2\beta-\gamma_0|\Delta_0{}^0|. \qquad (40)$$

Consequently, the spin of each soliton is 1/2.

For four types of solitons the behavior of the amplitude $f(x)$ is practically the same (the difference between the terms is of order γ_0), as shown in Fig. 2. On the other hand, the behavior of the phase $\varphi(x)$ is different even in the zeroth order and the functions $\varphi(x)$ for each case are plotted in

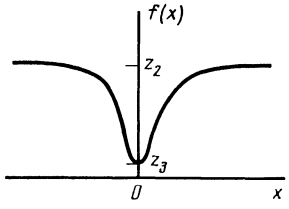

FIG. 2.

Figs. 3a–3d. It is clear from Eq. (22) [see also Eq. (35)] that the corrections due to the commensurability effects give rise to small (of order γ_0) and smooth (with a characteristic period of order φ_0) modulations of the functions $f(x)$ and (x) over distances $l \gg \xi_0$.

We shall now consider in greater detail the individual cases.

a) $\delta n = 1/3, q = 2\pi/3L, \beta = -\pi/3L, \varphi_0^0 = \pi/6$. According to the terminology of Refs. 5 and 6, this is a type-I kink. Among the rational values of ρ we can assign to this case $\rho = (N_{el}+1)/(N_0+1)$ on the basis of Ref. 6. However, if the change in the parameter ρ is due to doping, the charge transfer should be of order 1/3. We shall determine the energy of formation of solitons R as a contribution of one-particle terms. The value of $R_{1/3}$ can be obtained from Eq. (37):

$$R_{1/3} = \frac{2}{\pi} |\Delta_0^0| (1 - \gamma_0 + \gamma_0^2/3g_0). \tag{41a}$$

b) $\delta n = -1/3, q = 4\pi/3L, \beta = \pi/3L, \varphi_0^0 = -\pi/6$. This state represents a type-II kink, which corresponds to $\rho = (N_{el}-1)/(N_0-1)$. The value of $R_{-1/3}$ is given by

$$R_{-1/3} = \frac{2}{\pi} |\Delta_0^0| (1 - \gamma_0 - \gamma_0^2/3g_0). \tag{41b}$$

A comparison of Eqs. (41a) and (41b) shows that $R_{1/3}$ and $R_{-1/3}$ are different; in the present model the difference is of the order of γ_0^2. Both kink states correspond to the same

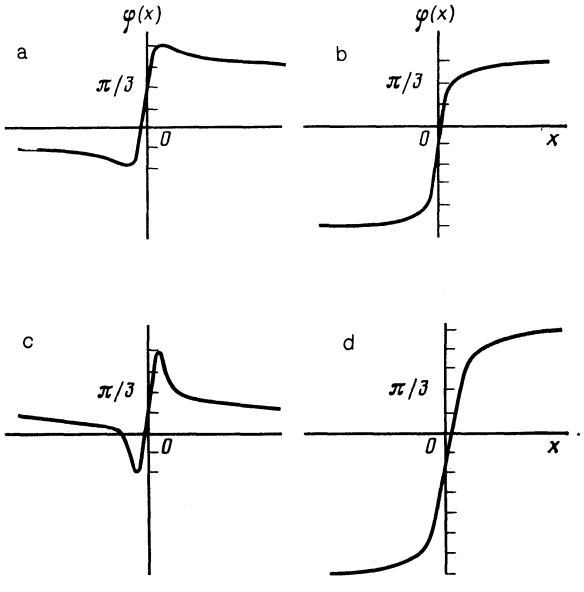

FIG. 3.

charge in the bulk energy δF_b, given by

$$\delta F_b = -\frac{L}{2\pi} |\Delta_0^0|^2 \left(1 + \frac{4\gamma_0}{\pi g_0}\right). \tag{42}$$

c) $\delta n = 1, q = 0, \beta = -\pi/L, \varphi_0^0 = \pi/6$. This is a symmetric type-I polaron characterized by $\rho = (N_{el}+1)/N_0$ and, to within terms of order $1/L$, we now have $R_1 \approx R_{1/3}$.

d) $\delta n = -1, q = 2\pi/L, \beta = -\pi/L, \varphi_0^0 = -\pi/6$. This is the case of a symmetric type-II polaron corresponding to $\rho = (N_{el}-1)/N_0$, $R_{-1} \approx R_{-1/3}$. Both polaron states are characterized by the same change in the bulk energy:

$$\delta F_b = -\frac{L}{2\pi} |\Delta_0^0|^2 \left(1 + \frac{4\gamma_0}{3\pi g_0}\right). \tag{43}$$

Comparison of Eqs. (42) and (43) shows that the polaron state is energetically less favorable. We note that minimization of Eq. (37) with respect to the parameter $\delta\rho$ gives a similar result.

