Phase diagrams of electronic and superconducting transitions to soliton lattice states

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The $T_c(\mu)$ and $T_c(n)$ phase diagram is constructed for a number of anisotropic systems that undergo electronic or superconducting transitions to an incommensurate structure of the soliton-lattice type (T_c is the critical temperature of the transition, μ is the chemical potential, and n is the number of particles). It is shown that at all temperatures the solution obtained by Brazovskii *et al.* [JETP Lett. **31**, 456 (1980)] and by Horvitz [Phys. Rev. Lett. **46**, 742 (1981)] at $T = 0$ in the one-dimensional Peierls model is exact also in a number of two- and three-dimensional models. The transition between a commensurate phase and a soliton-lattice phase is considered. This is a first-order transition at fixed μ and of second order at fixed n. The line of this transition and the superheating and supercooling lines are obtained. The results are used to analyze the experimental data, which points to formation of soliton lattices in antiferromagnetic chromium and in quasi-one-dimensional systems with spin-Peierls transition. The realizability is considered of soliton structures in quasi-one-dimensional superconductors of the $(TMTSF)_2X$ type, where the exchange field plays the role of the chemical potential.

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I. INTRODUCTION

Substantial progress was made recently in the study of the properties of quasi-one-dimensional systems that undergo a Peierls-type structural phase transition. In Refs. 1 and 2 the structure of the ground state was obtained for the continuum Peierls model at $T = 0$ and with bands slightly deviating from half-filled. This structure has the form of a soliton lattice with a period that is not commensurate with period of a purely doubled phase.

It is shown in this paper that the solution obtained in Refs. 1 and 2 is exact also at finite temperatures. This makes it possible to construct the phase diagram and find the temperature of the transition from the doubled phase into the soliton-lattice phase. This is a second-order phase transition in the case of systems with a fixed number n of the particles, and a first-order transition if the chemical potential μ is fixed, except for two special points—the beginning and the end of the $T_c(\mu)$ curve.

We discuss below the features of the phase diagrams for a number of physical systems, but we are mainly interested in the case of a fixed chemical potential. An important circumstance is the possibility of obtaining exact solution for certain two- and three-dimensional models. We consider the following systems.

1. Metals with almost flat sections of the Fermi surface, which become congruent upon translation by a vector Q. It is assumed that in one of the directions the width $W_\parallel$ of the electron band that forms the flat section is large compared with the band width $W_\perp$ in the transverse direction. The presence of Fermi-surface sections other than the congruent ones leads to preservation, as a whole, of the three-dimensional character of the electric and maganetic properties of the metal even upon the onset of one-dimensional charge- or spin-density waves (CDW or SDW). This situation obtains, for example, in chromium. The constants of the interelectron and of the electron-phonon interactions are also sufficiently isotropic, although the electron motion near the flat sections of the Fermi surface is quasi-one-dimensional. In this case transverse (to Q) modulation of the CDW or SDW is possible, in contrast to Ref. 3, where soliton solutions at $T = 0$ are considered in a quasi-one-dimensional Peierls model with a strongly anisotropic coupling constant.

2. Quasi-one-dimensional organic compounds that undergo spin-Peierls transitions.[4] Within the framework of the XY model,[4,5] the role of the chemical potential μ responsible for the appearance of the soliton lattice is assumed by an external magnetic field H.

3. Quasi-one-dimensional superconducting in an exchange field, which undergo a transition to the inhomogeneous Larkin-Ovchinnikov-Fulde-Ferrell (LOFF) *state.*[6,7] In this case the "non-one-dimensionality" must be large enough to separate the superconducting and structural instability channels (in all real quasi-one-dimensional compounds this condition is satisfied with large margin), but at the same time not strong enough to preserve the quasi-one-dimensional character of the electron spectrum. More precise criteria for the realization of a soliton lattice in quasi-one-dimensional superconductors are given below.

4. Two-band anisotropic semiconductors that go over into an "excitonic dielectric" state. The semiconducting character of the spectrum is assumed to be due to interband hybridization, and the band extrema are assumed to coincide in momentum space. In the absence of hybridization the system would be a one-dimensional semimetal, while the transverse mass and the effective two- or three-dimensionality are governed by the hybridization parameter γ_{12}. Such a system can go over into a ferroelectric or current state if the order parameter is real or imaginary, respectively.[9]

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2. BASIC EQUATIONS FOR THE CASE OF CDW AND SDW IN THE ONE-DIMENSIONAL APPROXIMATION

We consider first a model of a metal with almost flat sections of the electron and hole Fermi surfaces. The electron spectrum takes near the Fermi surface the form

$$\varepsilon_1(k)=\varepsilon(k_z)+\eta(k_\perp)-\mu_1, \quad \varepsilon_2(k+Q)=-\varepsilon(k_z)+\eta(k_\perp)+\mu_2, \tag{1}$$

where Q is a vector in the direction of the z axis and makes the electron and hole Fermi surfaces geometrically congruent at $\eta=0$ and $\mu_1=\mu_2$. The quantity $\eta(k_\perp)$ is the transverse corrugation of the Fermi surface and has in the strong-coupling approximation the form

$$\eta(k_\perp)=W^x\cos k_x a_x+W^y\cos k_y a_y. \tag{1'}$$

For simplicity we assume hereafter that $W^x=W^y=W^\perp$. All the remaining symbols are standard.

