a minimum of the free energy, while at the instability temperature the first *and* second derivatives of F cancel.

In summary, we have shown that, because of electron-phonon coupling, the tetrahedrally coordinated semiconductors undergo a plasma instability at high temperature which could be the cause of melting. For the case of silicon, we find that the electron-hole pair density near melting is much higher than the one predicted by the classical formula $n = (N_c N_v)^{1/2} \exp[-E_G(T)/2kT]$. The creation of a high-density electron-hole plasma by an external source decreases the instability temperature so that the crystal will melt at lower T.

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[14] The Auger effect gives $1/\tau(n) = Cn^2$ with $C = 4\times 10^{-38}$ $cm^6\ s^{-1}$. But, at very high density, one can even expect a four-particle process.

[15] With the Auger lifetime, G would be of the order of $10^{33}\ cm^{-3}\ s^{-1}$.

Solitons in Charge- and Spin-Density-Wave Systems

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(Received 28 December 1981)

A unified description of solitons in both charge-density-wave (CDW) and spin-density-wave (SDW) systems is presented within Hartree-Fock theory. Spin-carrying solitons correspond to a localized SDW region within a CDW ground state or vice versa. Solitons can have a fractional spin component when the CDW and SDW coexist in the ground state. In particular, a SDW in an odd-order commensurate system must coexist with a CDW and solitons have an irrational spin component.

PACS numbers: 72.15.Nj, 71.38.+i, 75.60.Ch

The ground state of most quasi-one-dimensional (1D) conductors is either a charge-density wave (CDW) or a spin-density wave (SDW).[1] The CDW system has been extensively studied and a variety of nonlinear soliton-type excitations were found.[2-10] The present work extends these theories to include also a SDW order parameter. In this scheme the previously known solitons are naturally manifest and the counting rule[8,11] for charge or spin is derived by use of derivative expansions. A table of all possible solitons is presented; new solitons with an irrational or fractional spin component are found to exist when the CDW and SDW coexist in the ground state. This is indeed the case for a SDW with odd-order commensurability.

The system under consideration is that of a quasi-1D electron gas with nonretarded coupling constants[12] g_1 for backward scattering, g_2 for forward scattering, and g_3 for umklapp scattering when the electron band is half filled. The system is studied in the Hartree-Fock scheme[13,14] which is a reasonable approximation to the SDW compounds of the (tetramethyl tetraselenafulvalene)$_2X$ family.[15]

Consider the electron spinor $\psi^\dagger(x) = (u_\uparrow^\dagger(x),$

$u_\downarrow^\dagger(x), v_\uparrow^\dagger(x), v_\downarrow^\dagger(x)$) where $u_\sigma(x)$ are right- and left-moving electrons, i.e., the electron field is $u_\sigma(x) \times \exp(ik_F x) + v_\sigma(x)\exp(-ik_F x)$, with k_F the Fermi momentum and $\sigma = \uparrow, \downarrow$ the spin values. If σ_i and τ_j are Pauli matrices in spin space and (u,v) space, respectively, then the electron Green's function satisfies the equation

$$[i\,\partial/\partial t + iv_F\tau_3\,\partial/\partial x - \sum_{j=1,2}(\Delta_j^C\tau_j + \Delta_j^S\sigma_3\tau_j)]\,G(x,t;x't') = \delta(x-x')\delta(t-t'), \tag{1}$$

where v_F is the Fermi velocity and the σ_3 polarization for the SDW is chosen. The CDW order parameter is $\Delta_1^C = \Delta_C\cos\theta_C$, $\Delta_2^C = -\Delta_C\sin\theta_C$ with Δ_C and θ_C its amplitude and phase, respectively; and similarly for the SDW order parameter, $\Delta_1^S = \Delta_S\cos\theta_S$, $\Delta_2^S = -\Delta_S\sin\theta_S$.

An equivalent set of order parameters are the amplitudes $\Delta_\uparrow, \Delta_\downarrow$ and phases $\theta_\uparrow, \theta_\downarrow$ for the CDW of the $\uparrow$ or $\downarrow$ components, respectively. ($\Delta_C\cos\theta_C + \Delta_S\cos\theta_S = \Delta_\uparrow\cos\theta_\uparrow$, etc.) In the following I assume that $\Delta_\uparrow = \Delta_\downarrow$ and that these amplitudes are space and time independent. This corresponds to $\theta_C = \theta_S + \pi/2 \equiv \theta$ and a constant amplitude $\Delta = \Delta_\uparrow = \Delta_\downarrow$, where

$$\Delta_C = \Delta\cos\varphi, \quad \Delta_S = -\Delta\sin\varphi. \tag{2}$$

Amplitude variations of either $\Delta_\uparrow$ or $\Delta_\downarrow$ reduce the condensation energy and face a large energy barrier.[3] Furthermore, variations in $\Delta_\uparrow$ or $\Delta_\downarrow$ do not carry topological charges[3,11] [Eqs. (5) and (6) below]; therefore the phases $\theta = \frac{1}{2}(\theta_\uparrow + \theta_\downarrow)$ and $\varphi = \frac{1}{2}(\theta_\uparrow - \theta_\downarrow)$ are sufficient for soliton classification in general and for detailed description of low-energy solitons in particular.

