Theory of magnetic-field-induced phase transitions in quasi-one-dimensional conductors

V. M. Yakovenko

L. D. Landau Institute of Theoretical Physics, Academy of Sciences of the USSR
(Submitted 1 December 1986)
Zh. Eksp. Teor. Fiz. **93**, 627–646 (August 1987)

A model of a layered quasi-one-dimensional metal in a strong magnetic field perpendicular to the layer is investigated. Renormalization-group equations for the model are derived in the "fast parquet" approximation. Numerical solution of these equations shows that for either sign of electron interaction a charge-density wave (CDW) or spin-density wave (SDW) arises in the system. If the sign of the interaction corresponds to superconductivity, a sequence of phase transitions between the various types of CDW or SDW occurs as the magnetic field strength increases. The type of CDW (SDW) is defined by its wave vector, the longitudinal component of which is quantized. The dependence of the CDW (SDW) type on the magnetic field strength H is determined by numerical solution of the renormalization-group equations for different values of H. The results can explain the experimental fact that the sequence of phase transitions in the $(TMTSF)_2X$ compounds is induced by a magnetic field from the superconducting phase only. The spin structure of the ordering, which may combine both CDW and SDW, is discussed by taking into account Zeeman splitting.

1. INTRODUCTION

The present article is devoted to a theoretical explanation of the anomalous behavior of the quasi-one-dimensional conductors $(TMTSF)_2X$, where $X = PF_6$, ClO_4, ReO_4, in a magnetic field lying along the axis **c*** of lowest conductivity (see the reviews of Refs. 1 and 2). For low temperatures $T \lesssim 1$ K in a weak magnetic field, $H < H_{c2} \sim 0.1$ T the materials are superconductors; in the region of fields $H_{c2} < H < H_{\text{thr}} \sim 4$ T, they are metals. In fields $H > H_{\text{thr}}$ they go into a semimetallic or an insulating phase, in which, according to the NMR data,[3] a spin-density wave (SDW) appears. The appearance of this phase is accompanied by a sequence of phase transitions, according to the magnetic field, between different types of SDW. As the magnetic field changes the phase transitions occur approximately periodically in H^{-1} with a frequency H_s: $1/H \approx n/H_s$. This is indicated by abundant data on the measurement of magnetoresistance,[4–7] Hall conductivity,[8,12] magnetization[13] and specific heat.[14] The effects described depend only on the sign of the projection of **H** on the **c*** axis, which testifies to their orbital origin.

It is remarkable that the sequence of phase transitions in a magnetic field is observed only if the material is superconducting in a zero magnetic field: for $X = PF_6$ (Refs. 4, 11), $X = ClO_4$ (Ref. 1), $X = ReO_4$ (Ref. 7). In fact, $(TMTSF)_2PF_6$ and $(TMTSF)_2ReO_4$ are superconducting only under pressure. The sequence of phase transitions in a magnetic field is observed in these materials only at the same pressures as superconductivity. The quasi-one-dimensional conductor $(TMTSF)_2ClO_4$ can be prepared in the two different phases R or Q; only the R phase is superconducting. The sequence of phase transitions is observed only in the R phase.

A theory of magnetic-field-induced SDWs was first proposed by Gor'kov and Lebed'.[2,15–17] It was further developed in Refs. 18–21. This theory explained the series of observed effects in terms of the ladder approximation. However, from the theoretical work mentioned it follows that the SDW in a magnetic field and superconductivity in the absence of a magnetic field are mutually exclusive, since their appearance would require opposite signs for the electron-electron interaction. Moreover, in Ref. 15 it was shown that in a magnetic field electrons are to some degree aligned, which leads in the ladder approximation to an increase in SDW instability. But it is well-known that in one-dimensional systems the electron-hole instability competes with superconductivity.[22] For a complete description it is necessary to employ the parquet approximation used in Refs. 23 and 24.