A similar model was considered in Ref. 3 under the assumption of a drastically anisotropic effective interaction constant, when the order parameter is only a function of the coordinate z. In the case of an almost isotropic interaction constant the order parameter can change also in the transverse direction. At $|\mu_1-\mu_2|=\mu\ll W_\parallel$, $W_\perp\ll W\parallel$ the electron and hole Fermi surfaces weakly corrugated planes. The model Hamiltonian of such a system is

$$H=\sum_{j=1,2}\int\left\{\Psi_j^+(\mathbf{r})\,\varepsilon_j\left(\frac{\nabla_r}{i}\right)\Psi_j(\mathbf{r})-\Delta_{ij}(\mathbf{r})\,\Psi_i^+(\mathbf{r})\,\Psi_j(\mathbf{r})\,(1-\delta_{ij})\right\}d\mathbf{r}+\int\frac{|\Delta(\mathbf{r})|^2}{g}d\mathbf{r}, \quad \Delta=\Delta_{12}=\Delta_{21}^*, \tag{2}$$

where g is the effective interaction constant and depends little on the momenta. It is assumed that $W_\perp\gg\Delta(\mathbf{r})$, so that the onset of one-dimensional CDW or SDW does not violate substantially the three-dimensionality of the system.

The eigenfunctions of the Hamiltonian (2) satisfy the Schrödinger equation

$$\begin{bmatrix}\varepsilon_1(\nabla_r/i)-E & \Delta(\mathbf{r})\\ \Delta^*(\mathbf{r}) & \varepsilon_2(\nabla_r/i)-E\end{bmatrix}\begin{pmatrix}\Psi_{1E}(\mathbf{r})\\ \Psi_{2E}(\mathbf{r})\end{pmatrix}=0. \tag{3}$$

The exact eigenvalues E_n and eigenfunctions $\psi_{1,2E_n}(\mathbf{r})$ can be obtained in the three-or two-dimensional case only for an extremely limited class of potentials, $\Delta=\Delta_1 e^{iQz}$. In the case of CDW the solution with the potential $\Delta=\Delta_1 e^{iQz}$ corresponds to pure doubling ($Q=\pi/a_z$) in the Peierls model. In the case of SDW this solution describes a linearly or helicoidally polarized antiferromagnetic structure. More complicated solution types are connected with slow spatial modulation of the order parameter $\Delta(\mathbf{r})$. We separate $\Delta(\mathbf{r})$ and $\psi_{1,2E}(\mathbf{r})$ the "fast" factors

$$\Delta(\mathbf{r})=\tilde{\Delta}(\mathbf{r})\exp(iQz+iQ_\perp\rho_\perp), \quad \rho_\perp=ix+jy,$$
$$\Psi_{1,2E}(\mathbf{r})=\varphi_{1,2E}(\mathbf{r})\exp[\pm iQz/2\pm iQ_\perp\rho_\perp/2]. \tag{4}$$

We assume next that $\tilde{\Delta}(\mathbf{r})$ is a purely real function that depends only on the coordinate z. By the same token we exclude from consideration for the time being solutions with slow spatial modulation in a transverse (relative to the z axis) directions. These solutions will be considered later.

It is convenient also to transform to the Fourier components $\varphi_{1,2}(z,q_\perp)$ with respect to the transverse coordinate. As a result we have the following system of equations:

$$\begin{bmatrix}iv_F\frac{d}{dz}+\eta\left(q_\perp+\frac{Q_\perp}{2}\right)-E & \tilde{\Delta}(z)\\ \tilde{\Delta}(z) & -iv_F\frac{d}{dz}+\eta\left(q_\perp-\frac{Q_\perp}{2}\right)-E\end{bmatrix}\begin{pmatrix}\varphi_{1E}\\ \varphi_{2E}\end{pmatrix}=0. \tag{5}$$

