Solitons with adjustable charge in a commensurate Peierls insulator

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We consider a one-dimensional electron gas with a half-filled band in which the electrons are coupled to both intersite and intrasite lattice distortions. In the region of parameter space in which both types of distortion develop nonzero expectation values, a new class of soliton which spontaneously breaks the charge conjugation symmetry of the model appears as the lowest-lying electronic excitation of the system. The soliton charge is a continuous function of the coupling constants.

I. INTRODUCTION: THE MODEL

The lowest-energy charged excitations in a commensurate, one-dimensional Peierls system appear to be solitons (domain walls) with fractional charge.[1] Originally it was imagined that the charge on a soliton is always a rational fraction of the electron charge, $Q^*=en/m$, where the fractional charge is related to the order of commensurability m. This is because the solitons are domain walls between equivalent ground states and hence have a winding number, $\Delta\theta=2\pi/m$, determined by the degeneracy of the ground state, which is also m. However, it was pointed out by Goldstone and Wilcek[2] (and implicitly by Rice *et al.*[1]) that if we admit solitons with arbitrary winding number $\Delta\theta$, then the charge associated with the soliton is $Q^*=e\,\Delta\theta/2\pi$, which can take on any value. It was recently shown by Brasovskii,[3] Rice and Mele,[4] and Jackiw and Semanoff[5] that in a simple model of a diatomic polymer in which there are two degenerate ground states, the solitons have a winding number, and hence a charge Q^*, which depends continuously on the difference in site energies of the two constituents.

In this paper we explore some effects of competing interactions on the nature of the commensurate Peierls state. In particular, we will show that for a class of physically reasonable models of the half-filled Peierls system, there is a finite region of parameter space in which there are *four* degenerate ground states and three different types of solitons (and their corresponding antisolitons) of which two have a winding number (hence charge) which is a continuous function of the interaction strengths. Since the model itself is initially charge conjugation symmetric, the irrational charge associated with these solitons appears as a consequence of a spontaneous breakdown of the charge conjugation symmetry.

Let us imagine a one-dimensional stack of molecules (which we will call sites), with one valence orbital per molecule and a band that is nearly half full. We include the coupling of the electrons to two lattice degrees of freedom, an intermolecular mode $\{u\}$, where u_n is the displacement of the center of mass of the nth molecule along the stack direction, and an intramolecular mode $\{v\}$, where v_n is the magnitude of the distortion of the nth molecule. The restriction to one intramolecular mode is not a fundamental limitation since in the generic case there is one most strongly coupled internal mode. The model can be easily generalized to include other internal modes, but they will have no qualitative effect on the results. To simplify the discussion, we will consider a model Hamiltonian which includes only harmonic terms in the lattice potential energy (quadratic in u_n and v_n) and a linear electron-phonon coupling (linear in u_n and v_n). Since some of the effects we will consider occur in next-to-leading order in the magnitude of the lattice displacements, this approximation is not formally justified. However, it can be easily shown that while the inclusion of higher-order terms in the Hamiltonian produces (usually small) quantitative corrections, it leaves the interesting physics qualitatively unchanged (see Ref. 6). Thus we will consider the Hamiltonian

$$H=-\sum_n\sum_{s=1}^{\nu}\{[t_0+\alpha(u_n-u_{n+1})](c^\dagger_{n,s}c_{n+1,s}+\text{H.c.})+\beta v_n c^\dagger_{n,s}c_{n,s}+\mu c^\dagger_{n,s}c_{n,s}\}+\tfrac{1}{2}\sum_n[K_1(u_n-u_{n+1})^2+K_2(v_n)^2+K_3v_nv_{n+1}]\,, \quad (1)$$

where ν is the spin degeneracy, $c^\dagger_{ns}$ creates an electron of spin s on site n, μ is the chemical potential, $4t_0$ is the bandwidth, and K_i are the various bare-lattice stiffness constants. Because of their different symmetries, the two lattice modes enter H in quite different ways. The translational symmetry of the system requires that the model be invariant under $u_n\to n_n+a$, and hence H can depend only on differences between the displacements of different sites. Because u_n-u_{n+1} is the change in the distance between sites n and $n+1$, we expect u_n to affect predominantly the electron hopping integral (coupling constant α). Since v_n is an intramolecular distortion, we expect it to modulate the site energy on site n (coupling constant β).

