Solitons in the Peierls condensate: Phase solitons

B. Horovitz
Department of Nuclear Physics, Weizmann Institute of Science, Rehovot 76100, Israel

J. A. Krumhansl
Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York 14853
(Received 3 June 1983)

The electron-phonon system in one dimension is studied within the adiabatic (Hartree) and Hartree-Fock approximations. The equations of motion for the Peierls order parameter at zero temperature are derived from a microscopic Hamiltonian and an effective Lagrangian is constructed. Charged phase solitons describe systems whose electron density is at or near M-fold commensurability with $M \geq 3$. For $M=2$, the order parameter is real in the adiabatic approximation, but becomes complex when both acoustic and optical phonons are coupled, or for a nonadiabatic theory. The latter is studied with a Coulomb exchange force and phase solitons are derived. The soliton charge is $2/M$ for all $M \geq 2$. When $M=4$, the pinning potential can be anomalously low, in agreement with data on TaS_3 and similar compounds.

I. INTRODUCTION

The electron-phonon system in one space dimension is of considerable interest, both theoretically and experimentally.[1,2] Peierls[3] noticed that the system is unstable towards formation of a charge-density wave (CDW) with wave vector $2k_F$, where k_F is the Fermi wave vector, and formation of a gap 2Δ at the Fermi level. The system is, however, not a simple semiconductor; as shown by Fröhlich,[4] the CDW can move rigidly and carry current.[5] This motion is pinned by either impurities, interchain coupling, or commensurability.[6] The Fröhlich mode then appears as an infrared "pinned mode" or in dc conduction when the field exceeds a threshold value.

Here we focus on commensurability pinning, which is present when the CDW wavelength is commensurate with the underlying lattice constant a, i.e., $2k_F/(2\pi/a)=N/M$ is rational. The integer M is defined as the order of commensurability. This system is of further interest as it leads to the well-known sine-Gordon equation for the phase field.[7,8] Rice, Bishop, Krumhansl, and Trullinger[7] showed that the soliton solutions of this sine-Gordon equation carry charge, and being thermally excited they contribute to the conductivity. The soliton is translationally invariant, unlike the commensurate system, and therefore restores the conductivity associated with the Fröhlich mechanism.

Another manifestation of solitons is the description of systems near commensurability. In these systems the ground state consists of commensurate regions separated by "discommensurations,"[9] or a "soliton lattice."[10–12] The single soliton is a limit of an incommensurate system becoming commensurate. Here the solitons are in the ground state and not thermally excited as in the commensurate case.

The derivation of the soliton-bearing equation from the microscopic Hamiltonian was reported in Ref. 8, where the nonlinear interaction was due to interchain coupling. In Sec. II the details of this derivation are given and the case of Mth-order commensurability, $M \geq 3$, is studied. The adiabatic (or Hartree) approximation is used and the effective Lagrangian is derived in terms of the amplitude, phase, and their derivatives up to second order. The adiabatic approximation is justified when the phonon frequency ω_0 satisfies $\omega_0 \ll \Delta$,[13] or when interchain tunneling is large compared with Δ.[14] In the latter case the system is three dimensional and solitons are then two-dimensional domain walls.

We study here solitons whose charge is $2/M$ and spin is zero. Spin-carrying solitons are also known[15–18]; these are usually described by singly occupied gap states.[15–17] The derivative expansion is useful in this case only if the system is near coexistence with a spin-density wave.[18] This will be further studied in a subsequent article.

The case of the half-filled band $M=2$ is studied in Sec. III. In the adiabatic (Hartree) approximation the order parameter is real and phase solitons do not exist. The effective Lagrangian does not allow amplitude solitons where the amplitude reverses sign, since the derivative expansion diverges when the amplitude vanishes. Thus the phenomenological derivation of amplitude solitons[19] is not justified. Indeed, when avoiding the derivative expansion, amplitude solitons can be found.[20–24] Another subsequent article will discuss these solitons in detail.

The order parameter for the $M=2$ system becomes complex when the electrons couple with two phonons whose coupling constants are out of phase, e.g., acoustic and optic phonons. Acoustic phonons prefer the CDW maxima to be in between sites, while optic phonons prefer them on sites. The phase variable describes, then, the interplay between these two positions.

A similar situation occurs when a single phonon coupling is considered beyond the adiabatic approximation or when direct electron-electron interactions are present. In particular, the system with an exchange long-range nonretarded (e.g., Coulomb) interaction is considered. The or-

der parameter is complex and phase solitons are found as reported in Refs. 25 and 26. The details of this derivation are given in Sec. III and the possibility of an attractive interaction between solitons is studied.

Section IV summarizes the results, and the relevance to experimental data is studied. In particular we find that when $M/4$ is an integer and the tight-binding approximation is used two relevant matrix elements vanish. The commensurability potential is then reduced to about that of an $M+2$ system. This can explain the low depinning fields of TaS_3,[27] ($M=4$), and similar compounds.

The Appendixes give derivative expansions, the relevant continuity equation, diagrammatic derivations, and a sufficient condition for attraction between solitons.

II. EFFECTIVE LAGRANGIAN: $M \geq 3$

In this section the electron-phonon system in one dimension is studied for incommensurate or $M \geq 3$ commensurate systems. The average charge density is $\rho_0 = 2k_F/\pi$ and the order of commensurability M is defined by

$$2k_F/(2\pi/a) = \rho_0 a/2 \equiv N/M \ , \tag{1}$$

with N,M reduced integers. Thus the fraction of filled states in the electron band is N/M.

The electron-phonon Hamiltonian is given by

$$H = \sum_{s,k} \epsilon_k C^\dagger_{s,k} C_{s,k} + \sum_{s,k,q} g_{k,q} R_q C^\dagger_{s,k} C_{s,k-q} + \sum_q \omega_q a^\dagger_q a_q \ , \tag{2}$$

where $C_{s,k}$ and R_q are the electron and phonon operators with momentum k and q, respectively, s is the spin index, $R_q = a_q + a^\dagger_{-q}$, ϵ_k and ω_q are the electron and phonon dispersions, and $g_{k,q}$ is the electron-phonon coupling constant. In the tight-binding model, which has been applied to polyacetylene,[15]

$$g_{k,q} = -4\alpha i \sin(\tfrac{1}{2}qa)\cos[(k-\tfrac{1}{2}q)a] \ , \tag{3}$$

where a is the lattice constant and α is a constant. In addition to the Hermiticity condition $g^*_{k,q} = g_{k-q,-q}$, Eq. (3) also satisfies $g_{k,q} = -g_{-k,-q}$. The latter condition is a result of an inversion symmetry which applies in general to acoustic phonons. On the other hand, coupling with a polarization field, i.e., optical phonons, has opposite parity and then $g_{k,q} = g_{-k,-q}$. An example is $g_{k,q} = g$, a constant.[28]

In the following we consider the weak coupling system where only phonons with $q \simeq \pm 2k_F$ are important and the relevant electron states are

$$C^{(m)}_{s,k} = C_{s,(3-2m)k_F+k}, \quad m = 1,2,\ldots,M, \quad |k| \ll k_F \ . \tag{4}$$

Thus $C^{(1)}_{s,k}$ and $C^{(2)}_{s,k}$ describe states near the Fermi surface while the states $3 \leq m \leq M$ are far from the Fermi surface. The range of wave vectors k can be formally extended to $|k| \leq k_F$ and then the states in Eq. (4) cover the whole phase space. The states $3 \leq m \leq M$ connect the important Fermi-surface states by multiple scattering of $2k_F$ phonons, as illustrated in Fig. 1.

We define the order-parameter field,

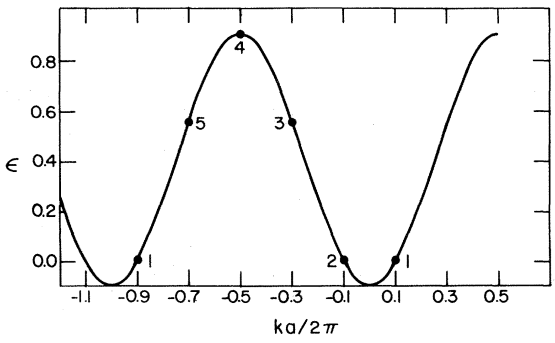

FIG. 1. Electron spectrum for an $M=5, N=1$ commensurate system, i.e., $k_F = \pi/(5a)$. Important regions of electron states [Eq. (4)] are marked. Commensurability energy involves five repeated $2k_F$ scatterings $1 \to 2 \to 3 \to 4 \to 5 \to 1$. Energy is measured from the Fermi level and is shown in units of $2t$ for a tight-binding spectrum with t the transfer integral. Extended-zone scheme is used.

$$\Delta_q = g_{k_F,2k_F} R_{2k_F+q} \ . \tag{5}$$

For the relevant states in Eqs. (4) and (5) with $|k| \ll k_F$ and $|q| \ll 2k_F$ the dependence of $g_{k_F+k,2k_F+q}$ on k,q is neglected and also ω_q is replaced by $\omega_0 \equiv \omega_{2k_F}$.

The approximated Hamiltonian is now decomposed into $H = H_{IC} + H_C$. The incommensurate part H_{IC} contains only the states $m = 1,2$ near the Fermi surface. With the use of linearized spectra,

$$\epsilon_{\pm k_F + k} = \pm v_F k \quad (|k| \ll k_F)$$

where v_F is the Fermi velocity, and a dimensionless coupling,

$$\lambda = 2|g_{k_F,2k_F}|^2/(\pi v_F \omega_0) \ , \tag{6}$$

we obtain

$$\begin{aligned} H_{IC} = & \sum_{s,k} v_F k (C^{(1)\dagger}_{s,k} C^{(1)}_{s,k} - C^{(2)\dagger}_{s,k} C^{(2)}_{s,k}) \\ & + \sum_{s,k,q} (\Delta_q C^{(1)\dagger}_{s,k} C^{(2)}_{s,k-q} + \text{H.c.}) \\ & + (\lambda \pi v_F)^{-1} \sum_q (|\Delta_q|^2 + |\dot{\Delta}_q|^2/\omega_0^2) \ . \end{aligned} \tag{7}$$

All sums involve $|k| \ll k_F$ and $|q| \ll 2k_F$, and $\dot{\Delta}_q$ is the conjugate momentum of Δ_q ($= \partial \Delta_q / \partial t$). In the last term of (7) we summed both $\pm 2k_F$ components.