After transforming to the sum and difference

$$\eta_\pm={}^1/_2[\eta(q_\perp+Q_\perp/2)\pm\eta(q_\perp-Q_\perp/2)]$$

and substituting

$$\varphi_{1,2E}=f_{1,2E}\exp\left[i\frac{\eta_-}{v_F}z\right] \tag{6}$$

we arrive at a system of equations for the functions $f_{1,2E}(q_\perp)$:

$$\left[-v_F^2\frac{d^2}{dz^2}+\tilde{\Delta}^2-(E-\eta_+)^2\right]\times\begin{pmatrix}f_{1E}\\ f_{2E}\end{pmatrix}+iv_F\frac{d\Delta}{dz}\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}\begin{pmatrix}f_{1E}\\ f_{2E}\end{pmatrix}=0. \tag{7}$$

The system (7) is obtained from (5) with allowance for (6) by squaring the right and left parts. It is analogous to the purely one-dimensional case, but now E is replaced by $E-\eta_+(q_\perp)$. By varying the thermodynamic potential Ω, expressed in standard fashion in terms of the eigenfunctions of the Hamiltonian (2), we easily obtain the self-consistency equation

$$\tilde{\Delta}(z)/g=\mathrm{Re}\sum_{q_\perp,E_n>0}f_{1E_n}^*(z,q_\perp)f_{2E_n}(z,q_\perp)[n(E_n-\eta_+-\mu)-n(-E_n-\eta_+-\mu)], \tag{8}$$

where E_n are the eigenvalues of the purely one-dimensional Hamiltonian obtained in continuum Peierls model after discarding the "fast" exponentials with the band close to half-filled; $n(x)$ is the Fermi distribution function.[1,2]

It was assumed in Ref. 3 that $Q_\perp=0$, in view of the abrupt decrease of the interaction constant at $Q_\perp\neq 0$. In our case the effective constant depends little on $Q_\perp$, so that the vector $Q_\perp$ should be chosen such as to minimize Ω (at fixed μ) or F (if the number n of the particles is fixed). The function

$$\eta_+(q_\perp)=W_\perp\cos q_y a_y\cos\frac{Q_y a_y}{2}+W_\perp\cos q_x a_x\cos\frac{Q_x a_x}{2}$$

vanishes at $Q_x a_x = Q_y a_y = \pi$ (this corresponds to pure doubling in the trasverse direction).

A formal analysis of the functions $\Omega(\eta_+)$ and $F(\eta_+)$ shows that at all temperatures T the conditions $\eta_+ = 0$ realizes the state that is energetically most favored at $W_\perp \gg \Delta$ (this relation is assumed satisfied in the model considered). Such a result is obvious, for the condition $\eta_+ = 0$ corresponds to the best geometric congruence of the electron and hole Fermi surfaces.

For two- and three-dimensional systems with CDW or SDW at $W_\parallel \gg W_\perp \gg \Delta$ the problem of finding $\tilde{\Delta}(z)$ can thus be reduced to one that is exactly solvable at all temperatures. In the case of the Peierls model it is necessary also to take into account the law of conservation of the number n of the particles.[1-3] In our case we can consider also a situation wherein it is the chemical potential μ which is fixed (this is valid if electron-hole pairing takes place only on a small part of the Fermi surface or there exists an additional zone with large density of states on the Fermi surface).

3. BOGOLYUBOV–DE GENNES EQUATIONS FOR QUASI-ONE-DIMENSIONAL SUPERCONDUCTORS IN AN EXCHANGE FIELD

The equations describing a Peierls transition in a system with a nearly half-filled band are analogous to the Bogolyubov–de Gennes equations in the quasiclassical approximation in the theory of superconductivity.[8] All the exact solutions for the order parameter $\Delta(z)$ are therefore applicable to one-dimensional superconducting systems in the self-consistent-field approximation. The ground state, however corresponds to the solution $\Delta = \text{const}$. This means that all the solutions of the soliton type could correspond only to excited states of the system in quasi-one-dimensional systems the energy of such excitations turns out to be infinitely large, since the purely one-dimensional solution $\Delta(z)$ has an energy $N\varepsilon_s$, where N is the number of filaments and $\varepsilon_s = 2\Delta_0/\pi$ is the soliton energy. These solutions can therefore not be realized (Δ_0 is the superconducting gap at $T = 0$). The situation changes in the exchange field, which plays the role of the chemical potential. It will be shown below that when the exchange field H exceeds a threshold value $H_c = 2\Delta_0/\pi\mu_B$ the energy minimum corresponds to the solution $\Delta(z) \sim \operatorname{sn} z$ of the soliton-lattice type. The appearance of an inhomogeneous state of superconductors in an exchange field was predicted in Refs. 6 and 7, but neither an exact solution for $\Delta(z)$ nor the field of the transition from the homogeneous into the inhomogeneous state could be found there. In quasi-one-dimensional superconductor the problem can be solved exactly and the (T, H) phase diagram of the inhomogeneous state can be constructed, in contrast to the three-dimensional case.[6,7] We write down the Bogolyubov equations for the functions[8] $(u_\uparrow, v_\downarrow)$ [the equations for $(u_\downarrow, v_\uparrow)$ are similar in form apart from the substitution $H \to -H$]:

$$Eu_\uparrow = (\hat{\varepsilon}-h)u_\uparrow - \Delta v_\downarrow, \quad -Ev_\downarrow = (\hat{\varepsilon}+h)v_\downarrow + \Delta^* u_\uparrow. \tag{9}$$