In Refs. 25 and 26 Brazovskiĭ and the present author developed a perturbation-theory approach to the electron hopping amplitude between stacks. It was shown that in very strong magnetic fields a SDW or CDW (charge-density wave) develops for both signs of the electron-electron interaction. If the interaction has the sign favorable to the appearance of superconductivity in the absence of a magnetic field, then in a very strong field electrons and holes on neighboring stacks pair up.[26] For the opposite sign of interaction (favorable to development of a SDW without a magnetic field) the pairing takes place on a single stack.[25] Unfortunately, this theory is inapplicable to the region of intermediate magnetic field where the sequence of phase transitions takes place.

In this work we use the parquet approximation to solve the problem. Within this approximation it is shown that in a broad range of magnetic fields a SDW or CDW forms for both signs of the electron-electron interaction. In the models (1) and (2) discussed below, the sequence of phase transitions takes place only if the sign of interaction corresponds to superconductivity, in agreement with experimental data. By numerical solution of the parquet equations we find the parameters of the SDW phase appropriate to the different values of magnetic field. For very strong fields the results obtained agree with the conclusions of the theory of Refs. 25 and 26.

2. DERIVATION OF THE PARQUET EQUATIONS

In the $(TMTSF)_2X$ compounds the electron hopping amplitude between stacks is relatively large in one direction (**b** axis) and small in the other (**c*** axis). Therefore we ne-

 0038-5646/87/080355-11$04.00 © 1988 American Institute of Physics

glect hops between layers. We look at a system of parallel stacks in a single (x, y) plane, at a distance b from each other. The magnetic field $\mathbf{H}$ lies perpendicular to the plane formed by the stacks. The model Hamiltonian has the form $\hat{H} = \hat{H}_0 + \hat{H}_{\text{int}}$,

$$\hat{H}_0 = \sum_{N,\alpha=\pm} \int dx \Big[-i\alpha\hbar v \hat{\psi}^+(x,N,\alpha) \frac{\partial}{dx} \hat{\psi}(x,N,\alpha) + t \sum_{M=\pm 1} \hat{\psi}^+(x,N,\alpha)\hat{\psi}(x,N+M,\alpha)\exp(-iMqx) \Big], \quad (1)$$

$$\hat{H}_{int} = G \sum_N \int dx \hat{\psi}^+(x,N,+)\hat{\psi}^+(x,N,-)\hat{\psi}(x,N,-)\hat{\psi}(x,N,+),$$

$$q = ebH/\hbar c. \quad (2)$$

Here v is the Fermi velocity, x is the coordinate along the stacks, and N is the number of stacks. The index $\alpha = \pm$ denotes electrons with momenta near $K \pm k_F$, where k_F is the Fermi momentum. The hopping amplitude between neighboring stacks is t, G is the amplitude of the electron interaction, e is the charge on the electron, and c is the speed of light. The $\exp(\pm ik_F x)$ factors in the $\hat{\psi}$-operators are separated out and cancelled. The oscillatory factor in the second term in (1) appears in the gauge $A_y = H_x$, $A_x = A_z = 0$. For simplicity, we will look at spinless fermions and CDW formation. The role of spins will be discussed in Sec. 7.

The eigenfunctions of the operator $\hat{H}_0$ are easily found:

$$[-i\alpha\hbar v\partial/\partial x + 2t\cos(k_y - qx)]\psi_{\varepsilon,k_y,\alpha}(x) = \varepsilon\psi_{\varepsilon,k_y,\alpha}(x), \quad (3)$$

$$\psi_{k_x,k_y,\alpha}(x,N,t) = \exp\{i[-\varepsilon t + k_x x + k_y N - \alpha\lambda\sin(k_y - qx)]\}, \quad (4)$$

$$\varepsilon = \alpha\hbar v k_x, \quad \lambda = 2tc/ebvH. \quad (5)$$

The dispersion relation (5) has a purely one-dimensional form; the energy does not depend on k_y. Therefore it is possible to transform the eigenfunctions of the operator $\hat{H}_0$ to the Wannier representation, by Fourier-transforming (4) in k_y:

$$\psi_{k_x,m,\alpha}(x,N,t) = \exp[i(-\varepsilon t + k_x x + (N-m)qx)]J_{N-m}(-\alpha\lambda). \quad (6)$$

Here $J_n(z)$ is a Bessel function. The wave function (6) is localized near stack with the label m, which is a quantum number.