Physically, the coupling constant α ($\alpha>0$) reflects the fact that the hopping integral between two sites increases in magnitude as they are brought closer together. β reflects the fact that the energy of an electron on a molecule is changed (increased if $\beta>0$) as the size (v_n) is decreased. It is necessary to include the term proportional to K_3 in Eq. (1) so that the internal phonon mode has a finite band-

width (dispersion). We expect that K_3 will usually be positive, hence favoring out-of-phase distortions on neighboring molecules. There could also be terms coupling u_n and v_n. However, these terms lead to unimportant complications without affecting the final results qualitatively.

There are, however, three qualitatively important simplifications inherent in this model. Most notably, we assume that the ionic masses are sufficiently large that the ion kinetic energy can be ignored ($M\to\infty$ limit). Thus we always consider static lattice configurations. We also ignore all direct electron-electron interactions, and all interchain or three-dimensional interactions.

II. GROUND-STATE PROPERTIES

The ground-state lattice configuration of H is the dimerized state $u_n=(-1)^n u$, $v_n=(-1)^n v-\bar{v}$. Since the dimerized lattice involves only two atoms per unit cell, the electronic energy and wave functions can be obtained by diagonalized a 2×2 matrix. The result for the total energy of the dimerized system is

$$E_T(\Delta,\theta)=\frac{2t_0\nu}{\pi}\left[-[1+(\Delta_2)^2]^{1/2}E(1-z^2)+\frac{\Delta_1^2}{2A_\alpha}+\frac{\Delta_2^2}{2A_\beta}-\pi\left[\epsilon+\frac{\mu}{2t_0}\right]+\frac{\epsilon^2}{2A_\epsilon}\right]. \tag{2}$$

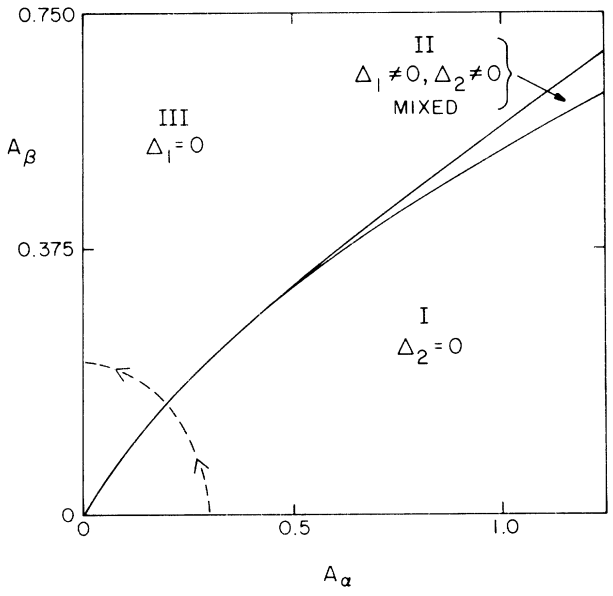

FIG. 1. Phase diagram: Region II is the coexistence region. The dashed line is a path through parameter space described in the text.

where

$$z^2=(\Delta_1^2+\Delta_2^2)/(1+\Delta_2^2),\quad \Delta_1=2\alpha u/t_0\equiv|\Delta|\cos(\theta),$$
$$\Delta_2=\beta v/(2t_0)\equiv|\Delta|\sin(\theta),\quad \epsilon=\beta\bar{v}/(2t_0),$$
$$A_\alpha=2\nu\alpha^2/(\pi K_1 t_0),\quad A_\beta=2\nu\beta^2[\pi t_0(K_2-K_3)],$$
$$A_\epsilon=2\nu\beta^2/[\pi t_0(K_2+K_3)],$$