Here $\Delta(z) = \tilde{\Delta}(z)\exp(iQ_\perp\rho_\perp)$ (only solutions of this type are considered), $\hat{\varepsilon} = p_z^2/2m + \eta(p_\perp)$, $h = \mu_B H$. We make the substitution:

$$u_\uparrow = \tilde{u}_\uparrow^+(z,\rho_\perp)\exp\left(-ip_F z + i\frac{Q_\perp\rho_\perp}{2}\right) + \tilde{u}_\uparrow^-(z,\rho_\perp)\exp\left(ip_F z + i\frac{Q_\perp\rho_\perp}{2}\right),$$

$$v_\downarrow = \tilde{v}_\downarrow^+(z,\rho_\perp)\exp\left(-ip_F z - i\frac{Q_\perp\rho_\perp}{2}\right) + \tilde{v}_\downarrow^-(z,\rho_\perp)\exp\left(ip_F z - i\frac{Q_\perp\rho_\perp}{2}\right). \tag{10}$$

The equations for $\tilde{u}_\uparrow^+$, $\tilde{v}_\downarrow^+$ and $\tilde{u}_\uparrow^-$, $\tilde{v}_\downarrow^-$ are similar, and we retain hereafter only the equations for $\tilde{u}_\uparrow^+$, $\tilde{v}_\downarrow^+$ and omit the superscripts $+$ and $-$.

Transforming to Fourier components with respect to the transverse coordinate $\rho_\perp$, we obtain

$$\begin{pmatrix} iv_F\frac{d}{dz} - h + \eta\left(q_\perp + \frac{Q_\perp}{2}\right) - E & -\tilde{\Delta}(z) \\ -\tilde{\Delta}(z) & -iv_F\frac{d}{dz} - h - \eta\left(q_\perp - \frac{Q_\perp}{2}\right) - E \end{pmatrix} \times \begin{pmatrix} \tilde{u}_\uparrow \\ \tilde{v}_\downarrow \end{pmatrix} = 0. \tag{11}$$

It can be seen right away that the system (11) is equivalent to the case (5) for CDW and SDW, accurate to the transformation $Q_\perp - \pi \to Q_\perp$. The equation for the superconducting order parameter $\tilde{\Delta}(z)$ is also obtained from (8) by a suitable substitution. Thus, in the case of superconductivity, even when no account is taken of the current connected with the choice of Δ in the form $\Delta(\mathbf{r}) \sim \exp(iQ_\perp\rho_\perp)$, the most suitable solution in accord with §2 is the one with $Q = 0$. The presence of a current when the phase of the order parameter is not fixed (i.e., $Q_\perp \neq 0$), leads to an additional energy loss.

We discuss now the feasibility in principle of realizing one-dimensional soliton structures in an exchange field in quasi-one-dimensional superconductors (it is assumed that $W_\parallel \gg W_\perp \gg \Delta$, so that this relation makes the mean-field theory applicable). The upper critical field $H_{c2}{}^0$, connected with the orbital effects in an isotropic superconductor is inversely proportional to the coherence length $H_{c2}{}^0 \sim \Phi_0/\zeta_0^2$, where $\zeta_0 = v_F/\Delta_0$ and Φ_0 is the flux quantum. In the quasi-one-dimensional case, when the field is directed along the z axis, the upper critical field is $H_{c2}'' \sim \Phi_0/\zeta_\perp^2$, where $\zeta_\perp = v_\perp/\Delta_0$ and $v_\perp$ is the velocity in the transverse direction. Thus, $H_{c2}'' \sim H_{c2}{}^0(W_\parallel/W_\perp)^2$ and can exceed substantially the paramagnetic limit: $H_{c2}'' \gg H_p \sim \Delta_0/\mu_B$. The influence of the exchange field is in this case decisive in fields $H \sim H_p$,

whereas the orbital effects in these fields are insignificant. A similar situation is realized apparently in organic quasi-one-dimensional superconductors such as $(TMTSF)_2X$ (Ref. 10) (we have in mind the case of a field parallel to the z axis in a sample with a transverse dimension along x smaller than λ_L). We are dealing throughout with magnetic fields $\mu_B H \ll \omega_D$ (ω_D is the Debye phonon frequency), where the BCS theory is valid at any rate. As will be seen from (T, H) phase diagram, superconductivity always sets in in such fields at a sufficiently low temperature.