We introduce the operators $\hat{a}^+(k_x, m, \alpha)$ and $\hat{a}(k_x, m, \alpha)$ which create and annihilate electrons in the states (6). In this representation the Hamiltonian has the form

$$\hat{H}_0 = \sum_{m,k_x,\alpha} \alpha\hbar v k_x \hat{a}^+(k_x,m,\alpha)\hat{a}(k_x,m,\alpha), \quad (7)$$

$$\hat{H}_{int} = \sum_{k_i,m_i,\ i=1-4} g(m_1,m_2,m_3,m_4)\delta(k_1+k_2-k_3-k_4 - (m_1+m_2-m_3-m_4)q) \quad (8)$$

$$\times\hat{a}^+(k_1,m_1,+)\hat{a}^+(k_2,m_2,-)\hat{a}(k_3,m_3,-)\hat{a}(k_4,m_4,+),$$

$$g(m,n,p,q) = G\sum_l J_{l-m}(-\lambda)J_{l-n}(\lambda)J_{l-p}(\lambda)J_{l-q}(-\lambda). \quad (9)$$

The expressions (7) and (8) can be considered as the Hamiltonian of an effectively quasi-one-dimensional system. The integer quantum numbers m, m_1–m_4 in (7) and (8) can be interpreted as the numbers of the stacks on which electrons are distributed. We will call them the numbers of the Wannier stacks, and denote them by small Latin letters to differentiate them from the stack numbers in the initial Hamiltonian (1) and (2). In contrast to the case in (1) and (2), hops between Wannier stacks are absent in (7), but in return the interaction term (8) is nonlocal in Wannier stack number.

The model (7) and (8) can be investigated with the help of the method of summation over parquet diagrams[23,27] or equivalently by the single-loop approximation in the renormalization-group (RG) method (see the review of Ref. 28). In the model defined by (7) and (8) we have two diagrams that are logarithmically divergent in the infrared: the Peierls and the Cooper. The problem of summing these diagrams reduces to writing down the RG equations for the renormalized interaction amplitudes $g(m_1, m_2, m_3, m_4, \omega)$, where ω is the infrared cutoff energy. These are the electron interaction amplitudes which have energy $\varepsilon \sim \omega$ and momentum $k_x \sim \omega/\hbar v$. In place of ω one can also use the temperature T. The expression (9) is the interaction amplitude for $\omega = \varepsilon_0$, where ε_0 is the energy of the ultraviolet cutoff, having the scale of the Fermi energy ε_F.

The RG equations have an intrinsically different form in the regions $\omega > \Omega$ and

$$\omega < \Omega = \hbar v q = ebHv/c, \quad (10)$$

where Ω is the characteristic magnetic field energy. We will look initially at the region $\omega > \Omega$. Let $\lambda = 2t/\Omega \gtrsim 1$. In this case the Bessel functions $J_n(\lambda)$ in (9) attain their maximum for $n \sim \lambda$; thus in (8) the characteristic values of m_1, m_2, m_3 and $m_4 \sim \lambda$. It follows that for $\omega > t$ we can neglect the term $(m_1 + m_2 - m_3 - m_4)q \sim \lambda q \sim t/\hbar v$ in the argument of the δ-function in (8) in comparison to the term $(k_1 + k_2 - k_3 - k_4) \sim \omega/\hbar v$. Then, transforming to the new operators

$$\hat{\tilde{a}}(x,N,\alpha) = \sum_{m,k_x} \hat{a}(k_x,m,\alpha)J_{N-m}(-\alpha\lambda)\exp(ik_x x),$$

we find that the Hamiltonian (7) and (8) takes the form $\hat{H}_0 = \hat{H}_{\text{int}}$, where $\hat{H}_0$ and $\hat{H}_{\text{int}}$ look like (1) and (2) with $t = 0$ in (1) and the substitution of $\tilde{a}(x, N, \alpha)$ for $\hat{\psi}(x, N, \alpha)$. Thus, in the region of energies $\omega > t$ the model described by (7) and (8) reduces to a purely one-dimensional model of spinless fermions. In this model there is only one interaction amplitude G [Eq. (2)] for which to write down the RG equation. However, it is known[29] that in this model the G-renormalization does not exist due to the mutual cancellation of the Peierls and Cooper diagrams. Thus, there is no renormalization in the energy interval (t, ε_0).