and $E(x)$ is the complete elliptic integral of the second kind. We have defined the angle θ for later convenience to allow us to express the two competing real order parameters Δ_1 and Δ_2 in terms of a single order parameter $\Delta=|\Delta|e^{i\theta}$. Δ_1 represents the magnitude of the bond alteration (the dimerization of the intersite separations) and Δ_2 the site alternation (the site energy dimerization); ϵ is a measure of the uniform distortion of all the molecules. Since it is proportional to the amplitude of a $k=0$ optical mode, while Δ_1 and Δ_2 are optical modes with $k=2k_F=\pi/a$, ϵ is in a sense irrelevant to the interesting physics. Thus in much of the discussion that follows we will take $A_\epsilon=0$. We will return to discuss the affect of $A_\epsilon\neq 0$ in Sec. IV. In the case of the half-filled band, the chemical potential lies at the band center, hence $\mu=-2t_0\epsilon$, and hence (if the lattice is held rigid) the electronic excitation spectrum has particle-hole or charge conjugation symmetry. The energy needed to add to the system an electron or hole with wave number k is

$$\epsilon_k=2t_0[\cos^2(ka)+(\Delta_1)^2\sin^2(ka)+(\Delta_2)^2]^{1/2}, \tag{3}$$

where a is the lattice constant. The minimum energy to create a fermion, the electronic gap or "mass," is $2t_0|\Delta|$.

The ground-state value of the order parameter is obtained by minimizing E_T with respect to Δ and θ. The resulting phase diagram is shown in Fig. 1.

Region I is characterized by pure bond alternation, $\theta=0$ or π, and

$$\Delta=4e^{-1/A_\alpha-1}[1+\mathcal{O}(\Delta^2)],$$

where Region III is characterized by pure site alternation, $\theta=\pm\pi/2$, and

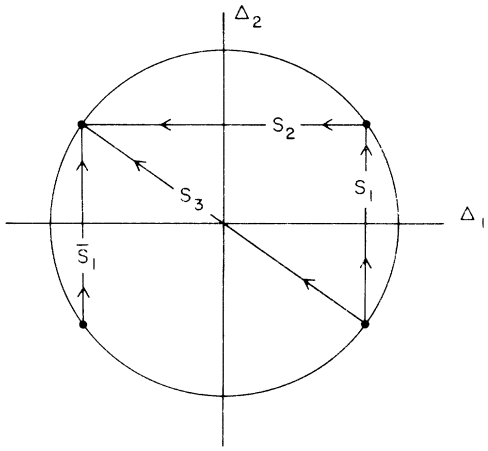

FIG. 2. Circle of constant $|\Delta|$ in the (Δ_1,Δ_2) plane. Ground-state configurations are indicated by the solid circles.

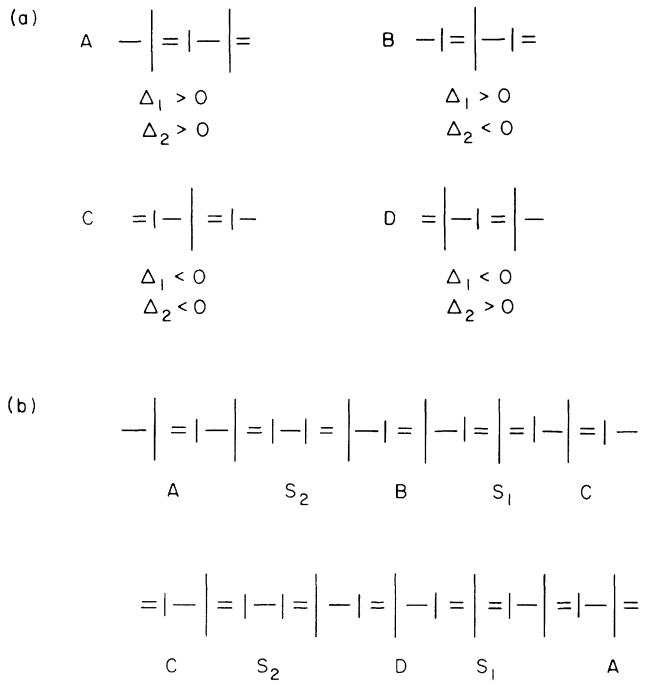

FIG. 3. (a) Schematic representation of the four possible ground states in the coexistence region. The bond alternation is represented by short double bonds ($u_n - u_{n+1} > 0$) and long single bonds ($u_n - u_{n+1} < 0$) while the site alternation is represented by stretched sites ($v_n > 0$) and compressed sites ($v_n < 0$). Note that A and C phases are related by an overall translation by one lattice site, as are B and D phases. (b) Schematic representation of the two types of irrationally charged solitons. Notice that the domain wall between A and B phases (S_2) is equivalent to the boundary between C and D phases. Similarly, an S_1 soliton is the boundary either between B and C or between D and A. By connecting the two illustrated segments together, we see that $2(S_1+S_2)$ is a topologically trivial combination of solitons (see discussion in the text).