4. SEMICONDUCTING MODEL WITH HYBRIDIZATION: ROLE OF THE PHASE OF THE ORDER PARAMETER

The Hamiltonian of the two-band model with interband hybridization is of the form[9]

$$\hat{H}=\begin{bmatrix} iv_F\dfrac{d}{dz} & \gamma_{12}\left(\dfrac{d}{d\rho_\perp}\right)-\tilde{\Delta}_{12}(z,\rho_\perp) \\ \gamma_{21}\left(\dfrac{d}{d\rho_\perp}\right)-\tilde{\Delta}_{21}(z,\rho_\perp) & -iv_F\dfrac{d}{dz} \end{bmatrix}. \tag{12}$$

In the models considered above the phase of the order parameter $\tilde{\Delta}$ was assumed fixed if it was possible, without loss of generality, to regard $\tilde{\Delta}$ as a real quantity. The situation is different for the Hamiltonian (12). Let $\gamma_{12}=\mathbf{P}^{12}(-id/d\rho_\perp)$, as is the case in the **k-p** approximation for the Kaane spectrum in the two-band model.[9] The hybridization vector $\mathbf{P}_{12}$ can be chosen to be purely imaginary ($\mathbf{P}_{12}=-\mathbf{P}_{12}$), but then the phase $\tilde{\Delta}(z,\rho_\perp)$ becomes real. Three-dimensionality of the spectrum is ensured in the model (12) only by the hybridization. Carrying out the procedure of "squaring" the Hamiltonian (12) in analogy with §2, we can obtain the following system of equations for its eigenfunctions $\varphi_{1,2E}(z,\mathbf{q}_\perp)$ under the assumption that $\tilde{\Delta}$ depends only on z:

$$\left[-v_F^2\frac{d^2}{dz^2}+|\gamma_{12}(\mathbf{q}_\perp)-\Delta_{12}|^2-E^2\right]\begin{pmatrix}\varphi_{1E}\\ \varphi_{2E}\end{pmatrix} + iv_F\begin{pmatrix} 0 & \dfrac{d\tilde{\Delta}_{12}}{dz} \\ -\dfrac{d\tilde{\Delta}_{21}}{dz} & 0 \end{pmatrix}\begin{pmatrix}\varphi_{1E}\\ \varphi_{2E}\end{pmatrix}=0. \tag{13}$$

If $\tilde{\Delta}_{12}$ is a real order parameter $\tilde{\Delta}_{12}=\tilde{\Delta}_{21}$, the system (13) reduces again to the one-dimensional exactly solvable case with the substitution $E^2\to E^2-|\gamma_{12}(\mathbf{q}_\perp)|^2$. But if $\tilde{\Delta}_{12}$ is imaginary and $\tilde{\Delta}_{12}=-\tilde{\Delta}_{21}$, it is impossible to reduce the problem to an exactly solvable second-order equation, in view of the presence of crossover terms of the type $\gamma_{12}(\mathbf{q}_\perp)\tilde{\Delta}_{21}$. A solution in the form of a soliton lattice does not satisfy the self-consistency equation in this case. It appears that in the class of single-period potentials there are no analytic solutions at all for the case of an imaginary order parameter, although we are unable to offer a rigorous proof of this statement. It is curious that approximate solutions can be obtained at $|\gamma_{12}|\gg|\Delta|$ and $|\gamma_{12}|\ll|\Delta|$ by perturbation theory. This makes it possible to find (at the accuracy indicated) the structure of the current state that arises when the order parameter is imaginary.[9,10] This question, however, is outside the scope of the present paper.

5. PHASE DIAGRAM AND LINE OF TRANSITIONS INTO THE SOLITON LATTICE STRUCTURE

Thus, for a large class of models of electronic phase transitions, including the quasi-one-dimensional superconducting transition, the problem of finding the spatial dependence of the order parameter can be reduced to an exactly solvable model at arbitrary temperatures. It is natural therefore to investigate the temperature phase diagram and find the region of existence of a soliton lattice. Greatest interest attaches to the case with fixed chemical potential μ (or its analog, a fixed magnetic field in the case of spin-Peierls and superconducting transitions). An analytic treatment is possible at $T\ll\Delta_0$ or $\Delta_1\ll T$, while in the intermediate case a numerical calculation is necessary [Δ_1 is the amplitude of the function $\Delta(z)$].