We can show that in the case of an unperturbed system the charge of solitons is delocalized and the commensurability effects give rise to a small charge of order γ_0, localized in a fairly wide range $l \gg \xi_0$; in this case the core of a soliton remains uncharged.

We shall now compare our results with those of the numerical calculations reported in Refs. 5 and 6. The two approaches yield four types of amplitude-phase solitons with different topological charges. The behavior of the amplitude and phase of the order parameter is in agreement with the results of numerical calculations. The soliton formation energies are practically identical. The main difference is in the number of discrete levels which appear as a result of formation of a soliton. In the present model there is always only one discrete level, whereas numerical calculations based on the three-band scheme yield two and three discrete levels for each band gap in the case of kinks and polarons, respectively. This circumstance is manifested most strongly by a local charge of a soliton core. According to the numerical calculations reported in Ref. 6, this core has a local charge because of the stronger polarization of the states in the continuous spectrum due to the formation of additional discrete levels.

The commensurability effects were analyzed also in Ref. 2 on the basis of an analogy between these effects and the interchain interaction. This interaction is described in terms of a certain model phase Hamiltonian. A comparison of the results allows us to draw the conclusion that qualitative agreement does exist and, in particular, this applies to the behavior of the order parameter and of the soliton charge. In view of the specific features of the various problems and because different methods are used to solve them, we cannot attempt any quantitative comparison; for example, in the present study, as in Ref. 10, commensurability effects are treated by means of perturbation theory and numerical contributions are small with respect to parameter γ_0. A "symmetric" solution approach is used in Ref. 2 to describe the behavior of the phase in the case of an amplitude soliton in a triply commensurate system. A direct calculation of the remaining parameters of this soliton was not carried out, but nevertheless the results of numerical calculations and those given above suggest that this soliton is of the amplitude type with $\delta n = 1/3$.

We shall now consider briefly the general situation

which arises in $|\rho-\rho_0| \ll 1$. If the values of the parameter ρ are such that $|\delta n| = m/3$ or $|\delta n| = n$, then lattices of m kinks or n polarons appear, respectively. The lattice periods are described by

$$m, n = L/l_0. \tag{44}$$

The formulas in the two preceding sections provide a complete account of these states. It follows from Eq. (37) that deviation of the parameter ρ from this value $\rho_0 = 2/3$ makes the inhomogeneous state less and less favorable from the energetic point of view and the commensurability energy decreases rapidly. An analysis shows that if

$$|\delta\rho| \gtrsim \gamma_0/2\pi \tag{45}$$

then energetic considerations favor a homogeneous state formed by a superstructure with a wave vector $Q = 2k_F$, although we cannot exclude the possibility that a commensurate phase of higher order may be more favorable in this range. Therefore, soliton states discussed above are possible only in a small region in the vicinity of the point $\rho = \rho_0$ and these states can be described quite satisfactorily using the approximation of a soliton grating with large internal spacings.

The numerical calculations of Refs. 5 and 6 show that this system can also have phase solitons and we can describe them in the continuum approximation if we dispense with perturbation theory. According to Refs. 5 and 6, two types of solitons with $\delta n = \pm 2/3$ are possible and both have zero spin; the energy of formation of these solitons is considerably less than that required for amplitude solitons. However, this does not mean that the properties of the system are determined briefly by phase solitons; it is most likely, as pointed out in Ref. 6, that mixed states are formed from phase and amplitude solitons.

The author is grateful to A. R. Its for discussing a number of topics.

APPENDIX

We shall now obtain expressions for the first-approximation wave functions $\Psi_i^{(1)}$ and the second-approximation potential $\Delta_2(x)$. In the first order of perturbation theory in respect of the parameter γ_0 we can obtain expressions for $\Psi_i^{(1)}$ by linearization of the relevant formulas for the three-band potential corresponding to opening up a small lacunae of width Δe_m. Following Ref. 11, we shall introduce two-component vectors $\mathbf{g}(x) = (g_1, g_2)$, $\mathbf{U}(\lambda) = (U_1, U_2)$, $\mathbf{r} = (r_1, r_2)$. This linearization corresponds to partial degeneracy of a hyperelliptic curve of the second kind and the Abel differentials occurring in the problem have to be calculated in the appropriate limit. Consequently, the two-dimensional Riemann θ function $\theta(\mathbf{g})$ is described by the formula

$$\theta(\mathbf{g}) = \theta_3(g_2) + A_0\chi(\mathbf{g}), \tag{A.1}$$

where

$$A_0 = \frac{\Delta e_m (z_1-z_3)^{1/2}\theta_1'}{4K(k')\theta_1(2w)(P_0(e_m))^{1/2}} \exp\left[-w_1^2\frac{K(k')}{K(k)}\right], \tag{A.2}$$

$$\chi(\mathbf{g}) = \theta_3(g_2+2w_1)\exp(2\pi i c g_1) + \theta_3(g_2-2w_1)\exp(-2\pi i c g_1). \tag{A.3}$$