The Green's function can be written as a power expansion in derivatives of $\Delta_j^C(x,t)$ and $\Delta_j^S(x,t)$.[3] To zeroth order in derivatives the fast varying parts of the charge and spin densities are

$$\rho_{\rm CDW} = -\frac{2\Delta}{\pi v_F}\ln\left(\frac{2E_c}{\Delta}\right)\cos\varphi\cos(2k_F x + \theta), \tag{3}$$

$$2S_{\rm SDW} = \frac{2\Delta}{\pi v_F}\ln\left(\frac{2E_c}{\Delta}\right)\sin\varphi\sin(2k_F x + \theta), \tag{4}$$

where E_c is the electron cutoff energy and spin refers here to its third component. The slowly varying charge and spin densities (ρ, S) and currents (j, j_S) are, to first order in derivatives,

$$\rho = 2k_F/\pi + \theta'/\pi, \quad j = -\dot{\theta}/\pi; \tag{5}$$

$$2S = \varphi'/\pi, \quad 2j_S = -\dot{\varphi}/\pi. \tag{6}$$

If $\Delta\theta = \theta(x=\infty) - \theta(x=-\infty)$ and $\Delta\varphi = \varphi(x=\infty) - \varphi(x=-\infty)$, then the counting rule[11] is that *the charge and spin of a localized configuration are* $\Delta\theta/\pi$ *and* $\Delta\varphi/2\pi$, *respectively.* The proof is made by spreading the conserved charge and spin continuously over a macroscopic length L so that $\theta'(x), \varphi'(x) \sim L^{-1}$ and Eqs. (5) and (6) can be used. This proof fails when $\Delta(x) = 0$ at some point where both phases are not defined.[4-6] This, however, happens only for special values of the coupling constants; by a continuous change in the latter the counting rule is recovered.[16] The counting rule can also be derived by bosonization of the theory.[17,18]

The equations of motion are now obtained from the Hartree-Fock self-consistency equation. Consider first the half-filled band:

$$\Delta_j^C = (i/4)(g_C \mp g_3)\mathrm{Tr}[\tau_j G(x,t;x,t^+)],$$
$$\Delta_j^S = (i/4)(g_S \pm g_3)\mathrm{Tr}[\sigma_3\tau_j G(x,t;x,t^+)], \tag{7}$$

where[13] $g_C = -2g_1 + g_2$, $g_S = g_2$, and the upper (lower) sign corresponds to $j=1$ ($j=2$). Both order parameters can coexist in the ground state only if $g_C = g_S$, which defines a coexistence line $g_1 = 0$.[12,13]

To derive equations of motion for both amplitude and phase an expansion to second order in derivatives is necessary.[3] However, for the phase-only problem the following procedure is

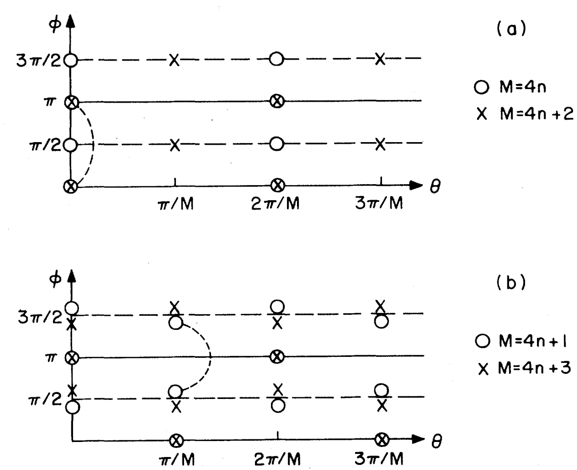

FIG. 1. Minima of the potential in Eq. (10). For $g_C > g_S$, the minima are on the solid lines $\varphi = \pi n$, while for $g_S > g_C$ they are on or near the dashed lines $\varphi = \pi(n + \frac{1}{2})$. (a) Circles, $M = 4n$; crosses, $M = 4n+2$. (b) Circles, $M = 4n+1$; crosses, $M = 4n+3$.