We consider first the case $T\ll\Delta_0$. The thermodynamic potential can then be expanded in the parameter T/Δ_0, where Δ_0 is the value of the order parameter at $T=\mu=0$.

Summing with the aid of the known density of states,[1] we get

$$\Omega=\Omega(0)+2\Delta_0^2N(0)\left\{-\frac{1}{4}+\left(\frac{T}{\Delta_0}\right)^{3/2}\left(\frac{\pi}{2}\right)^{1/2}\times\exp\left[\frac{-\Delta_0+|\mu|}{T}\right]\left(\frac{1}{L}-1\right)-\frac{\delta^2}{L}+\frac{(\gamma')^2}{4L}-\frac{\delta^2}{2L^2}\right\} \tag{14}$$

where

$$\gamma'=(1-\gamma^2)^{1/2},\ \delta=(|\mu|\pi/2\Delta_0)-1,\ L=\ln(4/\gamma').$$

Here $\Omega(0)$ is the potential of the normal phase.

When deriving (14) we also expanded in powers of γ', since we are interested in the region near the line of the transition from the commensurate structure ("doubled" in the case of a Peierls or spin-Peierls transition, homogeneous in the case of a superconductor) into an incommensurate one (i.e., into a soliton-lattice structure). With increasing μ the commensurate phase becomes unstable—the vanishing of the coefficient of $1/L$ (the principal term of the expansion in γ') in (14) determines the line of absolute instability $T_{c2}(\delta)$ of the commensurate phase:

$$\delta=\left(\frac{T_{c2}}{\Delta_0}\right)^{3/2}\left(\frac{\pi}{2}\right)^{1/2}\exp\left[\frac{-\Delta_0+|\mu_c|}{T_{c2}}\right],\quad \mu_c=\frac{2}{\pi}\Delta_0. \tag{15}$$

However, the presence of the term $-\delta^2/2L^2$ in (14) makes the transition into the soliton-lattice state a first-order transition. Thus, at a temperature $T_{c1}(\delta)>T_{c2}(\delta)$ a soliton lattice with finite soliton density ($\gamma'\neq0$) appears jumpwise:

$$T_{c1}=T_{c2}\left[1+\frac{T_{c2}}{\Delta_0-|\mu_c|}\left(\frac{T_{c2}}{\Delta_0}\right)^{3/2}\exp\left[\frac{-\Delta_0+|\mu_c|}{T_{c2}}\right]\right]\left(\ln\frac{16}{\delta^2}\right)^{-1}. \tag{16}$$

From (14) we also obtain easily the superheat line $T_{c3}(\delta)$ of the soliton lattice:

$$T_{c3}=T_{c2}[1+2(T_{c1}-T_{c2})/T_{c2}]. \tag{17}$$

To investigate the behavior of the system at $\Delta_1\ll T$ it is convenient to use a series expansion in terms of $\Delta(z)$ and its

derivatives (the Ginzburg-Landau functional). In the vicinity of the Lifshitz point $T^* = 0.31\Delta_0, \mu^* = 0.604\Delta_0$ (Ref. 11) it is necessary to retain the terms Δ^6, $(d\Delta/dz)^2\Delta^2$ and $(d^2\Delta/dz^2)^2$. The Lifshitz point is determined by the intersection of the line of transitions from the normal phase into the dielectric (superconducting) one and from the commensurate phase into the soliton-lattice phase. Since the solution $\Delta(z) = \Delta_1 \operatorname{sn} z$ is exact at all temperatures, it can be substituted in the corrresponding functional. The result is

$$\begin{aligned} \Omega &= \Omega(0) + 2N(0)\left[\alpha I_2\Delta_1^2 - 2AI_4\Delta_1^4 + BI_6\Delta_1^6\right], \\ I_2 &= J_2;\ I_4 = \gamma^{-2} + 2J_4 - (1+\gamma^{-2})J_2, \\ I_6 &= 16J_6 - 14(1+\gamma^{-2})J_4 + (1+12\gamma^{-2}+\gamma^{-4})J_2, \\ J_l &= \frac{1}{K(\gamma)}\int_0^{K(\gamma)} \operatorname{sn}^l(\zeta,\gamma)\,d\zeta. \end{aligned} \tag{18}$$

The coefficients α, A, and B are expressed in terms of digamma functions (see, e.g., Ref. 12):

$$\begin{aligned} &\alpha = \ln(T/T_0) + \psi_0 - \psi(1/2), \quad A = |\psi_2|/8, \quad B = \psi_4/24, \\ &\psi_n = (d^n/d\eta^n)\,\operatorname{Re}\psi(1/2 + i\eta), \quad \eta = \mu/2\pi T, \end{aligned} \tag{19}$$

$\psi(z)$ is the digamma function.