The commensurate part H_C involves the states which are far from the Fermi surface. We are concerned below with a small gap Δ at the Fermi surface, such that $\Delta \ll |\epsilon_{(3-2m)k_F}|$, $3 \leq m \leq M$. We therefore neglect the dependence of $\epsilon_{(3-2m)k_F+k}$ on k and obtain

$$H_C=\sum_{m=3}^{M}\sum_{s,k}\epsilon_m C_{s,k}^{(m)\dagger}C_{s,k}^{(m)} + \sum_{m=2}^{M}\sum_{s,k,q}\beta_m\Delta_q C_{s,k}^{(m)\dagger}C_{s,k-q}^{(m+1)}+\text{H.c.}\ , \tag{8}$$

where $C_{s,k}^{(M+1)}=C_{s,k}^{(1)}$ and

$$\beta_m=g_{(3-2m)k_F,2k_F}/g_{k_F,2k_F}\ , \tag{9}$$

$$\epsilon_m=\epsilon_{(3-2m)k_F}\ . \tag{10}$$

For the tight-binding model of Eq. (3),

$$\beta_m=\cos[(m-1)2\pi N/M]\ . \tag{11}$$

Note that for $N\geq 2$ some of the energies ϵ_m are negative. All the approximations made in the transition from Eq. (2) to Eq. (7) and Eq. (8) are justified in the weak coupling limit $\Delta \ll W$, where W is of order of the bandwidth [see Eq. (15)]; this is also known as the continuum limit.[21–23]

We define the Fourier transforms of the fields $C_{s,k}^{(m)}$ and Δ_q by $u_s^{(m)}(x)$ and $\bar{\Delta}(x)$, respectively, with $1\leq m\leq M$. These are slowly varying fields in the weak coupling case. The Hamiltonian Eq. (7) + Eq. (8) finally becomes

$$H=\sum_s\int dx\left[-iv_F u_s^{(1)\dagger}(x)\frac{\partial}{\partial x}u_s^{(1)}(x)+iv_F u_s^{(2)\dagger}(x)\frac{\partial}{\partial x}u_s^{(2)}(x)+\sum_{m=3}^{M}\epsilon_m u_s^{(m)\dagger}(x)u_s^{(m)}(x) + [\bar{\Delta}(x)u_s^{(1)\dagger}(x)u_s^{(2)}(x)+\bar{\Delta}(x)\sum_{m=2}^{M}\beta_m u_s^{(m)\dagger}(x)u_s^{(m+1)}(x)+\text{H.c.}]\right] +(\lambda\pi v_F)^{-1}\int dx[\,|\bar{\Delta}(x)|^2+|\dot{\bar{\Delta}}(x)|^2/\omega_0^2]\ . \tag{12}$$

The strategy which we use to solve the problem involves two steps. (a) The use of the equations of motion of $u_s^{(m)}(x)$ to eliminate the electronic degrees of freedom in favor of the phonon field $\bar{\Delta}(x)$ and its derivatives. This is accomplished by use of a derivative expansion in terms of the slowly varying field $\bar{\Delta}(x)$. (b) The second step uses the equation of motion of the phonon field. Here we consider the adiabatic approximation, i.e., $\bar{\Delta}(x)$ is a classical field and its equation of motion is derived from a variational principle. This can alternatively be derived from the Hartree term in a diagrammatic expansion. Finally, an effective Lagrangian in terms of $\bar{\Delta}(x,t)$ and its derivatives is constructed so that it reproduces the equations of motion.

A. Electron equations

In this subsection we use the electron equations of motion to obtain various electron expectation values in terms of $\bar{\Delta}(x)$ and its derivatives. The equations of motion from (12) are

$$i\frac{\partial}{\partial t}u_s^{(1)}(x,t)=-iv_F\frac{\partial}{\partial x}u_s^{(1)}(x,t)+\bar{\Delta}(x,t)u_s^{(2)}(x,t)+\beta_M^*\bar{\Delta}^\dagger(x,t)u_s^{(M)}(x,t)\ , \tag{13a}$$

$$i\frac{\partial}{\partial t}u_s^{(2)}(x,t)=iv_F\frac{\partial}{\partial x}u_s^{(2)}(x,t)+\bar{\Delta}^\dagger(x,t)u_s^{(1)}(x,t)+\beta_2\bar{\Delta}(x,t)u_s^{(3)}(x,t)\ , \tag{13b}$$

$$\epsilon_m u_s^{(m)}(x,t)=-\beta_m\bar{\Delta}(x,t)u_s^{(m+1)}(x,t)-\beta_{m-1}^*\bar{\Delta}^\dagger(x,t)u_s^{(m-1)}(x,t),\quad 3\leq m\leq M\ . \tag{13c}$$

The term $i\partial u_s^{(m)}(x,t)/\partial t$ for $3\leq m\leq M$ is neglected, since we are concerned with states near the Fermi surface, i.e., it is much less than $\epsilon_m u_s^{(m)}(x,t)$.

The states $3\leq m\leq M$ can be eliminated from Eqs. (13a) and (13b) by using Eq. (13c) successively. In this process the state m is shifted to $m\pm 1$, eventually reaching either $m=1$ or 2. Two types of corrections are generated: Diagonal terms with $m=1$ in (13a) and $m=2$ in (13b) or off-diagonal terms with $m=2$ in (13a) and $m=1$ in (13b). Diagonal terms involve only the amplitude $|\bar{\Delta}(x,t)|$ and amount to a shift in the chemical potential. These terms are present even in the incommensurate system and unless compensated for they will change the original value of k_F. We therefore add to the Hamiltonian a term which cancels the diagonal terms in the ground state,

$$\delta H=\sum_s\int dx\sum_{m=1}^{2}u_s^{(m)\dagger}(x)u_s^{(m)}(x)\int f(|\bar{\Delta}|)dx/\int dx\ . \tag{14}$$

To leading order $f=|\beta_2\bar{\Delta}|^2/\epsilon_{3k_F}$. (Note $|\beta_2|=|\beta_M|$ by inversion symmetry.) The diagonal corrections are neglected below. They lead to higher-order effects in $\bar{\Delta}/W$—renormalization of v_F and an asymmetry between solitons and antisolitons. (See Appendix A for details.)

The off-diagonal terms involve the product

$$W^{M-2}e^{-i\phi_0}=\frac{(-1)^M}{\beta_2}\prod_{m=3}^{M}\frac{\epsilon_m}{\beta_m}\ , \tag{15}$$

where $W>0$ is a large energy scale comparable to the bandwidth, and $-\phi_0$ is the phase of the right-hand side. We define a new order parameter by

$$\tilde{\Delta}(x,t)=\bar{\Delta}(x,t)+\frac{[\bar{\Delta}^{\dagger}(x,t)]^{M-1}}{W^{M-2}}e^{-i\phi_0}, \tag{16}$$

and the conventional[5,6] amplitude $\Delta(x,t)$ and phase $\phi(x,t)$, both real fields, by

$$\begin{aligned}\tilde{\Delta}(x,t)&=\Delta(x,t)e^{i\phi(x,t)}=\Delta_1(x,t)-i\Delta_2(x,t),\\ \Delta_1(x,t)&=\Delta(x,t)\cos\phi(x,t),\\ \Delta_2(x,t)&=-\Delta(x,t)\sin\phi(x,t).\end{aligned} \tag{17}$$

The ion displacement field (Fourier transform of R_q) is given by

$$R(x,t)=\bar{\Delta}(x,t)e^{2ik_Fx}/g_{k_F,2k_F}+\text{H.c.}=2\Delta(x,)\cos[2k_Fx+\phi(x,t)-\phi_g]/g+0(\Delta^{M-1}/gW^{M-2}), \tag{18}$$

where $g_{k_F,2k_F}=g\exp(i\phi_g)$.

The electron equations now reduce to

$$i\frac{\partial}{\partial t}\psi_s(x,t)=\left[-iv_F\sigma_3\frac{\partial}{\partial x}+\Delta_1(x,t)\sigma_1+\Delta_2(x,t)\sigma_2\right]\psi_s(x,t), \tag{19}$$

where ψ_s is a spinor field,

$$\psi_s(x,t)=\begin{bmatrix}u_s^{(1)}(x,t)\\ u_s^{(2)}(x,t)\end{bmatrix}, \tag{20}$$

and σ_i are the Pauli matrices.

Consider next the time-ordered Green's function (2×2 matrix),

$$G_s(x,t;x't')=-i\langle T[\psi_s(x,t)\psi_s^{\dagger}(x',t')]\rangle, \tag{21}$$

which, by using Eq. (19), satisfies

$$\left[i\frac{\partial}{\partial t}+iv_F\sigma_3\frac{\partial}{\partial x}-\Delta_1(x,t)\sigma_1-\Delta_2(x,t)\sigma_2\right]G_s(x,t;x',t')=\delta(x-x')\delta(t-t'). \tag{22}$$

By using the Fourier transform,

$$G_s(x,t;x't')=\sum_{\omega,p}e^{ip(x-x')-i\omega(t-t')}G_s(\omega,p,x,t), \tag{23}$$

Eq. (22) reduces to

$$\left[\omega-v_Fp\sigma_3-\Delta_1(x,t)\sigma_1-\Delta_2(x,t)\sigma_2+i\frac{\partial}{\partial t}+iv_F\sigma_3\frac{\partial}{\partial x}\right]\times G_s(\omega,p;x,t)=1. \tag{24}$$

The Green's function can now be solved in a derivative expansion as shown in Appendix A. This expansion is valid when $|\dot{\phi}|$, $v_F|\phi'|$, $|\dot{\Delta}/\Delta|$, and $v_F(\Delta'/\Delta)\ll\Delta$, i.e., for a slowly varying order parameter.

Consider first the density and current observables. The total density,

$$\sum_s\langle|u_s^{(1)}(x)e^{ik_Fx}+u_s^{(2)}(x)e^{-ik_Fx}|^2\rangle, \tag{25}$$

involves a slowly varying part, which is diagonal and gives the density,

$$\rho(x,t)=-i\sum_s\text{Tr}[G_s(x,t;x,t^+)], \tag{26}$$

and a fast varying part which is the CDW,

$$\rho_{\text{CDW}}(x,t)=-i\sum_s\text{Tr}\{[\sigma_1\cos(2k_Fx)+\sigma_2\sin(2k_Fx)]\times G_s(x,t;x,t^+)\}, \tag{27}$$

where t^+ approaches t from above.

The slowly varying part of the current operator is $v_F\sum_s\psi_s^{\dagger}\sigma_3\psi_s$ with the expectation value,

$$j(x,t)=-iv_F\text{Tr}[\sigma_3G_s(x,t;x,t^+)]. \tag{28}$$

By using the zeroth-order solution in derivatives [Eq. (A1)] and the sum Eq. (A11),

$$\rho_{\text{CDW}}(x,t)=-\rho_0\frac{\Delta(x,t)}{v_Fk_F}\ln\left[\frac{2E_c}{\Delta(x,t)}\right]\cos[2k_F+\phi(x,t)], \tag{29}$$

where E_c is the electron cutoff energy, of the order of the Fermi energy, or v_Fk_F.

The slowly varying observables, to first order in derivatives are derived in Appendix A [Eqs. (A7) and (A9)] with the result

$$\rho(x,t)=\rho_0+\phi'(x,t)/\pi,\quad j(x,t)=-\dot{\phi}(x,t)/\pi, \tag{30}$$

where the prime is $\partial/\partial x$ and the dot is $\partial/\partial t$.

Note that the equation of continuity $\dot{\rho}(x,t)=-j'(x,t)$ is satisfied by the first-order result Eq. (30). The equation of continuity is proven in general in Appendix B.

Although Eq. (30) is true locally only to first order in derivatives, it is very important to note that the global charge associated with any static localized configuration of $\Delta(x),\phi(x)$ (e.g., a soliton) is given to all orders in derivatives by

$$\rho_s=[\phi(\infty)-\phi(-\infty)]/\pi. \tag{31}$$

To prove this we start from a ground state (Δ,ϕ constant) and switch on the nonzero value of Eq. (31) adiabat-

ically. The exact conservation law (Appendix B) $\dot{\rho}(x,t)=-j'(x,t)$ implies that after the switch on ($t\to\infty$), $\rho(x)=F'(x)$, where $F(x)$ is a local function of $\Delta(x)$, $\phi(x)$, and their derivatives. In other words, the accumulated charge is the divergence of the time-integrated current at the boundaries. From Eq. (30) we identify $F(x)=\phi(x)/\pi+$ derivative terms. At the boundaries $x=\pm\infty$ the derivative terms vanish and Eq. (31) is obtained.

Thus to prove Eq. (31) we need the derivative expansion (30) only far from the soliton center, where the first-order term is sufficient. At the soliton center, (30) may not be sufficient or the derivative expansion may even diverge—still the proof holds and Eq. (31) is valid. There is, however, a single case for which the proof formally fails, and that is when the amplitude $\Delta(x)$ vanishes at some $x=x_0$. This case can be considered in a limiting procedure, but since the phase is not defined when $\Delta(x_0)=0$ various limiting procedures can differ by extra 2π rotations, and their charges then differ by even integers.