The region (Ω, t) of energies cannot be accurately investigated; therefore we confine ourselves to the condition

$$|G|\ln(t/\Omega)/2\pi\hbar v \ll 1. \quad (11)$$

In this case renormalization in the interval of energies (Ω, t) can be neglected due to condition (11) on the logarithmic narrowness of this interval. For fixed t and Ω the relationships (11) can be fulfilled for sufficiently small $|G|$. The condition (11) is equivalent to the inequality

$$\Omega \gg t \exp(-2\pi\hbar v/|G|) \sim T_{sc}, \tag{12}$$

where T_{sc} is the superconducting transition temperature for $H=0$. Therefore, when (12) is fulfilled renormalization in the energy interval (Ω, ε_0) can be neglected. The case $\lambda = 2t/\Omega \ll 1$ is treated in analog with the difference that the energy interval (Ω, t) is in general absent.

We now look at the energy region (10). The amplitudes $g(m_1, m_2, m_3, m_4, \omega)$ in (8) with $m_1 + m_2 \neq m_3 + m_4$ do not conserve the momentum k_x; therefore the logarithmic corrections to them are cut off at energy Ω. For $\omega < \Omega$ these amplitudes remain small ($\sim G$) and can be neglected. The remaining vertices with $m_1 + m_2 = m_3 + m_4$ can be parametrized in the following form:

$$\hat{H}_{int} = -\sum_{n,m,l} \tilde{g}(m, l, \omega)\hat{O}^+(x, n+m, l)\hat{O}(x, n, l), \tag{13}$$

$$\tilde{g}(m, l, \omega) = g(n+m, n+l, n+m+l, n, \omega), \tag{14}$$

$$\hat{O}^+(x, n, l) = \hat{a}^+(x, n, +)\hat{a}(x, n+l, -), \tag{15}$$

where $\hat{a}(x, n, \alpha)$ result from the Fourier transform in k_x of $\hat{a}(k_x, n, \alpha)$. The operator (15) creates an electron-hole pair with separation l between the particles. The operator (13) describes a hop of this pair at distance m. It is evident that in a hop the dipole moment el of the pair is conserved.

The parquet equations for the model (7), (13) and (15) are easy to derive using the method of Refs. 23 and 30. It is necessary to take account of the two diagrams depicted in Fig. 1:

$$d\Gamma(n, l, \xi)/d\xi = \sum_m \{\Gamma(m, l, \xi)\Gamma(n-m, l, \xi) - \Gamma(m, n+l-m, \xi)\Gamma(n-m, l-m, \xi)\}, \tag{16}$$

$$\xi = \ln(\Omega/\omega), \quad \Gamma(n, l, \xi) = \tilde{g}(n, l, \omega)/2\pi\hbar v.$$

The initial conditions for these equations, in accordance with (9) and (14), and taking account of the lack of renormalization in the energy interval (Ω, ε_0), has the form

$$\Gamma(n, l, 0) = g\sum_m J_{m-n}(-\lambda)J_{m-n-l}(\lambda)J_{m-l}(\lambda)J_m(-\lambda),$$

$$g = G/2\pi\hbar v. \tag{17}$$

3. ANALYSIS OF THE EQUATIONS

The Eqs. (16) represent an infinite system of ordinary differential equations. It is convenient to talk of ξ as the "time" for the system, and the solution $\Gamma(n, l, \xi)$ of the equations can be considered as the evolution in time starting from the initial condition (17).