Analysis of (18) leads to the following result: the transition from the normal to the soliton-lattice phase is of second order. The transition line is given by the relation $\alpha(\mu, T) = A^2/B$; near the transition we have $\Delta_1 \to 0$ and $\gamma \to 0$, but $\Delta_1/\gamma = Q = \text{const}$. The superheat line of the commensurate phase is given by

$$\alpha(T_{c2}, \mu) = 0.37A^2(T_{c2}, \mu)B^{-1}. \tag{20}$$

The transition from the commensurate (homogeneous in the case of a superconductor) phase into the soliton-lattice phase is of first order along a line T_{c1} that lies somewhat lower than T_{c2}:

$$\alpha(T_{c1}, \mu) - \alpha(T_{c2}, \mu) = 2\cdot 10^{-7}A^2(T_{c2}, \mu)B^{-1}. \tag{21}$$

Finally, the supercooling line $T_{c3}(\delta)$ is given by the relation

$$\alpha(T_{c3}, \mu) - \alpha(T_{c2}, \mu) = 3\cdot 10^{-7}A^2(T_{c2}, \mu)B^{-1}. \tag{22}$$

The (T,μ) phase diagram is shown in Fig. 1.

The intermediate part of the transition line from the commensurate to the soliton-lattice phase is drawn approximately. In the case of a fixed number of particles n, in the Peierls model, the transition between the doubled and soliton phases is of second order; near the Lifshitz point the equation for $T(n)$ is given by the relation

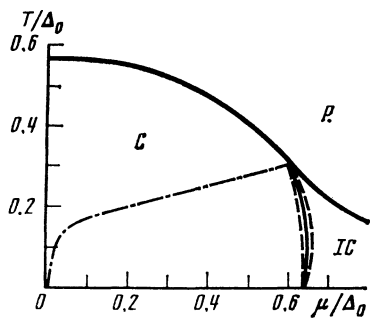

FIG. 1.

$$\psi_2\psi_1^2 = -|\alpha|(\psi_1\psi_3 + 0.072\psi_4). \tag{23}$$

An approximate $T(n)$ line is shown as a dash-dot line in Fig. 1 (in this case μ should be taken to mean n).

6. ROTATION OF SOLITON LATTICE IN TWO- AND THREE-DIMENSIONAL SYSTEMS

We consider now a more general class of solutions for $\Delta(z, \rho_\perp)$ in two-or three-dimensional systems. Let the "slow" part of $\Delta(z, \rho_\perp)$ depend only on one coordinate η along a certain θ direction making an angle θ with the z axis. We consider for simplicity a two-dimensional case. We transform into a coordinate frame (η, ζ) connected with the (z, y) system by an ordinary rotation:

$$\eta = \alpha z + \beta y, \quad \zeta = \alpha y - \beta z, \quad \alpha = \cos\theta, \quad \beta = \sin\theta. \tag{24}$$

We consider first the case of flat sections of the Fermi surface and seek $\Delta(z, y)$ in the form

$$\Delta(z,\ y) = \tilde{\Delta}(\eta)\exp[iQz + iQ_\perp y]. \tag{25}$$

The Fourier transforms of the wave functions $\varphi_{1,2}$ with respect to the variable ζ are conveniently represented in the form

$$\varphi_{1,2}(\eta,\ k_\zeta) = \tilde{\varphi}_{1,2}(\eta)\exp[ik_\zeta(\zeta - v_\zeta\eta/v_\eta)]; \tag{26}$$

$$v_\zeta = \alpha v_\perp - \beta v_F, \quad v_\eta = \alpha v_F + \beta v_\perp,$$

$$v_\perp = W_\perp a_y \sin(Q_\perp a_\perp/2) = W_\perp a_y. \tag{27}$$

With respect to the functions $\tilde{\varphi}_{1,2}(\eta)$ we obtain a system of equations completely analogous to (5), with the substitution $v_F \to v_\eta$. Taking the equality $\alpha^2 + \beta^2 = 1$ into account, as well as the fact that the energy gain in proportional to v_η, it is easy to verify that the most convenient solution is

$$v_\eta^{max} = (v_F^2 + v_\perp^2)^{1/2}, \quad \beta = v_\perp/v_\eta^{max}. \tag{28}$$

This means that in the two-dimensional case there is realized a soliton lattice rotated through an angle $\theta_2 = \arcsin(v_\perp/v_\eta^{max})$ away from the z axis.