Note that if $\Delta(x)\neq 0$ for all x, Eq. (31) is readily applied to each spin component separately, resulting in $\rho_{s\uparrow}=\rho_{s\downarrow}=\frac{1}{2}\rho_s$; the soliton spin is therefore zero. To obtain a spin-carrying soliton $\Delta(x)$ must pass through zero and then the difference $\rho_{s\uparrow}-\rho_{s\downarrow}$ may change by an integer. This can also be represented by different phases of the $\uparrow$ and $\downarrow$ density wave components.[16,18,29]

The soliton charge Eq. (31) is a well-defined observable when the charge is measured by a smooth sampling function $f(x)$ such that $f(x)\simeq 1$ over a region of width L around the soliton and then falls to zero in a distance l.[30,31] The fluctuations in the soliton charge vanish when $l,L\to\infty$. Note also that the integrated charge of the fast varying part Eq. (29) with the sampling function vanishes in the same limit.

B. Phonon equations

The model is now finally solved by considering the equations of motion for the phonons, or for the order-parameter fields $\bar{\Delta}(x,t)$. In the adiabatic limit $\bar{\Delta}(x,t)$ is considered a classical field which minimizes $\langle\psi|H|\psi\rangle$. The expectation value is taken with respect to the electron operators, and $|\psi\rangle$ is an electron eigenfunction, i.e., at any given time t, $\bar{\Delta}(x,t)$ is considered as a static potential and Eq. (13) is solved to find $|\psi\rangle$, i.e., $H|\psi\rangle=E\{\bar{\Delta}(x,t)\}|\psi\rangle$. This is the adiabatic limit—the electrons follow instantaneously the ion positions. The Feynman-Hellman theorem then states that

$$\frac{\delta\langle\psi|H|\psi\rangle}{\delta\bar{\Delta}(x,t)}=\left\langle\psi\left|\frac{\delta H}{\delta\bar{\Delta}(x,t)}\right|\psi\right\rangle . \tag{32}$$

The missing terms are

$$\left\langle\frac{\delta\psi}{\delta\bar{\Delta}}\middle|H\middle|\psi\right\rangle+\left\langle\psi\middle|H\middle|\frac{\delta\psi}{\delta\bar{\Delta}}\right\rangle=E\{\bar{\Delta}\}\frac{\delta\langle\psi|\psi\rangle}{\delta\bar{\Delta}}=0 , \tag{33}$$

since $\langle\psi|\psi\rangle$ is fixed by normalization.

By using Eq. (32) in the Hamiltonian Eq. (12) we obtain

$$\bar{\Delta}(x,t)+\frac{\ddot{\bar{\Delta}}(x,t)}{\omega_0^2}=-\lambda\pi v_F\sum_s\left[\langle u_s^{(2)\dagger}(x,t)u_s^{(1)}(x,t)\rangle+\sum_{m=2}^{M}\beta_m^*\langle u_s^{(m+1)\dagger}(x,t)u_s^{(m)}(x,t)\rangle\right] . \tag{34}$$

Equation (13c) is now used to eliminate $u^{(m)}$ in favor of $u^{(1)}$ or $u^{(2)}$. Diagonal contributions, $\langle u^{(m)\dagger}u^{(m)}\rangle$, $m=1,2$, are again neglected. Adding the contribution of (14) to (34) precisely cancels these terms in the ground state. For the effect on excitations see Appendix A. There are $M-1$ equal off-diagonal terms, and with definition (16) we obtain, to lowest order in $\tilde{\Delta}/W$ and $\ddot{\tilde{\Delta}}$,

$$\tilde{\Delta}(x,t)+\frac{\ddot{\tilde{\Delta}}(x,t)}{\omega_0^2}-M\frac{[\tilde{\Delta}^\dagger(x,t)]^{M-1}}{W^{M-2}}e^{-i\phi_0}=-\lambda\pi v_F\sum_s\langle u_s^{(2)\dagger}(x,t)u_s^{(1)}(x,t)\rangle . \tag{35}$$

This is also known as the self-consistency equation; the electron wave functions in presence of the potential $\tilde{\Delta}(x,t)$ [Eq. (19)] have to reproduce this potential via Eq. (35). A similar set of equations is known in the theory of superconductivity as the Bogoliubov–de Gennes equations.[32]

An alternative method[28] of deriving Eq. (35) is diagrammatic perturbation theory.[8,11] The Hartree approximation [Fig. 2(a)] is equivalent to the adiabatic limit. It is justified when $\omega_0\ll\Delta$ (Ref. 13) since all other diagrams involve virtual phonon lines which contribute powers of ω_0/Δ. This was also demonstrated for the phonon exchange term[14] [Fig. 1(b) with phonon exchange]. The condition $\omega_0\ll\Delta$ is the precise criterion for the validity of the adiabatic approximation. The Hartree approximation is also justified when the interchain tunneling is large compared with Δ, and small-momentum phonons are neglected.[14] Details of the diagrammatic approach are given in Appendix C.

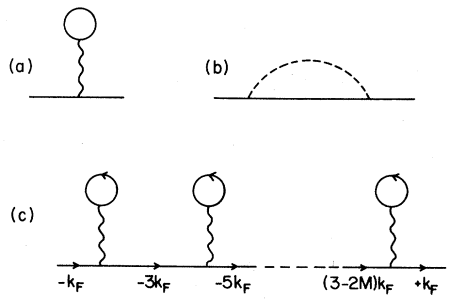

FIG. 2. Contributions to the electron equation of motion: (a) Hartree (or direct) term, and (b) exchange term. In both (a) and (b) solid line is the 2×2 electron's Green's function in the spinor representation, Eq. (22). Wavy line is the phonon's Green's function. (c) Umklapp scattering in an Mth-order commensurate system [Eq. (1)]. Electron with momentum $-k_F$ is scattered $M-1$ times to a $k_F-2\pi N/a$ (same as a $+k_F$) state. Here solid line is an electron in the normal (not spinor) representation.

We proceed now to eliminate the electron degrees of freedom from Eq. (35) by using the derivative expansion for the right-hand side to second order. Since this is a rather tedious calculation, it is worthwhile to consider first a simpler situation where the amplitude Δ is assumed constant, $\Delta(x,t)=\Delta_0$, and only a single equation for $\phi(x,t)$ is needed. In analogy with the derivation of the continuity equation (Appendix B), multiply Eqs. (22) and B1 by σ_3, substract their traces, and take the limit $t'\to t^+, x'\to x$. The result is

$$-\frac{1}{v_F}\frac{\partial}{\partial t}j(x,t)-v_F\frac{\partial}{\partial x}\rho(x,t) -4\,\mathrm{Im}[\tilde{\Delta}^{\dagger}(x,t)\langle u_s^{(2)\dagger}(x,t)u_s^{(1)}(x,t)\rangle]=0\ . \quad (36)$$

Now we can use the derivative expansions to *first* order Eq. (30), and from Eq. (35) we obtain

$$\left[1+\frac{4\Delta_0^2}{\lambda\omega_0^2}\right]\ddot{\phi}-v_F^2\phi''+\frac{4M}{\lambda}\frac{\Delta_0^M}{W^{M-2}}\sin(M\phi+\phi_0)=0\ . \quad (37)$$

The more general coupled equations for $\Delta(x,t),\phi(x,t)$ are obtained from the derivative expansion in Appendix A. Substituting Eq. (A17) in Eq. (35) we obtain (choosing for simplicity $\phi_0=0$)

$$\Delta=\lambda\Delta\ln\left[\frac{2E_c}{\Delta}\right]+\frac{1}{\omega_0^2}(\Delta\dot{\phi}^2-\ddot{\Delta}) -\frac{\lambda}{12\Delta^3}(v_F^2\Delta'^2-v_F^2\Delta\Delta''-\dot{\Delta}^2+\Delta\ddot{\Delta}) +M\Delta(\Delta/W)^{M-2}\cos(M\phi)\ , \quad (38)$$

$$\left[1+\frac{4\Delta^2}{\lambda\omega_0^2}\right]\ddot{\phi}-v_F^2\phi''+\frac{8\Delta}{\lambda\omega_0^2}\dot{\Delta}\dot{\phi} +\frac{4M}{\lambda}\Delta^2(\Delta/W)^{M-2}\sin(M\phi)=0\ . \quad (39)$$

Equation (36), in fact, leads to Eq. (39), which for a constant Δ, is the self-sustained Eq. (37).

Equations (38) and (39) correspond to the following Lagrangian density:

$$\mathcal{L}(\Delta,\phi)=N(0)\left\{\frac{1}{2}\Delta^2\left[\ln\left[\frac{2E_c}{\Delta}\right]+\frac{1}{2}\right]-\frac{\Delta^2}{2\lambda}+\frac{M_\phi(\Delta)}{m}\frac{\dot{\phi}^2}{8} -\frac{M_\Delta(\Delta)}{m}\frac{\dot{\Delta}^2}{24\Delta^2}-\frac{v_F^2}{8}\left[\phi'^2+\frac{\Delta'^2}{3\Delta^2}\right] +\frac{W^2}{\lambda}(\Delta/W)^M\cos(M\phi)\right\}, \quad (40)$$

i.e., the Euler-Lagrange equations of (40) for the fields $\Delta(x,t)$ and $\phi(x,t)$ reproduce precisely Eqs. (38) and (39). $N(0)=2/(\pi v_F)$ is the density of states, and the effective phase and amplitude masses are given by

$$M_\phi/m=1+4\Delta^2/\lambda\omega_0^2,\quad M_\Delta/m=1+12\Delta^2/\lambda\omega_0^2\ . \quad (41)$$

The overall prefactor in (40) is determined so that the corresponding Hamiltonian is the correct energy density, e.g., the first term in (40) is the electron condensation energy

$$\sum_{\epsilon_k<0}[(\epsilon_k^2+\Delta^2)^{1/2}-|\epsilon_k|]\ .$$

The space and time derivatives correspond to the energies involved with local fluctuations in the density or current[5] [see Eq. (30)] and to the ion kinetic energy.

An alternative method of deriving the commensurability effect is to diagonalize the Hamiltonian (12) in momentum space considering Δ and ϕ to zeroth order in derivatives.[6] This is in accord with the derivative expansion where both derivatives and Δ/W are small. The only phase-dependent term in the determinant of (12) is the product $\bar{\Delta}^M\prod_{m=2}^M\beta_m+\mathrm{H.c.}$ Neglecting the phase-independent terms as above, the low-lying eigenvalues $|E_k|\ll W$ are

$$E_k=\pm[(v_Fk)^2+|\bar{\Delta}|^2+2|\bar{\Delta}|^M\cos(M\phi+\phi_0)/W^{M-2}]^{1/2} =\pm[(v_Fk)^2+\Delta^2]^{1/2}\ , \quad (42)$$

where Eqs. (16) and (17) were used and lowest order in Δ/W is retained. To the same order, the phonon energy becomes

$$|\bar{\Delta}|^2/\lambda\pi v_F=[\Delta^2-2(\Delta^M/W^{M-2})\cos(M\phi+\phi_0)]/\lambda\pi v_F\ . \quad (43)$$

The last term in (43) is precisely the commensurability energy, i.e., the last term in Eq. (40). Thus instead of solving systematically the commensurate problem as we did in deriving (40), one can use this faster method, i.e., first solve the incommensurate case and then add the commensurability energy of Eq. (43).