$$\Delta = 4e^{-1/A_\beta}[1+\mathcal{O}(\Delta^2)] .$$

Region II is characterized by coexistence of site and bond alternation, so there is a ground state with $\theta=\theta_0$, where $0<\theta_0<\pi/2$. Since the energy is an even function of both Δ_1 and Δ_2, there are necessarily energetically equivalent ground states with $\theta=-\theta_0$, $\theta_0+\pi$, and $\pi-\theta_0$ as indicated by the solid circles in Fig. 2. The corresponding patterns of lattice distortions are shown schematically in Fig. 3(a).

The presence of a coexistence region is an intrinsically strong coupling effect, as can be seen from the Fig. 1. When Δ is small, the coexistence region has width of order Δ^2 about the line critical $A_\beta^{-1}=A_\alpha^{-1}+1$. The reason for this is that along this line, the energy is independent of θ to lowest order in Δ. Hence the ground-state values of θ are determined by higher-order terms. To make this explicit, we can express the total energy in the coexistence region as the sum of a θ-dependent and a θ-independent part:

$$E_T(|\Delta|,\theta)=\frac{-2t_0}{\pi}\left\{1+\frac{\Delta^2}{2}\left[\ln\left[\frac{4}{\Delta}\right]-\tfrac{1}{2}+\frac{1}{A}\right]+\mathcal{O}(\Delta^2)\right\}+\frac{t_0}{16\pi}\Delta^4 v(\theta) , \quad (4)$$

where $A^{-1}=\frac{1}{2}(A_\alpha^{-1}+A_\beta^{-1}-1)$ is the average coupling parameter, and

$$v(\theta)=d\cos(2\theta)+\tfrac{1}{2}[\cos^2(2\theta)-\tfrac{1}{2}]+\mathcal{O}(\Delta^2) , \quad (5)$$

where $d=(8D/\Delta^2-2A^{-1})$ and $D=\frac{1}{2}[A_\beta^{-1}-(1+A_\alpha^{-1})]$ is the distance in parameter space from the line $A_\beta^{-1}=(1+A_\alpha^{-1})$. It is easy to see by minimizing E_T with respect to $|\Delta|$ and θ that coexistence occurs only if

$$|\Delta|^2(2A^{-1}+1)>8D>|\Delta|^2(2A^{-1}-1) ,$$

that is, $|d|<1$ where, in the coexistence region, the ground-state value of the order parameter is

$$|\Delta| = 4\exp(1-A^{-1})$$

and

$$\theta_0=\cos^{-1}\{[\tfrac{1}{2}(1-d)]^{1/2}\} . \quad (6)$$

For systems in the vicinity of the coexistence region it is convenient to use the coupling constants A and d, rather A_α and A_β. By the "vicinity" of the coexistence region, we mean the narrow strip of the phase diagram in which d is of order 1.

III. THE SOLITONS: GENERAL TOPOLOGICAL CONSIDERATIONS

The solitons (kinks) which appear in the model are domain walls between regions of different possible ground states of the system. The intrinsic charge Q^* associated with a soliton is determined by its topology (that is, by the nature of the two ground states on either side of the soliton). In addition, if there is one or more localized electronic state associated with the soliton, it can exist in one of several charge states with charge Q, which differs from Q^* by an integral multiple of e, depending on the occupancy of these states. It is easily seen (see Refs. 1 and 2 and the next section) that in all the cases we will consider here, there is exactly one localized state in the band gap associated with each soliton. (There can also, in general, be a localized state beyond the band edge, but it plays no role in any interesting physical process.) Thus there are ν possible charge states of the soliton depending on the occupancy ν_0 ($\nu \le \nu_0 \le \nu$) of the gap state. The charge and spin of the soliton can be determined simply by any of a number of simple counting arguments.[1-3] We begin by classifying the solitons in the three regions of the phase diagram. Then we will give a simple intuitive version of the counting argument due to Schrieffer[1] to motivate the charge assignments.