more efficient: Consider Eq. (1) and its adjoint equation; multiply both equations by a matrix A, subtract the equations from each other, and then take the trace and the limit $x' \to x$, $t' \to t^+$. For $A = 1$, the equation of continuity $\dot{\rho}(x,t) + j'(x,t) = 0$ results. By using $A = \tau_3$ or $A = \sigma_3\tau_3$ and Eqs. (5), (6), and (7), equations to second order in derivatives of $\theta(x,t)$ or $\varphi(x,t)$ are obtained. Both equations can be considered as Euler-Lagrange equations of the Lagrangian

$$\mathcal{L}\{\theta,\varphi\} = (2\pi v_F)^{-1}\{\tfrac{1}{2}\dot{\theta}^2 - \tfrac{1}{2}v_F{}^2\theta'^2 + \tfrac{1}{2}\dot{\varphi}^2 - \tfrac{1}{2}v_F{}^2\varphi'^2 - \Delta^2 V(\theta,\varphi)\}, \tag{8}$$

where

$$V(\theta,\varphi) = 2\pi v_F\Big[g_3\Big(\frac{1}{g_C{}^2 - g_3{}^2} + \frac{1}{g_S{}^2 - g_3{}^2}\Big)\cos(2\theta) + \Big(\frac{g_C}{g_C{}^2 - g_3{}^2} - \frac{g_S}{g_S{}^2 - g_3{}^2}\Big)\cos(2\varphi) + g_3\Big(\frac{1}{g_C{}^2 - g_3{}^2} - \frac{1}{g_S{}^2 - g_3{}^2}\Big)\cos(2\theta)\cos(2\varphi)\Big]. \tag{9}$$

For a fixed θ or a fixed φ this is the well-known sine-Gordon system[2,12] which has a soliton solution. The soliton corresponds to a localized change of $\pm\pi$ in the phase, i.e., charge ± 1 and spin 0 or spin $\pm\frac{1}{2}$ and charge 0. A composite soliton with both spin and charge (the polaron) can also be considered.[5,7,18]

The derivative expansion is justified if the potential $V(\theta,\varphi)$ is small, i.e., for spinless solitons if $|g_3| \ll g_C$ in a CDW system ($\varphi = 0$) or $|g_3| \ll g_S$ in a SDW system ($\varphi = \pi/2$), and for charge neutral solitons if $|g_C - g_S| \ll g_C$.

The present approach gives a new insight into the nature of solitons with spin. The presence of spin requires a change in φ [Eq. (6)] which in turn interchanges CDW and SDW components [Eq. (2)]. For example, in a CDW system this soliton generates a localized region of a SDW. The unwinding of the phase $\theta_\uparrow = \theta + \varphi$ relative to $\theta_\downarrow = \theta - \varphi$ results in a localized SDW and a net spin. Similarly, in a SDW a spin-carrying soliton generates a localized CDW.

Consider next a system with a higher-order commensurability M, where the electron band is N/M filled, with $N < M$ reduced integers and $M \geq 3$. In such systems additional scatterings between $\pm k_F$ states arise through intermediate states with $k = (2m-3)k_F$, $3 \leq m < M$, whose energies ϵ_k are of order E_c. The scattering between these states involves a direct coupling to Δ_C and an exchange coupling to Δ_S by a momentum transfer $2k_F(m-2)$. (All these coupling constants are taken below to equal g_1.) Since this process involves the small parameter Δ/E_c, the Lagrangian of Eqs. (8) and (9) with $g_3 = 0$ can be used to describe the incommensurate system and then the commensurability energy can be added.

As shown by Lee, Rice, and Anderson,[19] the commensurability energy is found by evaluating an $M \times M$ determinant with the matrix elements discussed above. The potential in Eq. (8) becomes

$$V(\theta,\varphi) = 2\pi v_F\Big[\Big(\frac{1}{g_C} - \frac{1}{g_S}\Big)\cos(2\varphi) + \frac{4\eta}{g_C}\Big(\frac{g_1}{g_C}\Big)^{M-1}\cos(M\theta)\cos[(M-2)\varphi]\Big]. \tag{10}$$

The potential is given here to lowest order in the small parameter

$$\eta = \prod_{m=3}^{M}(\Delta/\epsilon_{(2m-3)k_F}) \sim (\Delta/E_c)^{M-2}$$

and in the umklapp coupling $g_1{}^{M-1}$. For $M = 2$ this corresponds to lowest order in g_3 which is equal or proportional to g_1.[15]