An unusual feature of the tight-binding result [Eq. (11)] is that when M is a multiple of 4, $\beta_m=0$ for $m=1+M/4$ and $1+3M/4$. In this case we expand $\beta(k)=\pm ka$ and the corrected electron dispersion is

$$E_k^2=(v_Fk)^2+\Delta^2-2a^2k^2\frac{\Delta^M}{\tilde{W}^{M-2}}\cos(M\phi)\ , \quad (44)$$

where $\tilde{W}$ is defined as in Eq. (15) but excluding the two vanishing β_m's. Thus v_F is renormalized and the leading term in the commensurability energy E_{com} comes from the $\ln(2E_c/\Delta)\simeq 1/\lambda$ term in Eq. (40), i.e.,

$$E_{\mathrm{com}}=N(0)\frac{1}{\tilde{\lambda}}\frac{\Delta^M}{\tilde{W}^{M-2}}\cos(M\phi)\ , \quad (45)$$

where

$$\tilde{\lambda}=2\lambda(v_F/\Delta a)^2\ . \quad (46)$$

Thus the vanishing of two β_m's reduces the commensurability energy by an additional $\sim(\Delta/\tilde{W})^2$ factor.

C. Solutions of the effective Lagrangian

The microscopic derivation is thus completed and the solutions for Eqs. (38) and (39) are now considered. The ground state is $\phi=0,\pm 2\pi/M,\pm 4\pi/M,\ldots,$ and $\Delta=\Delta_0$, where

$$\Delta_0=2E_c e^{-1/\lambda} . \tag{47}$$

Corrections of order Δ/W are neglected in (47). Small oscillations around the ground state give the amplitude and phase phonon dispersions,[6]

$$\omega_\Delta^2=\frac{m}{M_\Delta}(12\Delta_0^2+v_F^2q^2),\quad \omega_\phi^2=\omega_F^2+\frac{m}{M_\phi}v_F^2q^2 , \tag{48}$$

where the pinning frequency is

$$\omega_F^2=\frac{m}{M_\phi}\frac{4M^2}{\lambda}\Delta_0^2(\Delta_0/W)^{M-2} , \tag{49}$$

and the masses M_Δ, M_ϕ are evaluated at $\Delta=\Delta_0$. Equation (48) agrees with the results of the linearized theory[6] (except for a factor of 4 in the q^2 coefficient of ω_Δ^2, which is an algebraic error).

The commensurability effect is not neglected in the ω_ϕ equation; it is small but important when $q\to 0$, giving the pinning frequency of the CDW.[6] For an incommensurate system, $\omega_\phi(q=0)=0$, reflecting the translational invariance associated with the Fröhlich mechanism of a sliding CDW.

Consider now nonlinear solutions of Eqs. (38) and (39). Phase solitons, or "ϕ particles,"[7] are obtained from Eq. (39) if the amplitude is assumed to be constant. This is a reasonable assumption since the phase variation affects the amplitude with corrections of orders $(\Delta_0/W)^{M-2}\ll 1$. This leads to Eq. (37), i.e., the well-known sine-Gordon equation,[33]

$$\ddot{\phi}-\frac{m}{M_\phi}v_F^2\phi''-\frac{\omega_F^2}{M}\sin(M\phi)=0 . \tag{50}$$

The soliton represents a topological defect connecting adjacent ground states of ϕ. Thus its integrated charge from Eq. (31) is $\pm 2/M$.

As discussed above this is an observable fractional charge.[15,30,31] Note that the system is defined to have fractional charge $2N/M$ per unit cell [Eq. (1)]. This however is not a measurable fractional charge since one needs a sharply localized sampling function and the charge fluctuations are then finite. In contrast the soliton fractional charge is measurable, i.e., the charge fluctuations are arbitrarily small.

The soliton width is

$$d=\frac{v_F}{\Delta_0}[(\lambda/4M^2)(W/\Delta_0)^{M-2}]^{1/2} ,$$

and the static solution of Eq. (50) is

$$\phi_s(x)=(4/M)\tan^{-1}[\exp(\pm x/d)] , \tag{51}$$

corresponding to solitons (+) or antisolitons (−). By substituting $\phi_s(x)$ in Eq. (40) the soliton energy is obtained,

$$E_s=\frac{8\Delta_0}{\pi M}[(1/\lambda)(\Delta_0/W)^{M-2}]^{1/2} . \tag{52}$$

Since $W\gg\Delta_0$ $\phi_s(x)$ is slowly varying on the scale of the coherence length v_F/Δ_0, i.e., $d\gg v_F/\Delta_0$. Thus the soliton solution is consistent with the derivative expansion. When M is a multiple of 4, replace W by $\tilde{W}$ and λ by $\tilde{\lambda}$ [Eq. (46)] for the tight-binding model.

The incommensurate system with interchain coupling which produces on-chain backscattering was studied in Ref. 8. The nonlinear energy now involves $\Delta_l\Delta_m\cos(\phi_l-\phi_m)$ where l,m are indices of the interacting chains. Solitons exist also in this system[34]; to lowest order in the interchain coupling set $\phi_l=0$ on all chains except one, and the soliton then solves the sine-Gordon equation with $M=1$ in $\sin M\phi$. Therefore its charge is ± 2.

The effective Lagrangian is extremely useful for deriving the response of the system to external fields. The relevant interaction Lagrangian is added and the equations of motion are then derived. The interchain coupling of Ref. 8 can be introduced in this manner. Another important example is the response to an electromagnetic field. The interaction Lagrangian, using Eq. (30), is

$$\mathscr{L}_{\rm EM}=\frac{-A_0e\phi'}{\pi}-\frac{A_xe\dot{\phi}}{\pi} , \tag{53}$$

where $\vec{A}$ is the electromagnetic vector potential, x is the chain direction, and e is the electron charge. The equation of motion for the phase, Eq. (39), has now an additional term on the left-hand side which is $-2ev_FE$, where $E=-\dot{A}_x-A_0'$ is the electric field along the chain. This equation has been the basis for the study of nonlinear conductivity in CDW systems.[35,36] The CDW is depinned when $2ev_FE$ exceeds the coefficient of the $\sin M\phi$ term in Eq. (39). This defines a threshold field

$$E_t=\pi^2M^3E_s^2/(32ev_F) . \tag{54}$$

The linearized equation gives the low-frequency conductivity,[6]

$$\sigma(\omega)=\frac{i\omega\omega_p^2m/M_\phi}{\omega^2-\omega_F^2} , \tag{55}$$

where $\omega_p^2=8v_Fe^2$ is the plasma frequency.

The situation near commensurability is also easily handled. Since $\phi'(x,t)$ represents addition of charge to the commensurate system the Hamiltonian has an additional term, $-(M/2\pi)\mu\phi'(x,t)$. The coefficient μ is the chemical potential for solitons, or $\mu M/2$ is the chemical potential for the electron charge. For the phase-only problem (constant amplitude) there is a commensurate-to-incommensurate (C-I) transition as function of μ when $\mu=E_s$. For $\mu>E_s$ the single-soliton energy is negative and the ground state is a soliton lattice.[9–12] The transition is continuous, implying that solitons repel each other (see Appendix D).

III. EFFECTIVE LAGRANGIAN: $M=2$

The case of the half-filled band needs a special treatment since in the case considered in Sec. II with $k_F=\pi/2a$, the order parameter has only one component. The states $\pm 2k_F=\pm\pi/a$ are identical and from Eq. (5), $\bar{\Delta}(x)$ must have the same phase as $g_{k_F,2k_F}$, i.e., the phase is frozen and only amplitude variations are allowed. Another way to see this is through the ion displacement at the site n,

$$R_n \sim \Delta\cos(2k_F na+\phi-\phi_g)=(-1)^n\Delta\cos(\phi-\phi_g)$$

[Eq. (18)]. Thus only the product $\Delta\cos(\phi-\phi_g)$ is relevant and the ion field is determined by a single component.

Since the ground state is doubly degenerate at $\pm\Delta_0$ it should be possible to have a soliton connecting $\pm\Delta_0$ with a constant phase such that it passes through $\Delta=0$. This is an "amplitude soliton." However, near $\Delta=0$ the derivative expansion is not valid; its expansion parameter Δ'/Δ diverges. The effective Lagrangian (40) diverges at $\Delta=0$ and cannot be used to study amplitude solitons.

Thus the use of a phenomenological Lagrangian which allows amplitude solitons, as attempted in Ref. 19, is not justified. Amplitude solitons can be found by other methods[20–24] avoiding the derivative expansion. Here we extend the model of Sec. II into situations where the order parameter is complex and the method of derivative expansions can be applied.

The frozen phase is a consequence of considering a single phonon coupling in the adiabatic limit. The electrons are enslaved by the ions and do not have independent dynamics; the order parameter is then just a single-phonon field. More general cases allow for a complex order parameter. We consider here the following situations.

(a) Adiabatic limit of electrons coupled to two phonons with coupling constants which have different phases. Variations of ϕ are now allowed and represent the interplay between the two phonon fields.

(b) A single phonon field beyond the adiabatic limit. The order parameter, defined as an electronic response [Eq. (22)], acquires higher-order contributions through virtual phonons and becomes complex.

(c) Addition of direct electron-electron interactions. As in case (b) the electrons feel each other directly and not just through the static phonon field. This allows for additional self-mass terms and the order parameter is complex.

First, consider case (a) of two phonons in the adiabatic limit. As an example we take an acoustic phonon with a pure imaginary coupling [Eq. (3)] and an optical phonon with a real coupling constant. The coupling constants $g_{k_F,2k_F}$ are $g_{\rm ac}$ and $g_{\rm op}$, the bare frequencies are $\omega_{\rm ac}$ and $\omega_{\rm op}$, and the dimensionless couplings, Eq. (6), are $\lambda_{\rm ac}$ and $\lambda_{\rm op}$, respectively.

We define the order parameters $\Delta_i(x)$ $(i=1,2)$ by their Fourier transform,

$$\Delta_1(q)=g_{\rm op}R^{\rm op}_{2k_F+q},\quad \Delta_2(q)=ig_{\rm ac}R^{\rm ac}_{2k_F+q}\ , \tag{56}$$

with $R^{\rm op}$ and $R^{\rm ac}$ the two phonon fields. The fields $\Delta_i(x)$ are real since $\pm 2k_F$ are identical states and $g_{\rm op}$ and $ig_{\rm ac}$ are real. This feature is the manifestation of the $M=2$ commensurability. The Hamiltonian in the spinor notation [Eq. (20)] is then

$$H=\sum_s\int dx\left[-iv_F\psi_s^\dagger(x)\sigma_3\frac{\partial}{\partial x}\psi_s(x)+\Delta_1(x)\psi_s^\dagger(x)\sigma_1\psi_s(x)+\Delta_2(x)\psi_s^\dagger(x)\sigma_2\psi_s(x)\right]$$
$$+\int dx\{(2\lambda_{\rm op}\pi v_F)^{-1}[\Delta_1^2(x)+\dot{\Delta}_1^2(x)/\omega_{\rm op}^2]+(2\lambda_{\rm ac}\pi v_F)^{-1}[\Delta_2^2(x)+\dot{\Delta}_2^2(x)/\omega_{\rm ac}^2]\}\ . \tag{57}$$

Note that λ in Eq. (12) is replaced here by $2\lambda_{\rm op}$ or $2\lambda_{\rm ac}$. The extra factor 2 is an important feature of the $M=2$ system; it arises from the single $2k_F$ mode, while in (12) we summed on the two independent $\pm 2k_F$ modes. Thus the restoring force when $M=2$ is reduced by a factor of 2, strongly enhancing the Peierls instability in this case. Note also that if one of the couplings vanishes, say $\lambda_{\rm op}=0$, then $\Delta_1(x)$ is frozen to $\Delta_1(x)\equiv 0$ and the order parameter has only a Δ_2 component.