In regions I and III there are only two ground states and so there can be only one type of soliton (and its corresponding antisoliton). The soliton is thus a region of finite extent over which the order parameter changes sign (θ

changes by π). These solitons are well known[1,3] to have charge $Q=e/2(\nu-2\nu_0)$ and spin $\frac{1}{2}\nu_0(\nu-\nu_0)$.

In the coexistence region (III) there are three possible solitons (S_1, S_2, and S_3) and their corresponding antisolitons ($\bar{S}_1$, $\bar{S}_2$, and $\bar{S}_3$) as shown schematically in Figs. 2 and 3(b). S_1 is the boundary between the state with $\theta=-\theta_0$ and $\theta=+\theta_0$, S_2 is the boundary between $\theta=\theta_0$ and $\theta=\pi-\theta_0$, and S_3 is the boundary between θ_0 and $\theta_0+\pi$. The spin of all the solitons is, as before, $\frac{1}{2}\nu_0(\nu-\nu_0)$. S_3 is topologically equivalent to the solitons in regions I and III and so its charge is the same as those solitons. The strange charges on S_1 and S_2 derive from the fact that the change in the phase of the order parameter across the soliton, $\Delta\theta$, is a function of the coupling constant d. The charge on the soliton is

$$Q_j=e(\nu\Delta\theta_j/2\pi-\nu_0)\ , \tag{7}$$

where for S_1, $\Delta\theta_1=2\theta_0$, and for S_2, $\Delta\theta_2=\pi-2\theta_0$. [The charge of the corresponding antisoliton is obtained by letting $\Delta\theta_j\rightarrow-\Delta\theta_j$ and $\nu_0\rightarrow(\nu-\nu_0)$.] If we imagine changing d, the fractional charge associated with S_1 goes monotonically from $Q_1^*=\frac{1}{2}e\nu$ on the $d=+1$ side of the coexistence region to $Q_j^*=0$ on the $d=-1$ side, while Q_2^* goes from 0 to $\frac{1}{2}e\nu$.

To obtain an intuitive feeling for the origin of these charges, imagine the following construction: We start with a chain in one of its uniform ground states, the A phase, for example. We then introduce a series of two S_1- and S_2-type solitons in the manner shown in Fig. 3(b), allowing there to be a sufficient region of uniform ground state between each soliton so that they can be treated as independent and noninteracting. Since the net effect of the introduction of these four solitons is to shift the Peierls condensate one wavelength to the right (without altering the boundary conditions) the total charge associated with the solitons is $+e\nu$. Since the two S_1-type solitons are equivalent to each other, they must have the same charge, as must the two S_2's, so $Q_1^*+Q_2^*=e\nu/2$. In region I the amplitude of the site-diagonal distortions is zero ($\Delta_2=0$), so the S_1-type soliton illustrated is a mathematical construct with no physical manifestation, and hence $Q_1^*=0$ and $Q_2^*=e\nu/2$. Similarly, in region III, S_2 exists only in the mind of the illustrator, and hence $Q_1^*=e\nu/2$ and $Q_2^*=0$. However, as the coexistence region is traversed from region I toward region III, the magnitude of Δ_1 decreases from $\Delta_1=\Delta$ to $\Delta_1=0$, and Δ_2 increases correspondingly. Hence, the charges Q_1^* and Q_2^* necessarily interpolate continuously between their values in regions I and III. Since from a topological point of view $S_3=S_1+S_2$, in all regions $Q_3^*=Q_1^*+Q_2^*=e\nu/2$.

IV. SOLITON ENERGIES

Having established the quantum numbers of the solitons it remains only to determine the lattice configurations which minimize the total adiabatic energy for each charge and spin state of the system, and hence to calculate the appropriate soliton shapes and creation energies. This can be done quite simply for H in Eq. (1) by finding the minimum of the adiabatic potential energy by direct numerical calculation.[1] However, in the weak coupling limit, $\Delta\ll 1$ ($A<1$), analytic results can be obtained as well. For the present we will ignore coupling to the $k=0$ intramolecular phonon. (We set $A_\epsilon=0$.)