Note that for $g_S > g_C$ and odd M the terms in Eq. (10) have incompatible minima; the resulting ground state is not a pure SDW, i.e., $\varphi \neq \pi/2$, and the commensurability energy is of order η^2. This result is also obvious from symmetry considerations: An odd invariant $\sim \Delta_S{}^M$ of a SDW is not allowed by time reversal ($\Delta_S \to -\Delta_S$) while the invariant $\Delta_C\Delta_S{}^{M-1}$ is allowed and generates a finite Δ_C. Thus for *odd* M the ground state cannot be a pure SDW; it is either a pure CDW ($g_C > g_S$) or a *coexisting* SDW and CDW ($g_S \geq g_C$). When $\Delta_C \ll \Delta_S$ a minimum of Eq. (10) (for $\theta = 0$) is at $-\tan^{-1}(\Delta_S/\Delta_C) = \varphi_0 \simeq [1 - \tilde{\eta}(-)^{(M-1)/2}]\pi/2$, where

$$\tilde{\eta} = \eta(M-2)(g_1/g_C)^{M-2}/\pi. \tag{11}$$

The degenerate minima of the potential (10) are shown in Fig. 1. The elementary solitons which connect nearest minima are listed in Table I. Also bound states of these solitons may be possible, depending on values of the coupling constants.

Some of the solitons in Table I are known from previous studies. The spinless soliton with charge $2/M$ is the "φ particle,"[2,8] the $M = 2$ sys-

TABLE I. Soliton charge ρ, spin S, and energy E_S for Mth-order commensurate systems.

Ground-state system	$\pm\rho$	$\pm 2S$ [a]	$\sim E_S/\Delta$
CDW or SDW, M even	$\{2/M$	0	$\sqrt{\eta}$
	0	1	1 [c]
CDW, M odd	$\{2/M$	0	$\sqrt{\eta}$
	$1/M$	1	1
SDW, M odd[b]	$\{1/M$	$\tilde{\eta}$	η
	0	$1\pm\tilde{\eta}$	1 [d]
CDW or SDW, incommensurate	0	1	1

[a] For ground states with a SDW only, the spin component parallel to the SDW polarization is defined.

[b] The irrational $\tilde{\eta}$ is given by Eq. (11).

[c] For $M=4n$ $(n\geq 1)$ soliton has an electric dipole.

[d] Two types, one of which has an electric dipole.

tem has the polyacetylene-type solitons,[4-6] and for the $M=3$ CDW system the $S=\frac{1}{2}, \rho=\frac{1}{3}$ is also known.[8,9] In the incommensurate limit $M\to\infty$ and $\eta\to 0$, only a spin-$\frac{1}{2}$ neutral soliton survives.[5,6,10]

The new types of solitons with irrational spins are associated with CDW-SDW coexistence. This is also obvious from Eq. (7) where a change of φ which is not $n\pi$ results in a different CDW-SDW mixture. To visualize such a soliton consider the ground state discussed above ($g_S > g_c$, M odd) where $\theta_\uparrow - \theta_\downarrow = 2\varphi_0$ with φ_0/π irrational, and the degenerate ground state obtained by interchanging the $\uparrow$ and $\downarrow$ components $\theta_\uparrow - \theta_\downarrow = -2\varphi_0$. The soliton which interpolates between these states has an irrational spin $\varphi_0/2\pi$.

A few comments on the meaning of these results are appropriate: (a) A ground-state SDW polarized in the σ_3 direction breaks the rotation symmetry and a soliton spin cannot be defined in the perpendicular directions, i.e., $\langle\sigma_1\rangle = \langle\sigma_2\rangle = 0$ but $\langle\sigma_1^2\rangle$ and $\langle\sigma_2^2\rangle$ diverge. The soliton spin then represents only rotations around the polarization axis which allow irrational eigenvalues. Similarly the soliton charge can in principle be irrational, as in some field theory models.[17] (b) The counting rule gives the expectation values of the charge and spin component σ_3. These, however, are true eigenvalues since the soliton configuration is nondegenerate,[8,17] i.e., the corresponding fluctuations vanish in the limit of a slowly varying sampling function.[20,21] (c) Rotations of the SDW polarization axis with an angle θ_p in a plane lead to an additional term in the Lagrangian, $L_1 = \sin^2\varphi(\dot{\theta}_p^2 - v_F^2\theta_p'^2)/4\pi v_F$; this shows the stability of solitons with a constant θ_p.