The equations of motion are obtained by variation with respect to $\Delta_1(x)$ and $\Delta_2(x)$ [using Eq. (32)] or by the Hartree term (Appendix C). The result is

$$\Delta_1(x,t)+\ddot{\Delta}_1(x,t)/\omega_{\rm op}^2=-\lambda_{\rm op}\pi v_F\sum_s\langle\psi_s^\dagger(x)\sigma_1\psi_s(x)\rangle\ ,$$
$$\Delta_2(x,t)+\ddot{\Delta}_2(x,t)/\omega_{\rm ac}^2=-\lambda_{\rm ac}\pi v_F\sum_s\langle\psi_s^\dagger(x)\sigma_2\psi_s(x)\rangle\ . \tag{58}$$

By using the derivative expansion (A17) the equations in terms of Δ and ϕ [Eq. (17)] are readily obtained. These equations correspond to the following effective Lagrangian density:

$$\mathcal{L}(\Delta,\phi)=N(0)\left\{\frac{1}{2}\Delta^2\left[\ln\left[\frac{2E_c}{\Delta}\right]+\frac{1}{2}\right]-\frac{\Delta_1^2+\dot{\Delta}_1^2/\omega_{\rm op}^2}{4\lambda_{\rm op}}-\frac{\Delta_2^2+\dot{\Delta}_2^2/\omega_{\rm ac}^2}{4\lambda_{\rm ac}}-\frac{v_F^2}{8}\left[\phi'^2+\frac{\Delta'^2}{3\Delta^2}\right]+\frac{1}{8}\left[\dot{\phi}^2+\frac{\dot{\Delta}^2}{3\Delta^2}\right]\right\}. \tag{59}$$

The ground state for, say, $\lambda_{ac} > \lambda_{op}$, is

$$\Delta_c = 2E_c e^{-1/(2\lambda_{ac})} , \tag{60}$$

and $\phi = \pi/2 + n\pi$ (n is an integer). Note the significance of the factor 2 in the exponent of Eq. (60) as compared with Eq. (47). The small-oscillation spectra are similar to Eq. (48) with the replacement $\lambda \to 2\lambda_{ac}$, and the pinning frequency is

$$\omega_F^2 = 8\beta(m/M_\phi)\Delta_c^2 , \tag{61}$$

where $\beta = (\lambda_{op}^{-1} - \lambda_{ac}^{-1})/4$.

Soliton-type solutions interpolate between degenerate minima with a phase change of $\pm\pi$. The soliton charge from Eq. (31) is therefore ± 1. This system was also studied with strong coupling terms retained.[37] It was then found that the soliton charge may be irrational.

The derivative expansion is justified when $\beta \ll 1$, i.e., the energy difference between $\phi = \pi/2$ and $\phi = 0$ is small. In this limit the amplitude is constant and the static soliton energy becomes

$$E_s = 2\Delta_c \sqrt{2\beta}/\pi . \tag{62}$$

The soliton energy as function of β is plotted in Fig. 3 (dashed line). The plot is based on a mapping to the system, which is considered next [Eqs. (68) and (69)], its numerical solution,[26] and the known value for $\beta \to \infty$.[21-24] A more detailed discussion follows the case considered next.

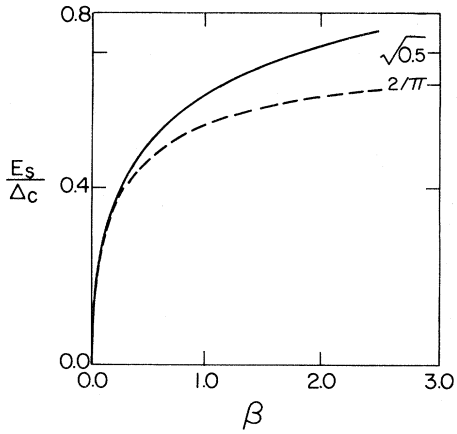

FIG. 3. Single soliton energy E_s as function of $\beta = (\lambda_{op}^{-1} - \lambda_{ac}^{-1})/4$ in case (a) [Eq. (57)] or of $\beta = \lambda[\gamma(2\lambda+\gamma)]^{-1}$ in case (c) [Eq. (64)]. Solid line is the numerical solution (Ref. 26) of Eqs. (69) and (70) valid for small β, and dashed line is the expected exact solution of Eq. (58) or Eq. (67) approaching the known result $2/\pi$ at $\beta \to \infty$.

Cases (b) and (c) extend perturbation theory beyond the adiabatic or Hartree limit. We consider, in particular, case (c) with electron-electron forward scattering in the Hartree-Fock approximation and electron-phonon coupling in the adiabatic limit. Case (b) is qualitatively similar[14] but more difficult to handle since phonon exchange is a retarded interaction and then the order parameter in Eq. (22) is nonlocal in time, i.e., $\Delta_i = \Delta_i(x,t,t')$.

The electron-electron Coulomb interaction is represented by

$$H_1 = \gamma\pi v_F \sum_{s,s'} \int dx\, \psi_s^\dagger(x) 1 \psi_s(x) \psi_{s'}^\dagger(x) 1 \psi_{s'}(x) . \tag{63}$$

This interaction involves only forward scattering, i.e., small momentum transfer. (It corresponds to the conventional nonretarded g_2 and g_4 couplings.[38,39]) The corresponding potential in real space has a range r_0 with $a \ll r_0 \ll v_F/\Delta_c$,[23] where $2\Delta_c$ is the gap in the commensurate system. The condition $r_0 \gg a$ means that only small momentum transfer is involved, while the condition $r_0 \ll v_F/\Delta_c$ allows the use of a local interaction in Eq. (38) for the slowly varying field $\psi_s(x)$.

The total Hamiltonian is then

$$H = \sum_s \int dx \left[-iv_F \psi_s^\dagger(x)\sigma_3 \frac{\partial}{\partial x} \psi_s(x) + \bar{\Delta}(x) \psi_s^\dagger(x)\sigma_1 \psi_s(x) \right] + (2\lambda\pi v_F)^{-1} \int dx [\bar{\Delta}^2(x) + \dot{\bar{\Delta}}^2(x)/\omega_0^2] + H_1 , \tag{64}$$

with $\bar{\Delta}(x)$ a real field. The ion displacement field at site n ($x = na$) is $R(x) \sim (-1)^n \bar{\Delta}(x)$.

The Hartree-Fock scheme is justified when interchain tunneling is large compared with Δ_c.[14] Instead of tunneling, the phonon field can be the source of interchain coupling which allows the long-range order, and reduces the fluctuations. More precisely, if the electron-phonon interaction is dominated by the Hartree term (for $\omega_0 \ll \Delta_c$) then perturbation theory in γ involves powers of[38] $\gamma \ln(2E_c/\Delta_c) \sim \gamma/\lambda$ for $\gamma \ll \lambda$. Thus the Hartree-Fock scheme is also valid when $\omega_0 \ll \Delta_c$ and $\gamma \ll \lambda$.

We assume that the system is charge neutral on the scale of the coherence length v_F/Δ so that the direct (Hartree) term of (63) is canceled while the exchange decoupling gives

$$H_1^{ex} = -2\gamma\pi v_F \sum_s \int dx [u_s^{(1)\dagger}(x) u_s^{(2)}(x) \langle u_s^{(2)\dagger}(x) u_s^{(1)}(x) \rangle + \text{H.c.} - |\langle u_s^{(1)\dagger}(x) u_s^{(2)}(x) \rangle|^2] . \tag{65}$$

The order parameter, as the off-diagonal electron self-mass, becomes

$$\tilde{\Delta}(x) = \bar{\Delta}(x) - 2\gamma\pi v_F \langle u_s^{(2)\dagger}(x) u_s^{(1)}(x) \rangle . \tag{66}$$

Since we consider here spinless excitations, $\tilde{\Delta}(x)$ is independent of which spin states are summed. The self-consistency equation is obtained by variation of (64) with respect to $\bar{\Delta}(x)$,

$$\bar{\Delta}(x,t)+\ddot{\bar{\Delta}}(x,t)/\omega_0^2=-\lambda\pi v_F\sum_s\langle\psi_s^\dagger(x,t)\sigma_1\psi_s(x,t)\rangle\ . \tag{67}$$

In terms of the amplitude and phase fields [Eqs. (17), (66), and (67)] the real field $\bar{\Delta}(x)$ satisfies

$$\Delta(x,t)\cos\phi(x,t)=\frac{2\lambda+\gamma}{2\lambda}\bar{\Delta}(x,t)+\frac{\gamma}{2\lambda\omega_0^2}\ddot{\bar{\Delta}}(x,t)\ . \tag{68}$$

Use of the derivative expansion [Eq. (A17)] in Eq. (67) yields equations for Δ and ϕ. The same result is obtained by diagrammatic approach from Fig. 2(a) for the phonon coupling and Fig. 2(b) for H_1 (see Appendix C). After some algebra these equations become

$$\frac{\gamma+\lambda(1-\cos2\phi)}{\gamma(2\lambda+\gamma)}\Delta=\Delta\ln\left[\frac{2E_c}{\Delta}\right]-\frac{1}{12\Delta^3}(v_F^2\Delta'^2-v_F^2\Delta\Delta''-\dot{\Delta}^2+\Delta\ddot{\Delta})-\frac{2\lambda}{(2\lambda+\gamma)^2\omega_0^2}\cos\phi\frac{\partial^2}{\partial t^2}(\Delta\cos\phi)\ , \tag{69}$$

$$\frac{\gamma\Delta^2}{\gamma(2\lambda+\gamma)}\sin(2\phi)=\tfrac{1}{4}(v_F^2\phi''-\ddot{\phi})+\frac{2\lambda\Delta}{(2\lambda+\gamma)^2\omega_0^2}\sin\phi\frac{\partial^2}{\partial t^2}(\Delta\cos\phi)\ . \tag{70}$$

These equations correspond to the following effective Lagrangian density:

$$\mathscr{L}(\Delta,\phi)=N(0)\left\{\frac{1}{2}\Delta^2\left[\ln\left[\frac{2E_c}{\Delta}\right]+\frac{1}{2}\right]-\frac{\Delta^2}{2(2\lambda+\gamma)}-\frac{\lambda\Delta^2}{2\gamma(2\lambda+\gamma)}[1-\cos(2\phi)]-\frac{v_F^2}{8}\left[\phi'^2+\frac{\Delta'^2}{3\Delta^2}\right]\right.$$
$$\left.+\frac{1}{8}\left[\dot{\phi}^2+\frac{\dot{\Delta}^2}{3\Delta^2}\right]+\frac{\lambda}{(2\lambda+\gamma)^2\omega_0^2}\left[\frac{\partial}{\partial t}\Delta\cos\phi\right]^2\right\}. \tag{71}$$

The commensurability is manifested by the pinning potential $\sim\Delta^2\cos2\phi$ which has the same form as in Eq. (40) with $M=2$. The peculiar feature of this pinning potential is that its coefficient diverges when $\gamma\to0,\lambda\neq0$. In this limit the phase must be frozen to its ground-state value $\cos2\phi=1$ and the order parameter is real. Indeed, it was noted above that in the Hartree approximation (for $\gamma\to0$ the exchange contribution vanishes) phase excitations are not possible.

Note that the ion kinetic energy [last term in Eq. (70)] involves the product $\Delta\cos\phi$, in agreement with Eq. (68). Nonadiabatic interactions, such as the exchange term, do not confine the electrons to the ion positions and allow dependence on both $\Delta\cos\phi$ and $\Delta\sin\phi$. In other words, the charge can now oscillate relative to the ions, as well as with the ions.