In Ref. 24 equations analogous in form to the Eqs. (16) were investigated. Following this work, we take the Fourier transform of (16) and (17) in the first argument:

$$f(k_y, l, \xi) = \sum_n \Gamma(n, l, \xi)\exp(-ik_y n), \quad -\pi \leqslant k_y \leqslant \pi,$$

$$\frac{df(k_y, l, \xi)}{d\xi} = f^2(k_y, l, \xi) - \sum_{l_1, l_2}\int\int_{-\pi}^{\pi} \frac{dk_1\, dk_2}{(2\pi)^2} f(k_1, l_1, \xi)f(k_2, l_2, \xi) \cdot \exp[-ik_y(l_1 - l_2) + il(k_1 - k_2) - i(k_1 l_2 - k_2 l_1)], \tag{18}$$

$$f(k_y, l, 0) = gJ_l^2\left(2\lambda\cos\frac{k_y}{2}\right), \quad \lambda = \frac{2t}{\Omega}. \tag{19}$$

For an approximate solution of the Eqs. (18) we neglect for the time being the second term on the right-hand side. The remaining equations have the general solution

$$f(k_y, l, \xi) = [C(k_y, l) - \xi]^{-1} \tag{20}$$

for some function $C(k_y, l)$. The transition temperature T_c is determined by the minimum of $C(k_y, l)$, which is reached at a point (k_0, l_0):

$$\xi_c = \ln(\Omega/T_c) = \min C(k_y, l) = C(k_0, l_0). \tag{21}$$

In the neighborhood of the transition point the singular part of $f(k_y, l, \xi)$ can be rewritten in the form

$$f(k_y, l, \xi) \approx A\delta_{l, l_0}[\tau + \beta(k_y - k_0)^2]^{-1}, \quad \tau = \xi_c - \xi \tag{22}$$

with coefficients $A \sim 1$ and $\beta \sim |g|^{-1}$. Substituting (22) in (18), we find that the first term on the right side of (18) is of order τ^{-2}, and the second of order $|g|\tau^{-1}$ (the singularity is weaker due to the integration over k_1 and k_2). Thus for

$$|\tau| \ll |g|^{-1} \tag{23}$$

the above approximation is self-consistent. A solution of the type (22) is called a "moving pole" since the location of the pole depends on a continuous parameter, the momentum.

If we neglect the first term on the right side of Eqs. (18) we get a "stationary pole" type solution:

$$f(k_y, l, \xi) = \theta(k_y, l)/\tau, \tag{24}$$

where $\theta(k_y, l)$ is some function. This is shown in Appendix A for the case $g < 0$, that is, when the interaction sign corresponds to superconductivity. This approximation is not self-consistent, since when (24) is substituted into (18) both terms on the right side of (18) are of the same order: τ^{-2}. Of course, a stationary pole can in principle arise also when both terms in (18) are calculated simultaneously. Jumping ahead, we note that for numerical solution of the Eqs. (18) with both terms for $g < 0$ in the intermediate region of values of ξ the behavior of $f(k_y, l, \xi)$ is essentially like a stationary pole. However as ξ increases it sooner or later is converted to a moving pole. From this we can conclude that the stationary-pole solution is unstable, and the only stable asymptotic solution is the moving pole (22).

We now discuss the character of the ordering that arises in the system for $T < T_c$. The singular behavior of the extremum $f(k_0, l_0, \xi)$ in (22) leads to a singular growth of the

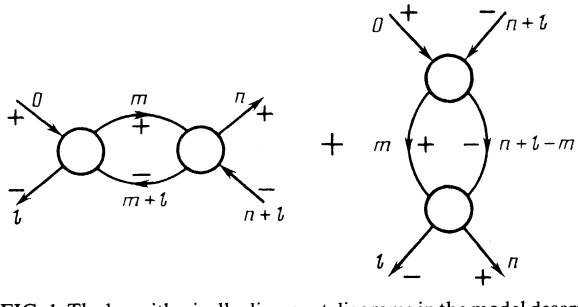

FIG. 1. The logarithmically divergent diagrams in the model described by (7), (13). The $\pm$ signs signify electrons with momenta near $\pm k_F$. The letters signify the numbers of the Wannier stacks on which the interacting electrons are located.

corresponding generalized susceptibility for $T \to T_c$.[24,30] The structure of the order parameter for the low-temperature phase is determined by the structure of the moving pole (22) [see (13)]:

$$\langle \hat{O}(x,\ n,\ l)\rangle = Y_{k_0,l_0}(x,\ n)\delta_{l,l_0}\exp(ik_0 n). \tag{25}$$