Another peculiar result is that some solitons have an electric dipole (footnotes c and d in the table). These solitons correspond to the curved trajectories in Figs. 1(a) and 1(b), where θ which minimizes the potential shifts as φ varies.

Table I also lists the order of magnitude of the soliton energy E_S in powers of η. The derivative expansion is self-consistent if $E_S \ll \Delta$. Cases with $E_S \sim \Delta$ are consistent with known results[4-6,10] although the derivative expansion is valid for $|g_c - g_S| \ll g_c$, or $g_3 \ll \max(g_c, g_S)$ for an $M=2$ charged soliton. The charge and spin values, however, are determined by the counting rule which is independent of the derivative expansion.

In conclusion, a unified description for solitons in both CDW and SDW is shown. New types of solitons are found with an irrational spin component for systems with a coexisting CDW and SDW.

I wish to thank Jason Ho for several illuminating comments and also J. R. Schrieffer and S. Kivelson for stimulating and helpful discussions.

This research was supported in part by the National Science Foundation under Grant No. PHY77-27084.

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Ti NMR Study of the Nearly Ferromagnetic System $TiBe_2$

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(Received 3 February 1982)

NMR data on $TiBe_2$ have been taken from 1.3 to 270 K in magnetic fields up to 60 kG. The linear dependence of the Knight shift and the NMR linewidth with $\chi = M/H$ show that the increase of χ versus applied field at low temperatures is due to a homogeneous property of the electron gas. The d-electron contribution to the spin-lattice relaxation rate is found to scale linearly with χT in a wide temperature range spanning the spin-fluctuation temperature.

PACS numbers: 76.60.Cq, 75.20.En, 76.60.Es

The properties of the intermetallic compound $TiBe_2$ have attracted considerable interest in recent years. This cubic C-15 type material has a strongly enhanced, temperature-dependent susceptibility[1,2] and at low temperatures the $\chi = M/H$ susceptibility changes with the magnetic field[3,4] and shows a maximum at about 50 to 60 kG. The large enhancement of the susceptibility without any long-range magnetic ordering at low temperature, together with the specific heat, resistivity,[5,6] and ESR data[7] show that the electronic system in $TiBe_2$ exhibits the properties of an interacting Fermi liquid with a low spin-fluctuation temperature[8] ($T_{sf} \sim 20$ to 50 K). The consequences of the interactions on a microscopic scale, the behavior of the dynamic susceptibility, and the origin of the field-dependent χ are open problems which call for more experimental work. On the other hand, the influence of sample preparation on some macroscopic properties, such as the magnitude of the maximum of M/H, is apparent in the early publications.[3,4] More systematic investigations as a function of preparation techniques are presently attempted.[6] It is quite important to determine whether the differences in the macroscopic parameters are induced mainly by homogeneous modifications of the electronic structure, by sample inhomogeneities, or by local environment effects around impurities. NMR as a microscopic probe is well suited to clear up this point and to provide information on the dynamical susceptibility through nuclear relaxation measurements.

In this Letter we present NMR investigations on the Ti nuclei in a wide range of fields and temperatures. The $TiBe_2$ sample was prepared by Monod *et al.*[4] and before reduction into powder for the NMR measurements it has been heat treated in vacuum at 800 K for 100 h. The resistivity ratio $r = \rho(300\text{ K})/\rho(4.2\text{ K})$, the low-field susceptibility χ (10 kG), and the susceptibility ratio $p = \chi(60\text{ kG})/\chi(10\text{ kG})$ were $r = 36$, $\chi(10) = 8.4 \times 10^{-3}$ emu/mole, and $p = 1.18$, respectively, after annealing. On the other hand $r = 110$, $\chi(10) = 9.7 \times 10^{-3}$ emu/mole, and $p = 1.27$ were found on a sample prepared in Los Alamos, which confirms the different results of Refs. 3 and 4 and shows that our sample is adequate for investigating any problem linked with sample homogeneity.

The NMR spectra were taken with a phase-coherent spectrometer operating at a fixed frequency in the range from 5 to 16 MHz. The magnetic field was calibrated by measuring the NMR signal of ^{109}Ag in a silver sample[9] located in the same sample holder as the $TiBe_2$. We recorded the full integral of the spin echo versus magnetic field. The pulse separation time ($\tau \lesssim 400$ μsec) was always much shorter than the time decay of the spin echo.

At 272 and 77 K the Knight shifts were $\boldsymbol{K} = (0.09 \pm 0.01)\%$ and $-(0.49 \pm 0.005)\%$ in good agreement with the results of Saji *et al.*[1] and slightly differing from the values estimated from the more recent measurements of Takayi *et al.*[10] At 1.3 K