Consider next the solutions for the coupled-phase-amplitude equations. The ground state has $\phi=0,\pm\pi,\pm2\pi,\ldots$ with amplitude,

$$\Delta_c=2E_c\exp[-1/(2\lambda+\gamma)]\ . \tag{72}$$

Small oscillations around the ground state yield the dispersion for amplitude and phase phonons,

$$\omega_\Delta^2=\left[1+\frac{24\lambda\Delta_c^2}{(2\lambda+\gamma)^2\omega_0^2}\right]^{-1}(12\Delta_c^2+v_F^2q^2)\ ,$$
$$\omega_\phi^2=\frac{8\lambda}{\gamma(2\lambda+\gamma)}\Delta_c^2+v_F^2q^2\ . \tag{73}$$

The derivative expansion is valid for $\omega\ll\Delta_c$ which from (73) implies $\lambda\ll\gamma$. In particular the phase-mode frequency is independent of ω_0; to reduce its frequency the pinning potential from the electron-phonon coupling must be reduced, i.e., $\lambda\ll\gamma$.

Before studying soliton solutions, we note that the static solutions of this case are equivalent to those of the previous case of two coupled phonons. This is achieved by the correspondence $2\lambda_{ac}\leftrightarrow2\lambda+\gamma$ and $2\lambda_{op}\leftrightarrow\gamma$ for $\lambda_{ac}>\lambda_{op}$, or an interchanged correspondence when $\lambda_{op}>\lambda_{ac}$. To show this we note that Eqs. (17), (66), and (67) for static solutions, are identical to those of Eq. (58) with the required correspondence in coupling constants. [The absence of spin sum in Eq. (66) implies a factor $\frac{1}{2}$ in this comparison.] Furthermore, the energy $\langle H\rangle$ of Eqs. (64) and (65) is equal to that of Eq. (57) when the equations of motion are satisfied. This completes the proof for the equivalence; note that it is independent of the derivative expansion.

We proceed now to study the soliton solutions. The degeneracy of the ground state implies the existence of phase solitons which interpolate between $\phi=0$ and $\phi=\pm\pi$ with total charge ±1 [Eq. (31)]. This conclusion is exact to all orders in the derivative expansion as shown below Eq. (31).

The static soliton solution of Eqs. (69) and (70) were studied numerically by Grabowski *et al.*[26] as function of the parameter $\beta=\lambda/[\gamma(2\lambda+\gamma)]$. Their result for the soliton energy is shown in Fig. 3 (solid line). For $\beta\ll1$ the

soliton is wide compared with v_F/Δ_c which is the validity condition for the derivative expansion. The parameter β maps into $\beta=|\lambda_{op}^{-1}-\lambda_{ac}^{-1}|/4$ of the previous case; thus Eq. (62) applies here also (for $\beta \ll 1$).

For $\beta > 1.48$ an unusual behavior appears—bound states of two or more solitons exist. At $\beta=1.48$ the single-soliton width is $\sim 4v_F/\Delta_c$,[26] so that the derivative expansion is not rigorously valid. The result shows, however, that a strong pinning potential is more likely to produce an attractive force between solitons. A strong pinning potential implies a large soliton energy.

This statement is made rigorous in Appendix D where we show that when the soliton energy E_s satisfies $E_s > \Delta_c/\sqrt{2}$ then solitons attract each other; the proof is independent of the derivative expansion. Figure 3 indeed shows that if the Lagrangian (71) is maintained for large β then $E_s > \Delta_c/\sqrt{2}$ for $\beta \gtrsim 1.6$, rather close to the observed value for attraction. Note that the condition of Appendix C is a *sufficient* one, i.e., if $E_s < \Delta_c/\sqrt{2}$, solitons may or may not attract.

However, for all values of β in the weak coupling system ($\lambda, \gamma \ll 1$) the soliton energy satisfies $E_s < 2\Delta_c/\pi$. To show this we use the mapping to case (a) and note that a solution to Eq. (58) with $\Delta_2(x) \equiv 0$ is possible—this is just the pure amplitude soliton[20–24] whose energy for the form (57) is well known to be $2\Delta_c/\pi$. The variational principle then yields that E_s at the minimum-energy configuration is $E_s < 2\Delta_c/\pi$. Therefore, by allowing an additional degree of freedom (the phase when $\gamma \neq 0$), the soliton energy can only decrease.

The correct form of the soliton energy is shown by the dashed line in Fig. 3. This is a universal function of the parameter β, which can be defined for all local Hartree-Fock theories. This function connects the various forms of charged solitons in $M=2$ systems: pure-phase solitons [Eq. (62)] for $\beta \ll 1$, coupled-phase-amplitude solitons [Eqs. (69) and (70) solved in Ref. 26] for $\beta \lesssim 0.5$, and pure amplitude solitons for $\beta \to \infty$.

The condition of Appendix D is not satisfied ($2/\pi \simeq 0.67 < 1/\sqrt{2} \simeq 0.71$), implying that the solitons of the original system [Eqs. (64) and (65)] probably do not attract each other. [The conclusions of Ref. 26 are, of course, valid for the Lagrangian (71) as such, without relating it to Eq. (64).]

The soliton energy can increase when additional terms are present in the Hamiltonian, e.g., a phonon dispersion term $\sim \Delta'^2(x)$. The criterion of Appendix D is an efficient method for relating this energy to the interaction between solitons.

IV. DISCUSSION

The formalism of the effective Lagrangian was developed and applied to $M \geq 3$ fold commensurate systems in Sec. II and to $M=2$ commensurate systems in Sec. III. The "phase-only" problem, where amplitude variations can be neglected, is appropriate to $M \geq 3$, or to $M=1$, which is the case of interchain coupling.[8] The effective Lagrangian of this problem has been inferred[7,19] from the small-oscillation theory.[6] The present derivation gives a microscopic basis for the nonlinear equations. It shows that the picture of phase solitons[7] is basically correct; however, the picture of amplitude solitons[17] is misleading. In the latter case the derivative expansion fails and an effective Lagrangian cannot be obtained.

Experimental manifestations of phase solitons are their contribution to the conductivity and their effect on the nonlinear I-V curves.[35,36] It has been shown that the I-V curves in tetrathiafulvalenium—tetracyanoquinodimethane (TTF-TCNQ) at low temperatures are nonlinear,[40] and the contribution of phase solitons has been suggested. In this incommensurate system the nonlinearity can come from the interchain coupling, as discussed in Ref. (8).

The case of the half-filled band, or $M=2$, is of more recent interest as it applies to polyacetylene. There is considerable evidence that addition of charge by doping or by photogeneration creates spinless charge carriers.[41] The phase solitons of Sec. III indeed carry charge but not spin. They are the continuation of charged amplitude solitons[20–24] into situations which require a complex order parameter.

It is useful to have results for the soliton energy for the most frequent applications, namely $M=3$ and 4. For the tight-binding model, using Eqs. (11), (15), and (52) for $M=3$ and the modification of Eq. (46) for $M=4$, we obtain

$$E_s = \begin{cases} \dfrac{4\Delta_0}{3\pi\sqrt{3\lambda}} \left[\dfrac{\Delta_0}{t}\right]^{1/2}, & M=3 \quad (74) \\ \dfrac{\Delta_0}{2\pi\sqrt{2\lambda}} \left[\dfrac{\Delta_0}{t}\right]^{2}, & M=4 \quad (75) \end{cases}$$

where t is the transfer integeral ($\epsilon_k = -2t\cos ka$). An extra factor of Δ_0/t in Eq. (75) is a consequence of $\beta_2=\beta_4=0$ [Eq. (11)].

If the electron-phonon coupling constant is independent of the electron momentum (e.g., for optical phonons) then $\beta_m=1$ for all m. The soliton energies become (assuming still a tight-binding dispersion for the electrons)

$$E_s = \begin{cases} \dfrac{8\Delta_0}{3\pi\sqrt{3\lambda}} \left[\dfrac{\Delta_0}{t}\right]^{1/2}, & M=3 \quad (76) \\ \dfrac{\Delta_0}{\pi\sqrt{2\lambda}} \dfrac{\Delta_0}{t}, & M=4\,. \quad (77) \end{cases}$$

The depinning field is readily found from Eq. (54) and the relevant soliton energy [Eqs. (74)–(77)].

The Fröhlich mechanism of a sliding CDW was confirmed so far only in systems which are at or near $M=4$ commensurability, e.g., $NbSe_3$,[42] TaS_3 (Ref. 27) (orthorhombic and monoclinic), and $K_{0.30}MoO_3$.[43] In particular, orthorhombic TaS_3 becomes $M=4$ commensurate below 130 K with a threshold field of $E_t=0.2$–0.4 V/cm.[27] From conductivity and magnetic susceptibility data[44] $\Delta_0 \simeq 700$ K, $t \simeq 1.3$ eV and then $\lambda=0.22$ [Eq. (47) with $E_c \simeq 2t$]. Equations (54) and (75) yield $E_t=0.3$

V/cm (with $E_s=0.36$ K), while Eqs. (54) and (77) yield $E_t\simeq 600$ V/cm (with $E_s=16$ K). The tight-binding model is therefore in good agreement with experiment. The vanishing of the matrix elements β_2 and β_4 account for the rather low depinning field in TaS_3 and in similar systems.

A critical field can also be defined for near-commensurate systems.[45] The fact that only systems at or near $M=4$ commensurability manifest a sliding CDW may be related to the anomalously low depinning field of such systems.

In conclusion, we have shown the existence of phase solitons in all $M\geq 1$ commensurate CDW systems. The $M=1$ case corresponds to interchain coupling[8] and may be relevant to TTF-TCNQ.[40] The $M=2$ case corresponds to the half-filled band and is relevant to polyacetylene.[41] The $M=4$ case is relevant to TaS_3 and similar compounds. The $M\geq 3$ systems are of special interest as they allow fractionally charged solitons.

The soliton-bearing equations were derived from a microscopic Hamiltonian by developing the methods of derivative expansions and effective Lagrangians. These methods are efficient tools in the study of a growing number of physical systems.

ACKNOWLEDGMENTS

We wish to thank J. R. Schrieffer, S. A. Brazovskii, E. Domany, and Y. Frishman for very useful discussions.

APPENDIX A: DERIVATIVE EXPANSIONS

In this appendix the procedure for the derivative expansion of the Green's function in Eq. (24) is shown and the relevant traces are evaluated to second order in derivatives.

The zeroth-order solution of Eq. (24) is (spin index is omitted)

$$G_0(\omega,p;x,t)=\frac{\omega+v_F p\sigma_3+\Delta_1(x,t)\sigma_1+\Delta_2(x,t)\sigma_2}{\omega^2-E^2+i\delta}\ , \tag{A1}$$

where $E^2=(v_F p)^2+\Delta^2$, $\Delta^2=\Delta_1^2(x,t)+\Delta_2^2(x,t)$, and $\delta=+0$. The exact Green's function has the form

$$G(\omega,p;x,t)=\sum_{n=0}^{\infty}G_n(\omega,p;x,t)\ , \tag{A2}$$

where

$$G_n(\omega,p;x,t)=(-1)^n G_0(\omega,p,x,t)\left[\left[iv_F\sigma_3\frac{\partial}{\partial x}+i\frac{\partial}{\partial t}\right]\times G_0(\omega,p;x,t)\right]^n , \tag{A3}$$

and each derivative acts on all terms to its right.