Similar reasoning in the three-dimensional case yields a soliton-lattice rotation angle:

$$\theta_3 = \arcsin\left[2\tilde{v}_\perp^2/(v_F^2 + 2\tilde{v}_\perp^2)\right]^{1/2}, \quad \tilde{v}_\perp = W_\perp a_\perp \tag{29}$$

(for simplicity we assume that $a_x = a_y = a_\perp$).

It is noteworthy that all the equations are valid if $v_\perp \ll v_F$, i.e., in the case of an open Fermi surface. It was assumed that only a small region of transverse momenta near $Q_\perp$ is significant, so that the relations $\Delta \ll W_\perp \ll W_\parallel$ are satisfied. If, however, $W_\perp \sim W_\parallel$, i.e., the system is isotropic, nothing definite can be said concerning the $\Delta(z, \rho_\perp)$ structure. In the case of a superconductor in an exchange field we have $v_\perp = 0$ and no rotation of the soliton structure occurs. We cannot, of course, guarantee the absence of some specific two-dimensional exact solution, but it is hoped that in strongly anisotropic superconductors the one-dimensional solution considered above is energetically most favored, inasmuch as in the purely one-dimensional case it is precisely this solution which realizes the ground state.

In the case of the model with hybridization, we also seek a solution for $\tilde{\Delta}$ in the rotated coordinate system (η, ζ). The wave functions $\varphi_{1,2}$ are presented in the form

$$\varphi_{1,2}(\eta,\ \xi)=\tilde{\varphi}_{1,2}(\eta)\exp[ik_\xi(\xi+A\eta)], \tag{30}$$

where

$$A=\frac{v_F^2-|\mathbf{P}_{12}|^2}{v_F^2\alpha^2+|\mathbf{P}_{12}|^2\beta^2}\alpha\beta. \tag{31}$$

For $\tilde{\varphi}_{1,2}(\eta)$ we obtain a system of equations similar to (13) but with the substitutions $v_F\to\tilde{v}_\eta$, $\mathbf{P}_{12}\to\mathbf{P}_{12}$, where

$$\tilde{v}_\eta=[v_F^2\alpha^2+|\mathbf{P}_{12}|^2\beta^2]^{1/2},\quad \tilde{\mathbf{P}}_{12}=\mathbf{P}_{12}v_F/\tilde{v}_\eta. \tag{32}$$

The presence of hybridization leads to an energy loss and hinders the phase transition; on the other hand, the most favorable for the transition is the presence of a maximum $\tilde{v}_\eta$. It is easily seen from (32) that the maximum value of $\tilde{v}_\eta$ and the minimum hybridization $\mathbf{P}_{12}$ are reached simultaneously at $\beta=0$, i.e., in the absence of soliton-lattice rotation.

7. CONCLUSION

We have constructed a phase diagram for an entire series of physical models in which a transition into the soliton-lattice state is possible. The transition from the commensurate ("doubled") phase into the soliton phase is of first order at finite temperatures and fixed μ, but of second order at $T=0$. Recent numerical calculations using a large number of harmonics confirm this conclusion.[13] We note also that the result of Ref. 14, that the transition is of second order at fixed μ, is wrong. There exist at present a number of experimental data in evidence of a transition into a soliton-lattice phase in real systems. Thus, a transition into a state with an incommensurate SDW in chromium and its alloys is accompanied by the onset of higher harmonics of SDW and CDW. Analysis of these harmonics,[15] based on neutron-diffraction data, revealed a distinct modulation of CDW of the soliton type. The transition from an incommensurate into a commensurate ($AF_1\to AF_0$) structure in chromium alloys is of first order, in agreement with our present results. We note that we are speaking only of an approximate comparison, since chromium contains an electron "reservoir" of finite size, (i.e., the case realized in intermediate between fixed μ and n).

Within the framework of the XY model a spin-Peierls transition in a magnetic field[5] is similar to the Peierls model with fixed μ. A transition to an incommensurate structure (a soliton lattice) in a magnetic field was observed in experiment,[4] where a substantial difference was revealed between the static and dynamic magnetic susceptibilities near the critical field H (the latter was substantially smaller). Within the framework of the soliton-lattice theory this difference has a natural explanation: owing to the large mass of the soliton, the characteristic oscillation frequencies of the soliton lattice are quite low and in the dynamic regime the soliton lattice may be unable to attune itself to the field.

Quasi-one-dimensional superconductors in an exchange field can likewise turn out to be unstable to a transition into a soliton phase $\Delta(z)\sim\mathrm{sn}\,z$. This is in fact the LOFF state—in quasi-one-dimensional superconductors it is possible to obtain an exact solution of the problem of the transition from the homogeneous state to the inhomogeneous phase. One can hope that such a state will appear in the quasi-one-dimensional organic superconductors $(TMTSF)_2X$ (Ref. 10) in a field parallel to the chains.

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