Let us first consider the lowest-energy charge excitations in the coexistence region, which are the solitons of types 1 and 2 with $\nu_0=0$. As we shall see, these are phase solitons with width large compared to the electron correlation length,

$$\xi_0=\hbar v_F/|\Delta|\approx 2t_0a/|\Delta|\ ,$$

where v_F is the Fermi velocity. Because of their large width, we can derive their properties by considering an effective phase Hamiltonian, $H^{\rm eff}(\theta)$, obtained by expanding the adiabatic potential energy in powers of $\nabla\theta(x)$. The result is

$$H^{\rm eff}(\theta)=\frac{t_0}{2\pi}\int\frac{dx}{a}\left\{\frac{|\Delta|^4}{8}v(\theta)+|\Delta|^2\left[\left[\frac{\xi_0 d\theta}{dx}\right]^2+\mathcal{O}\left[\frac{\xi_0 d\theta}{dx}\right]^4\right]\right\}, \tag{8}$$

where $v(\theta)$ is defined in Eq. (5). The optimal S_1-type soliton is obtained by minimizing $H^{\rm eff}$ with respect to $\theta(x)$ subject to the boundary condition $\theta(x)\rightarrow\pm\theta_0$ as $x\rightarrow\pm\infty$. The result is

$$\theta(x)=\tan^{-1}\left[\tan(\theta_0)\tanh\left[\frac{x-x_0}{l}\right]\right], \tag{9}$$

where $l=2\sqrt{2}\xi_0/\Delta(1-d^2)^{1/2}$ is the soliton width and the soliton creation energy is

$$E_s=\frac{t_0}{\sqrt{2}\pi}|\Delta|^2\{2\theta_0[1-2\cos^2(\theta_0)]+\sin(2\theta_0)\}\ . \tag{10}$$

Notice that the soliton creation energy is of order $|\Delta|^2$, and hence much smaller than the electron creation energy which is $2t_0|\Delta|$. This is due to the large width of the soliton compared to the electronic correlation length, $l/\xi_0\sim|\Delta|^{-1}$. Also, because of this large width, the empty localized gap state has energy at the edge of the gap, just below the conduction-band edge. E_s has its largest value at the lower edge of the coexistence region, $d\lesssim+1$, where $E_s=t_0|\Delta|^2\sqrt{2}$, and drops monotonically as d decreases, until, for $d\gtrsim-1$,

$$E_s=(2t_0|\Delta|^2/3)(1-|d|)^{3/2}\ .$$

Near the edges of the coexistence region, the characteristic exponential length l diverges with exponent $\frac{1}{2}[l\sim(1-d^2)^{-1/2}]$. For d near 1, the soliton is no longer exponentially localized,

$$\theta(x)\approx\tan^{-1}[\tan(\theta_0)(x-x_0)/l]\approx\tan^{-1}[\sqrt{2}|\Delta|(x-x_0)/\xi_0]\ .$$

However, as seen in the second equality, it is still algebraically localized in a region of width $\sim\xi_0/|\Delta|$. For d near -1,

$$\theta(x)\approx\theta_0\tanh[(x-x_0)/l] ,$$

so that as $d\rightarrow -1$, the magnitude of the kink vanishes in the same fashion as its width diverges. The type-2 kinks are the same as type 1 with $\pi-\theta_0$ replacing θ_0. It should be noted that a single S_3-type soliton with $\nu_0=0$ is unstable with respect to the process $S_3\rightarrow S_1+S_2$.

A second interesting class of excitations is comprised of those that involve a change in the occupancy of the gap state associated with the soliton. A soliton in which the gap state is full (ν-fold) occupied (or an antisoliton in which is unoccupied) is always unstable,

$$S_j(\nu_0=\nu)\rightarrow S_j(\nu_0=0)+2\bar{S}_1(\nu_0=\nu)+2\bar{S}_2(\nu_0=\nu) .$$