First consider Eq. (26),

$$\rho(x,t)=-i\sum_{\omega,p}{}'\,\mathrm{Tr}[G(\omega,p;x,t^+)]\ . \tag{A4}$$

The prime indicates a factor 2 for the spin sum so that

$$\sum_{\omega,p}{}'=\tfrac{1}{2}N(0)\int d\epsilon\int d\omega/2\pi,\quad \epsilon=v_F p$$

and $N(0)=2/\pi v_F$ is the density of states for both spins. The zeroth-order solution gives $\sum_p{}'1=\rho_0$, while to first order,

$$\rho(x,t)=\rho_0+i\sum_{\omega,p}{}'\mathrm{Tr}\left[G_0(\omega,p;x,t)\left[iv_F\sigma_3\frac{\partial}{\partial x}+i\frac{\partial}{\partial t}\right]\times G_0(\omega,p;x,t)\right] . \tag{A5}$$

The $\partial/\partial t$ term can be written as

$$-\tfrac{1}{2}\frac{\partial}{\partial t}\sum_{\omega,p}{}'\mathrm{Tr}[G_0^2(\omega,p;x,t)]=-\tfrac{1}{2}\sum_{\omega,p}{}'\frac{3\omega^2+E^2}{(\omega^2-E^2+i\delta)^3}\frac{\partial\Delta^2}{\partial t}=0\ . \tag{A6}$$

Therefore,

$$\begin{aligned}\rho(x,t)&=\rho_0+4iv_F\sum_{\omega,p}{}'\frac{\Delta_1\Delta_2'-\Delta_2\Delta_1'}{(\omega^2-E^2+i\delta)^2}\\&=\rho_0+(2\pi)^{-1}\Delta^2\phi'\int d\epsilon(\epsilon^2+\Delta^2)^{-3/2}\\&=\rho_0+\phi'(x,t)/\pi\ .\end{aligned} \tag{A7}$$

For the current Eq. (28) we obtain, to first order,

$$j(x,t)=iv_F\sum_{\omega,p}\mathrm{Tr}\left[\sigma_3 G_0(\omega,p;x,t)\times\left[iv_F\sigma_3\frac{\partial}{\partial x}+i\frac{\partial}{\partial t}\right]G_0(\omega,p;x,t)\right] . \tag{A8}$$

The $\partial/\partial x$ term is written in the form of (A6) and vanishes, while the $\partial/\partial t$ term corresponds to $-\partial/\partial x$ in (A7), so that

$$j(x,t)=-\dot{\phi}(x,t)/\pi\ . \tag{A9}$$

Next consider the trace

$$\mathrm{Tr}[\sigma_1 G(x,t;x,t)]=\sum_{\omega,p}{}'\mathrm{Tr}[\sigma_1 G(\omega,p;x,t)]\ . \tag{A10}$$

The zeroth-order solution gives

$$2\sum_{\omega,p}{}'\frac{\Delta_1}{\omega^2-E^2}=N(0)\Delta_1\ln\frac{2E_c}{\Delta}\ . \tag{A11}$$

The first-order term vanishes, while the second-order term involves the following integrals:

$$\sum_{\omega,p}\frac{\omega^2+\epsilon^2}{(\omega^2-E^2)^n}=0,\quad n\geq 3 \tag{A12}$$

$$\sum_{\omega,p}\frac{2\omega^2+\Delta^2}{(\omega^2-E^2)^3}=\sum_{\omega,p}\frac{4\omega^2+\Delta^2}{(\omega^2-E^2)^4}=\sum_{\omega,p}\frac{18\omega^2+3\Delta^2}{(\omega^2-E^2)^5}=0\ , \tag{A13}$$

$$\frac{i}{N(0)}\sum_{\omega,p}{}'\frac{\Delta^2}{(\omega^2-E^2)^2}=-\tfrac{1}{4}\ , \tag{A14}$$

$$\frac{i}{N(0)}\sum_{\omega,p}{}'\frac{\Delta^4}{(\omega^2-E^2)^3}=\tfrac{1}{8}\ , \tag{A15}$$

$$\frac{i}{N(0)}\sum_{\omega,p}{}'\frac{\Delta^6}{(\omega^2-E^2)^4}=-\tfrac{1}{12}\ . \tag{A16}$$

All these integrals are converging and the momentum cutoff (or E_c) is taken to be infinite. The corrections which are neglected are powers of $\Delta/E_c \ll 1$.

The trace of the second-order term is a straightforward although lengthy calculation, with the result

$$\mathrm{Tr}[\sigma_1 G(x,t;x,t)]=-iN(0)\left[\Delta\cos\phi\ln\left[\frac{2E_c}{\Delta}\right]-\frac{1}{4\Delta}\sin\phi(v_F^2\phi''-\ddot{\phi})-\frac{1}{12\Delta^3}\cos\phi(v_F^2\Delta'^2-\dot{\Delta}^2-v_F^2\Delta\Delta''+\Delta\ddot{\Delta})\right]\ . \tag{A17}$$

The trace of $\sigma_2 G$ is obtained from (A17) by replacing ϕ with $\phi+\pi/2$.

Consider next the effect of the diagonal renormalization, as discussed below Eq. (14). The equations of motion, with the shift (14) in the chemical potential, are [the average in (14) replaces Δ by Δ_0]

$$\left[i\frac{\partial}{\partial t}+|\beta_2|^2[\Delta^2(x,t)-\Delta_0^2]/W+iv_F\sigma_3\frac{\partial}{\partial x}-\Delta_1(x,t)\sigma_1-\Delta_2(x,t)\sigma_2\right]\psi(x,t)=0\ , \tag{A18}$$

and Eq. (35) has an additional term on the left-hand side,

$$\tilde{\Delta}(x,t)[\rho_0-\rho(x)]\,|\beta_2|^2\lambda\pi v_F/W\ , \tag{A19}$$

where ρ_0 is the space average of $\rho(x)$.

The diagonal correction in (A18) shifts the zeroth-order Green's function by

$$\delta G_0(\omega,\rho;x,t)=-G_0^2(\omega,p;x,t)[\Delta^2(x,t)-\Delta_0^2]\,|\beta_2|^2/W\ . \tag{A20}$$

The second term in (A18) can be eliminated by a shift in the frequency summation except for derivatives which act directly on it. The change in electronic expectation values is at least of first order in derivatives, i.e.,

$$\mathrm{Tr}[\sigma_1\delta G_1(x,t;x,t^+)]=\sum_{\omega,p}\mathrm{Tr}\left[\sigma_1 G_0(\omega,p;x,t)\left[iv_F\sigma_3\frac{\Delta\Delta'}{2W}+i\frac{\Delta\dot{\Delta}}{2W}\right]G_0^2(\omega,p;x,t)\right]=\frac{-i\Delta'\sin\phi}{2\pi W}\ , \tag{A21}$$

where the integrals (A12)–(A15) were used. Replacing σ_1 in (A21) by σ_2 results in replacing $\sin\phi$ by $\cos\phi$, while replacing it by 1 or σ_3 results in zero. Substituting these results with Eq. (30) in the phonon equation (35) plus (A19) yields the additional terms $-|\beta_2|^2\lambda v_F\Delta\phi'/W$ and $4|\beta_2|^2 v_F\Delta\Delta'/W$ on the left-hand sides of Eqs. (38) and (39), respectively. This corresponds to an additional term in the Lagrangian Eq. (40),

$$\delta\mathcal{L}=N(0)(|\beta_2|^2 v_F/2W)[\Delta^2(x,t)-\Delta_0^2]\phi'(x,t)\ . \tag{A22}$$

Linearizing the $\Delta(x,t)$ equation around Δ_0 and substituting the result in the phase equation yields

$$\ddot{\phi}-\frac{m}{M_\phi}v_F^2\left[1-|\beta_2|^2\frac{\Delta_0^2}{W}\right]\phi''-\frac{\omega_F^2}{M}\left[1-M|\beta_2|^2\frac{v_F\phi'}{W}\right]\sin(M\phi)=0 \tag{A23}$$

instead of Eq. (50). The effect of diagonal corrections is to renormalize the Fermi velocity and shift the commensurability term. The latter correction introduces a small asymmetry between solitons and antisolitons which is of higher order in Δ/W than the terms retained in Eq. (50).

APPENDIX B: EQUATION OF CONTINUITY

Consider the Green's-function equation (21) and the adjoint of Eq. (22). Interchanging primed and unprimed variables yields

$$G(x,t;x't')\left[-i\frac{\overleftarrow{\partial}}{\partial t'}-iv_F\sigma_3\frac{\overleftarrow{\partial}}{\partial x'}-\Delta_1(x',t')\sigma_1-\Delta_2(x',t')\sigma_2\right]=\delta(t-t')\delta(x-x')\ . \tag{B1}$$

Substracting the traces of Eqs. (22) and (B1) and then taking the limit $t'\to t^+$, $x'\to x$ gives

$$\frac{\partial}{\partial t}\rho(x,t)+\frac{\partial}{\partial x}j(x,t)=0\ , \tag{B2}$$

where the density and current are defined in Eqs. (26) and (28). The fact that the Hamiltonian involves only a first-order $\partial/\partial x$, as does Eq. (B1), leads to the equation of continuity (B2) with only the slowly varying fields.

The derivation is the same also if nonlocal interactions are considered, and the order parameters have the general form $\Delta_i(x,t;x',t')$.

APPENDIX C: DIAGRAMMATIC APPROACH

Consider first the incommensurate case of Sec. II, i.e., only the states $m=1,2$ in the Hamiltonian equation (12) are retained. The equation of motion in the Hartree approximation [Fig. 2(a)] is[23]

$$\left[i\frac{\partial}{\partial t}+iv_F\sigma_3\frac{\partial}{\partial x}\right]G_s(x,t;x't')=\delta(x-x')\delta(t-t')-\tfrac{1}{2}i\,|\,g_{k_F,2k_F}\,|^2\int dx''dt''D_0(x,t;x'',t'')\sum_{i=1,2}\sigma_i\mathrm{Tr}[\sigma_i G_{s'}(x,t;x'',t'')]$$

$$\times G_s(x,t;x',t')\ , \tag{C1}$$

where the trace includes the s' spin sum and the phonon propagator is

$$D_0(x,t;x',t')=\sum_{\omega}\frac{2\omega_0}{\omega^2-\omega_0^2}e^{-i\omega(t-t')}\delta(x-x')=\frac{-2}{\omega_0}\left[1+\frac{1}{\omega_0^2}\frac{\partial^2}{\partial t^2}\right]^{-1}\delta(t-t')\delta(x-x')\ . \tag{C2}$$

Comparing Eqs. (22) and (C1), the self-consistency equation is obtained,

$$\Delta_i(x,t)+\ddot{\Delta}_i(x,t)/\omega_0^2=\tfrac{1}{2}i\pi\lambda v_F\mathrm{Tr}[\sigma_i G_s(x,t;x,t^+)],\quad i=1,2 \tag{C3}$$

which is the same as Eq. (35) except for the commensurability term.

The effect of commensurability can now be added. When Eq. (1) is satisfied, then a $+2k_F$ phonon can scatter a $+k_F$ electron to a $-k_F$ state in $M-1$ steps. This is in addition to its previous effect of scattering a $-k_F$ electron into a $+k_F$ state. The umklapp process is demonstrated in Fig. 2(c), completing Eq. (35). Each interaction involves a factor of $\tilde{\Delta}(x,t)$ from the loop and a factor β_m/ϵ_m, $3\le m\le M$ from the internal electron line.

Consider next the Hartree-Fock scheme for the Hamiltonian Eq. (64). The direct term [Fig. 2(a)] with the interaction (63) involves the density

$$\sum_s\mathrm{Tr}[G_s(x,t;x,t^+)]$$

and affects the diagonal elements of the Green's function. This direct term is neglected here by the assumption of "charge neutrality."