Suitable calculations yield the following expression for the first-approximation function $\Psi_1^{(1)}$:

$$\Psi_1^{(1)} = \Psi_{10}\left\{1 + \sum_m A_0(m)\left[\frac{\chi(\mathbf{g}(x)-\mathbf{U})}{\theta_2(g_2(x)-U_2)} - \frac{\chi(\mathbf{g}(0)-\mathbf{U})}{\theta_2(g_2(0)-U_2)} + \frac{\chi(\mathbf{g}(0)+\mathbf{r})}{\theta_2(g_2(0)+r_2)} - \frac{\chi(\mathbf{g}(x)+\mathbf{r})}{\theta_2(g_2(x)+r_2)}\right]\right\}. \tag{A.4}$$

The following notation is used in Eqs. (A.2)–(A.4):

$$g_2(x) = iv + w, \quad U_2 = -u_0, \quad r_2 = -w,$$
$$cg_1(x) = bx + \frac{1}{2} + \frac{i}{2\pi}\ln\frac{\theta_2(w+w_1)}{\theta_2(w-w_1)}, \quad w_1 = \frac{F(\varkappa_3, k')}{2K(k')},$$
$$cU_1 = \frac{i}{2\pi}\ln\frac{\theta_2(u_0-w_1)}{\theta_2(u_0+w_1)},$$
$$\sin\varkappa_3 = \left[\frac{(E_3-E_1)(E_4-e_m)}{(E_4-E_1)(E_3-e_m)}\right]^{1/2}, \tag{A.5}$$
$$b = \frac{1}{2\pi}(P_0(e_m))^{1/2}\left[\frac{1}{E_2-e_m} - \left(\frac{z_1-z_3}{P_0(e_m)}\right)^{1/2} Z(\varkappa_3, k')\right],$$

where the quantities v, u_0, and w are defined by Eqs. (10) and (12). The expression for $\Psi_2^{(1)}$ is obtained from Eq. (A.4) by replacing Ψ_{10} with Ψ_{20} and the argument of the θ function $\mathbf{g}(x) - \mathbf{U}$ with $\mathbf{g}(x) - \mathbf{U} + 2\mathbf{r}$. The summation in Eq. (A.4) is carried out over all doubly degenerate points, but since an increase in m causes a rapid reduction of the contributions of such points, we can confine ourselves to a finite number of terms. Substituting the functions $\Psi_i^{(1)}$ into the self-consistency equation (6), we find that when the conditions of Eq. (23) are satisfied, the following expression describes the second-order potential:

$$\Delta_2(x) = \Delta_1(x) + \Delta_0(x) \times \sum_m A_0(m)\left[\frac{\chi(\mathbf{g}(x)-\mathbf{r})}{\theta_2(g_2(x)-r_2)} - \frac{\chi(\mathbf{g}(x)+\mathbf{r})}{\theta_2(g_2(x)+r_2)}\right]. \tag{A.6}$$

[1] W. P. Su, J. R. Schrieffer, and A. J. Heeger, Phys. Rev. B **22**, 2099 (1980).
[2] S. A. Brazovskiĭ, Zh. Eksp. Teor. Fiz. **78**, 677 (1980) [Sov. Phys. JETP **51**, 342 (1980)].
[3] H. Takayama, Y. R. Lin-Liu, and K. Maki, Phys. Rev. B **21**, 2388 (1980).
[4] S. A Brazovskiĭ, I. E. Dzyaloshinskiĭ, and I. M. Krichever, Zh. Eksp. Teor. Fiz. **83**, 389 (1982) [Sov. Phys. JETP **56**, 212 (1982)].
[5] W. P. Su, Phys. Rev. B **27**, 370 (1983).
[6] Y. Ono, Y. Ohfuti, and A. Terai, J. Phys. Soc. Jpn. **24**, 2641 (1985).
[7] J. T. Gammel and J. A. Krumhansl, Phys. Rev. B **27**, 7659 (1983).
[8] V. P. Lukin, Fiz. Tverd. Tela (Leningrad) **19**, 379 (1977) [Sov. Phys. Solid State **19**, 217 (1977)].
[9] I. M. Krichever, Dokl. Akad. Nauk SSSR **270**, 1312 (1983).
[10] I. E. Dzyaloshinskiĭ and I. M. Krichever, Zh. Eksp. Teor. Fiz. **83**, 1576 (1982) [Sov. Phys. JETP **56**, 908 (1982)].
[11] A. R. Its, Vestn. Leningr. Univ. Fiz. Khim. No. 7(2) (1976).
[12] A. Erdélyi (ed.), *Higher Transcendental Functions* (California Institute of Technology H. Bateman MS Project), 3 vols., McGraw-Hill, New York (1953, 1955).
[13] V. E. Zakharov, S. V. Manakov, S. P. Novikov, and L. P. Pitaevskiĭ, Soliton Theory: Inverse Scattering Method [in Russian], Nauka, Moscow (1980).

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