However, for $\nu=2$, it is possible to have a soliton with a singly occupied gap state, $\nu_0=1$. For instance, the lowest-energy triplet excitation is a widely separated soliton-antisoliton pair, each of which has $\nu_0=1$. The soliton creation energy for $\nu_0=1$ can clearly be reduced by lowering the energy of the localized gap state. This can be done only by making the soliton width or order $\xi_0(l\sim\xi_0)$. Thus the soliton shape cannot be derived from the phase Hamiltonian in Eq. (7). It can, however, be obtained by considering the continuum limit of the full Hamiltonian in Eq. (1) and ignoring terms of order Δ^4. We will do so below. The results of this continuum theory are valid in the weak coupling limit ($a/\xi_0\ll 1$). The result[2] is the following: The soliton profile is given by the expression

$$\Delta(x)=|\Delta|e^{i\theta_0}\tanh(x-x_0/\xi_0) \tag{11a}$$

and the soliton creation energy is

$$E_s=(\nu/\pi)|\Delta| . \tag{11b}$$

The electronic spectrum in the presence of this type of soliton is charge conjugation symmetric, so the localized state lies at exactly midgap. The lowest triplet excitation is thus an $S_3\bar{S}_3$ pair, each with charge $Q^*=0$ and spin $\frac{1}{2}$.

Finally, we note that although irrationally charged solitons only appear in the coexistence region, the presence of the two competing order parameters is also felt in regions I and III in the vicinity of the coexistence regime. To explore these effects, let us consider the nature of the solitons as a function of the coupling constant over the entire parameter space. $H^{\rm eff}(\theta)$ in Eq. (8) provides an adequate description of the system only in the vicinity of the coexistence region ($|d|$ not much greater than 1) and only when the characteristic length scales, such as the charged soliton width $l\sim\xi_0/|\Delta|$, are much greater than the correlation length ξ_0. Far from the coexistence region, where the gradient expansion in $H^{\rm eff}$ breaks down, the weak coupling system can be described by a different sort of continuum model. This is possible because when $|d|\gg|1$, the higher-order θ-dependent terms in the energy $\mathcal{O}(\Delta^4)$, which play a central role in region II, can be ignored. Thus we begin our discussion by describing the continuum limit of the model in Eq. (1). (We use the technique described in Ref. 8. See also Refs. 3 and 9.) For the sake of completeness, we will at the same time discuss the qualitative effects of the heretofore neglected coupling to the $k=0$ intramolecular optical phonon $A_\epsilon\neq 0$. The resulting Hamiltonian is

$$\frac{H}{2t_0}=\sum_{S=1}^{\nu}\int dx\,\psi_s^\dagger(x)\left[-i\hbar v_F\frac{\partial}{\partial x}+\Delta_1(x)\sigma_x+\Delta_2(x)\sigma_y+\epsilon(x)\right]\psi_s(x)+\int\frac{dx}{a}\left[\frac{\Delta_1^2(x)}{2A_\alpha}+\frac{\Delta_2^2(x)}{2A_\beta}+\frac{[\epsilon(x)-\bar{\epsilon}]^2}{2A_\epsilon}\right]+E_{\rm kin} , \tag{12}$$

where $\psi_s^\dagger(x)$ is the creation operator of a spinor field with components corresponding to left and right moving electron branches, σ_a are the Pauli matrices in the branch index, $\hbar v_F=2t_0a$ is the Fermi velocity, $\epsilon(x)$ is the local amplitude of the long-wavelength optical phonon measured relative to its equilibrium value, $\bar{\epsilon}=\beta\bar{v}/(2t_0)$ [in the continuum model with cutoff energy $W\sim 2t_0$, $\bar{\epsilon}=\nu W(2A_\epsilon/\pi)$], and, $E_{\rm kin}$ is the lattice kinetic energy. Note that in deriving the continuum model we have ignored not only higher-order terms in Δ [$\mathcal{O}(\Delta^4)$] but also some terms of order Δ^2. Thus the continuum model is only valid (in detail) in the extreme weak coupling limit when terms of order Δ^2 can be ignored relative to terms of order Δ^2/A.