The contribution of the electron-phonon coupling to the exchange term [Fig. 1(b)] is small if $\omega_0\ll\Delta_c$.[13,14] Therefore the exchange term is dominated by the nonretarded interaction (63) which contributes to the equation of motion the terms

$$\frac{4i\gamma}{N(0)}G_s(x,t;x,t)G_s(x,t;x',t')=\frac{i\gamma}{N(0)}\sum_i\sigma_i\mathrm{Tr}[\sigma_i G_s(x,t;x,t)]G_s(x,t;x',t')\ . \tag{C4}$$

In the last sum only the $i=1,2$ terms are retained and the corrections to the diagonal elements are neglected. These corrections correspond to the g_4 coupling,[38,39] i.e., interactions between electrons on the same side of the Fermi surface, and usually lead to a renormalization of v_F.[38]

Combining Eq. (C1) (with $g^2\to 2g^2$ and the sum has only $i=1$) with Eq. (C4), the self-consistency equations become

$$\Delta_1(x,t)=\tfrac{1}{2}i\pi v_F\left[2\lambda\left[1+\frac{1}{\omega_0^2}\frac{\partial^2}{\partial t^2}\right]^{-1}+\gamma\right]$$

$$\times\mathrm{Tr}[\sigma_1 G_s(x,t;x,t^+)]\ , \tag{C5}$$

$$\Delta_2(x,t)=\tfrac{1}{2}i\gamma\pi v_F\mathrm{Tr}[\sigma_2 G_s(x,t;x,t^+)]\ .$$

These equations are identical to Eq. (67) when expressed in terms of $\tilde{\Delta}(x)$ of Eq. (66).

APPENDIX D: ATTRACTING SOLITONS

In this appendix the following statement is proven: In a Hartree or Hartree-Fock theory, if $E_s>\Delta_c/\sqrt{2}$, then solitons attract each other at long distances. Here E_s is the energy of adding an isolated unit charge to the system (called here for convenience a soliton) and $2\Delta_c$ is the Peierls gap. This result is of interest only to $M=2$ systems, since for $M\ge 3$, $E_s\ll\Delta_c$ [Eq. (52)].

The proof involves the following three steps.

(a) When the electron chemical potential is varied a commensurate-to-incommensurate (C-I) transition occurs.

This transition is of first order if and only if solitons attract each other at long distance. To see this consider the charge density (relative to the commensurate density) $\delta\rho$ as a function of the chemical potential μ. ($\delta\rho$ is the order parameter for the *C-I* transition.) Now if solitons attract each other at long distance then the system with a too small $\delta\rho$ is unstable since the attraction favors smaller distances between the solitons. Thus the curve $\delta\rho(\mu)$ does not include states with too low densities, i.e., it is discontinuous. On the other hand, if the transition is of first order, jumping from $\delta\rho=0$ to a finite $\delta\rho=\delta\rho^*$, then a system with $0<\delta\rho<\delta\rho^*$ must phase separately into regions which have either $\delta\rho=0$ or $\delta\rho^*$. Therefore solitons tend to approach each other, i.e., their long-distance interaction is attractive. Note that this interaction is not necessarily a two-body effect which leads to a two-soliton bound state; it can be a collective interaction.

(b) Consider the Gibbs free energy $G(\mu)=E-\mu\delta\rho$. In the commensurate phase $\delta\rho=0$, and the energy E is just the condensation energy of the Peierls phase. For the Hartree of Hartree-Fock theory of Secs. II and III this gives

$$G_c(\mu)=-\Delta_c^2/2\pi v_F \ . \tag{D1}$$

In the incommensurate limit the gap is $\Delta_0 \ll \Delta_c$ [Eqs. (47) and (60)] so that its condensation energy is small compared with (D1). The energy is then just the energy of adding $\delta\rho$ electrons to a metal, or changing k_F by $\pi\delta\rho/2$,

$$E_m=4\int_0^{\pi\delta\rho/2} v_F q\frac{dq}{2\pi}=\frac{\pi}{4}v_F(\delta\rho)^2 \ . \tag{D2}$$

The chemical potential is

$$\mu=\frac{\partial E_m}{\partial\rho}=\pi v_F\delta\rho/2 \ , \tag{D3}$$

and therefore the Gibbs free energy for a metal is

$$G_m(\mu)=-\mu^2/(\pi v_F) \ . \tag{D4}$$

Comparing Eqs. (D1) and (D4) shows that the metal has a lower Gibbs free energy if $\mu>\mu_c$, where

$$\mu_c=\Delta_c/\sqrt{2} \ . \tag{D5}$$

(c) The final step is to show that if $E_s>\Delta_c/\sqrt{2}$ then the *C-I* transition is of first order. For $\mu_c<\mu<E_s$ a state with low $\delta\rho$ is not favored as compared with commensurate phase since it costs an energy of $(E_s-\mu)\delta\rho>0$ (low $\delta\rho$ means sufficiently low so that higher-order terms in G can be neglected). However, for $\mu>\mu_c$ $G_m<G_c$, i.e., the metal is favored as compared with the commensurate phase. Thus at $\mu=\mu_c$ there is a *C-I* transition which excludes low soliton density states, i.e., it is a first-order transition. From (a) solitons then attract each other, completing the proof.

Since there is some condensation energy from the incommensurate phase gap the condition may be improved, giving a slightly lower bound on E_s as a sufficient condition for attraction.[26]

For spinless fermions (the spin-Peierls system[46]) the same derivation applies except for spin factors of 2. The density $\delta\rho$ of solitons, each with half-charge, is half the charge density. The result is that solitons attract each other for $E_s>\Delta_c/\sqrt{8}$.

[1]For recent reviews, see Proceedings of the International Conference on Synthetic Low Dimensional Conductors and Superconductors (Les-Arc, 1982) [J. Phys. (Paris) Colloq. 44-C3, (1983)].

[2]For further reviews, see Proceedings of the International Conference on Low Dimensional Conductors (Boulder, 1981) [Mol. Cryst. Liq. Cryst. 77-86, 1 (1981) and (1982)].

[3]R. E. Peierls, *Quantum Theory of Solids* (Clarendon, Oxford, 1955), p. 108.

[4]H. Fröhlich, Proc. R. Soc. London Ser. A 223, 296 (1954).

[5]D. Allender, J. W. Bray, and J. Bardeen, Phys. Rev. B 9, 119 (1974).

[6]P. A. Lee, T. M. Rice, and P. W. Anderson, Solid State Commun. 14, 703 (1974).

[7]M. J. Rice, A. R. Bishop, S. E. Trullinger, and J. A. Krumhansl, Phys. Rev. Lett. 36, 432 (1976).

[8]B. Horovitz and J. A. Krumhansl, Solid State Commun. 26, 81 (1978).

[9]W. L. McMillan, Phys. Rev. B 14, 1496 (1976); A. E. Jacobs and M. B. Walker, *ibid.* 21, 4132 (1980).

[10]P. Bak, in *Solitons and Condensed Matter Physics,* edited by A. R. Bishop and T. Schneider (Springer, Berlin, 1978), p. 264.

[11]T. Ohmi and H. Yamamoto, Prog. Theor. Phys. 58, 743 (1977).

[12]B. Horovitz, J. Phys. C 15, 161 (1982).

[13]S. A. Brazovskii and I. E. Dzyaloshinskii, Zh. Eksp. Teor. Fiz. 71, 2338 (1976) [Sov. Phys.—JETP 44, 1233 (1976)].

[14]B. Horovitz, Phys. Rev. B 16, 3943 (1977).

[15]W. P. Su and J. R. Schrieffer, Phys. Rev. Lett. 46, 738 (1981); J. R. Schrieffer in Proceedings of the International Conference on Low Dimensional Conductors (Boulder, 1981), Ref. 2, p. 209.

[16]J. Tinka Gammel and J. A. Krumhansl, Phys. Rev. Lett. 49, 899 (1982); Phys. Rev. B 27, 7659 (1983).

[17]J. A. Krumhansl, B. Horovitz, and A. J. Heeger, Solid State Commun. 34, 945 (1980).

[18]B. Horovitz, Phys. Rev. Lett. 48, 1416 (1982).

[19]M. J. Rice, Phys. Lett. 71A, 152 (1979).

[20]W. P. Su, J. R. Schrieffer, and A. J. Heeger, Phys. Rev. Lett. 42, 1698 (1979); Phys. Rev. B 22, 2099 (1980).

[21]S. A. Brazovskii, Zh. Eksp. Teor. Fiz. Pis'ma Red. 28, 656 (1978) [JETP Lett. 28, 606 (1978)]; Zh. Eksp. Teor. Fiz. 78, 677 (1980) [Sov. Phys.—JETP 51, 342 (1980)].

[22]H. Takayama, Y. R. Lin-Liu, and K. Maki, Phys. Rev. B 21, 2388 (1980).

[23]B. Horovitz, Phys. Rev. B 22, 1101 (1980).

[24]B. Horovitz, Phys. Rev. Lett. 46, 742 (1981).

[25]B. Horovitz, Solid State Commun. 34, 61 (1980).

[26]M. Grabowsky, K. R. Subbaswamy, and B. Horovitz, Solid State Commun. 34, 911 (1980).

[27]Z. Z. Wang, H. Salva, P. Monceau, M. Renard, C. Roucau, R. Ayroles, F. Levy, L. Guemas, and A. Meerschaut, J. Phys.

Lett. 44, L311 (1983); P. Monceau, H. Salva, and Z. Z. Wang, in *Proceedings of the International Conference on Synthetic Low Dimensional Conductors and Superconductors* (Les-Arc, 1982), Ref. 1; J. Phys. (Paris) Colloq. 44-C3, 1639 (1983).

[28]A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinskii, *Methods of Quantum Theory in Statistical Physics* (Prentice-Hall, Englewood Cliffs, N.J., 1963).

[29]J. T. Ho, Phys. Rev. Lett. 48, 946 (1982).

[30]S. Kivelson and J. R. Schrieffer, Phys. Rev. B 25, 6447 (1982).

[31]Y. Frishman and B. Horovitz, Phys. Rev. B 27, 2565 (1983).

[32]P. G. de Gennes, *Superconductivity of Metals and Alloys* (Benjamin, New York, 1966).

[33]A. C. Scott, F. Y. F. Chu, and D. W. McLaughlin, Proc. IEEE 61, 1443 (1973).

[34]B. Horovitz, J. A. Krumhansl, and E. Domany, Phys. Rev. Lett. 38, 778 (1977).

[35]S. E. Trullinger, M. D. Miller, R. A. Guyer, A. R. Bishop, F. Palmer, and J. A. Krumhansl, Phys. Rev. Lett. 40, 206 (1978).

[36]K. Maki, Phys. Rev. B 18, 1641 (1978).

[37]S. Kivelson, Phys. Rev. B 28, 2653 (1983).

[38]J. Solyom, Adv. Phys. 28, 201 (1979).

[39]B. Horovitz, Solid State Commun. 18, 445 (1976).

[40]M. J. Cohen, P. R. Newman, and A. J. Heeger, Phys. Rev. Lett. 37, 1500 (1976); M. J. Cohen and A. J. Heeger, Phys. Rev. B 16, 688 (1977).

[41]For a review see A. J. Heeger and A. G. MacDiarmid in Proceedings of the International Conference on Low Dimensional Conductors (Boulder, 1981), Ref. 2, p. 1, J. D. Flood and A. J. Heeger, in Proceedings of the International Conference on Synthetic Low Dimensional Conductors and Superconductors (Les-Arc, 1982), Ref. 1; J. Phys. (Paris) Colloq. 44-C3, 397 (1983).

[42]R. M. Fleming, C. H. Chen, and D. E. Moncton, in *Proceedings of the International Conference on Synthetic Low Dimensional Conductors and Superconductors* (Les-Arc, 1982), Ref. 1; J. Phys. (Paris) Colloq. 44-C3, 1651 (1983).

[43]J. Dumas, C. Schlenker, J. Marcus, and R. Buder, Phys. Rev. Lett. 50, 757 (1983).

[44]D. C. Johnston, J. P. Stokes, P. L. Hsieh, and G. Gruner, in *Proceedings of the International Conference on Synthetic Low Dimensional Conductors and Superconductors (Les-Arc, 1982),* Ref. 1; J. Phys. (Paris) Colloq. 44-C3, 1749 (1983).

[45]M. Weger and B. Horovitz, Solid State Commun. 43, 583 (1982).

[46]E. Pytte, Phys. Rev. B 10, 4637 (1974).