We can immediately deduce several important conclusions concerning the effect of the third field $\epsilon(x)$ on the properties of the model. Since $\epsilon(x)$ couples to the local charge density $\psi_s^\dagger(x)\psi_s(x)$, the same considerations apply throughout the phase diagram, even in the coexistence region (II). It is clear that in region II, where the charged soliton widths are very large and the charge densities correspondingly small, the effect of the coupling to $\epsilon(x)$ is small (so long as A_ϵ is not too large). Thus in this regime we were justified in considering the model with $A_\epsilon=0$. Moreover, in all regions of the phase diagram, the properties of the neutral soliton (i.e., an S_3-type soliton for $\nu=2$ and $\nu_0=1$) are totally unaffected by the presence of $\epsilon(x)$. This is a consequence of the fact that the soliton is not only globally neutral, but locally neutral as well.[10] However, far from the coexistence region, where as we will see, the soliton widths are of order ξ_0, the presence of $\epsilon(x)$ has a significant effect on the charged soliton shape and creation energy. Specifically, $\epsilon(x)$ tends to cause a reduction in both the soliton width and creation energy relative to the values of these quantities when $A_\epsilon=0$. Having thus determined the effect of $A_\epsilon\neq 0$, let us once again take $A_\epsilon=0$ to simplify the discussion.

We now are in a position to discuss the qualitative na-

ture of the soliton solutions along the dashed curve in Fig. 1. At the edges of the phase diagram, where $A_\beta=0$, or $A_\alpha=0$ Eq. (12) becomes equivalent to the well-known (TLM) model of polyacetylene. The minimum energy soliton is thus a pure amplitude soliton with a field configuration and creation energy the same as that given in Eq. (3), regardless of its charge state. In the case of normal electrons ($\nu=2$), the degeneracy between the neutral and charged solitons is lifted as we move into the interior of the phase diagram. The neutral soliton has the same shape and creation energy anywhere along this curve (and for any value of A_ϵ). However, the charged soliton becomes monotonically more phaselike, more spread out, and its creation energy decreases as we approach the coexistence region. Finally, at the border of the coexistence region ($|d|=1$) the minimum energy charged soliton can be found from $H^{\text{eff}}(\theta)$ to be a pure phase soliton with

$$\theta(x)=\tan^{-1}[\sqrt{2}\,|\Delta|\,(x-x_0)/\xi_0]\ ,$$

and with creation energy $E_s=\nu|\Delta|^2/\sqrt{2}$. Thus in the vicinity of the coexistence region we expect the conductivity activation energy to be a factor of $|\Delta|$ smaller than at the edges of the phase diagram.

V. EXPERIMENTAL PROSPECTS AND CONCLUSIONS

We conclude with a few brief remarks. Any commensurability-2 system with both intermolecular and intramolecular phonon modes has the possibility, in principle, of having a phase diagram of the sort in Fig. 1. A possible way to change the relative magnitudes of A_α and A_β is to apply pressure to the material. Since A_α depends exponentially on the intermolecular spacing, while A_β is probably not very sensitive to pressure, we expect that pressure will tend to drive the system in the direction of increasing A_α. For example, it appears that in $(MNP)_{0.5}(Phen)_{0.5}$ tetracyanoquinodimethane at ambient pressure, can be thought of[11] as a half-filled band with spinless electrons ($\nu=1$) and A_β greater than A_α. By applying pressure to this system, it may be possible to drive it into the coexistence region. This has the possibility of being a rather clean experiment. The difficulty is in finding the very narrow coexistence region.

In contrast, there are serious worries concerning the prospects of seeing fractionally charged solitons in a diatomic polymer, as suggested in Refs. 3–5. These models envisage a rigid uniform background field, analogous to Δ_2 in Eq. (12), which is due to the presence of alternating A and B atoms along the polymer chain. The irrationally charged solitons in that model are analogous to our S_2-type solitons, as they are domain walls between different senses of the band alternation. However, defects in the perfect alternating structure of the AB alloy appear in the model as static (possibly charged) local defects associated with deformations of Δ_2. If the defect is topological in character, it is analogous to a trapped S_1-type soliton, while if it is substitutional it is analgous to a trapped $S_1\bar{S}_1$ pair or, in other words, to a polaron. In either case, these defects interact strongly with the mobile S_2 solitons and either bind them or tend to confine them to the region between two such defects depending on the sign of the interaction with the particular defect. In either case it will make the observation of properties associated with the fractional charge very difficult unless the polymer is remarkably defect free.

Finally, we note that we have ignored all quantum-mechanical effects associated with the lattice. However, as the soliton width increases, we expect quantum effects to become increasingly important.[4] Thus we expect quantum effects to be largest in the coexistence region, exactly where the irrationally charged solitons occur.

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