The order parameter $Y_{k_0,\,l_0}(x,\,n)$ is characterized by the distance l_0 between the electron and hole in the direction perpendicular to the stack, and by the center-of-mass momentum k_0 of the electron-hole pair in that direction. The distance l_0 takes discrete integer values, but the momentum k_0 takes on a continuous range of values within the Brillouin zone. The dependence of $Y_{k_0,\,l_0}(x,n)$ on (x,n) describes the fluctuations of the order parameter at large distances. The quantity el_0 is the dipole moment of the electron-hole pair. This is a purely microscopic parameter, with no relation to the macroscopic dipole moment of the system

$$\mathbf{d} = \sum_{\mathbf{r}} \mathbf{r}\rho(\mathbf{r}), \tag{26}$$

where $\rho(\mathbf{r})$ is the deviation of the charge density at the point $\mathbf{r} = (x, N)$ from a uniform distribution. A pairing with $l_0 \neq 0$ does not lead to the appearance of $\mathbf{d} \neq 0$, since, as will be seen below, $\rho(\mathbf{r})$ has the form (59) or (60).

We now determine the CDW wave vector described by the order parameter $Y_{k_0,\,l_0}$. This can be measured with the help of x-ray or neutron scattering. The CDW wave vector is equal to the change of photon or neutron momentum upon scattering. The scattering of interest to us is described by the Hamiltonian

$$\hat{H}_1 = \sum_{N,\alpha}\int dx \hat{b}^+(x,N)\hat{b}(x,N)\langle\hat{\psi}^+(x,N,-\alpha)\hat{\psi}(x,N,\alpha)\rangle \times \exp(2i\alpha k_F x), \tag{27}$$

where $\hat{b}^+(x,N)$ is the creation operator for photons or neutrons. Using the formula (6), the determination (15) and (25) of the order parameter, and the sum rule for Bessel functions, we find

$$\begin{aligned}\sum_{\alpha}&\langle\hat{\psi}^+(x,N,-\alpha)\hat{\psi}(x,N,\alpha)\rangle\exp(2i\alpha k_F x)\\ &= \sum_{\alpha,m_1,m_2}\langle\hat{a}^+(x,m_1,-\alpha)\\ &\quad\times\hat{a}(x,m_2,\alpha)\rangle J_{N-m_1}(\alpha\lambda)J_{N-m_2}(-\alpha\lambda)\\ &\quad\times\exp\{2i\alpha k_F x + i(m_1-m_2)qx\}\\ &= Y_{k_0,l_0}F(k_0,l_0,\lambda)\exp[i(2k_F+l_0 q)x + ik_0 N] + \text{comp. conj.},\end{aligned} \tag{28}$$

where the scattering amplitude $F(k_0, l_0, \lambda)$ has the form

$$F(k_0,\,l_0,\,\lambda) = (-1)^{l_0}J_{l_0}(2\lambda\cos(k_0/2))\exp(-ik_0 l_0/2). \tag{29}$$

Having substituted the expression (28) in the scattering Hamiltonian (27) and carried out a Fourier transform in x, N, we find

$$\hat{H}_1 = \sum_{\mathbf{K}_1,\mathbf{K}_2}\hat{b}^+(\mathbf{K}_1)\hat{b}(\mathbf{K}_2)\delta(\mathbf{K}_1-\mathbf{K}_2-\mathbf{K}(l_0,k_0))\, Y_{k_0,l_0}F(k_0,l_0,\lambda) + \text{e.f.}, \tag{30}$$

where the momentum $\mathbf{K}(l_0, k_0) = (K_x, K_y)$ transferred to the photon or neutron is equal to

$$K_x = 2k_F + l_0 q, \quad K_y = k_0. \tag{31}$$

Thus, the longitudinal component of the CDW wave vector takes quantized values in accordance with (31), and the perpendicular component equals k_0. The quantization of k_x is described in References 2, 17 and 19. We shall see that this effect is tied to the quantization of the perpendicular dipole moment el_0 of the electron-hole pair. We note also the nontrivial form of the scattering amplitude $F(k_0, l_0, \lambda)$ in (29). For $k_0 = \pi$ it goes to zero for all $l_0 \neq 0$, which makes it difficult to observe a structure with such parameters.

We note that the initial conditions (19) are symmetric under the interchange $k_y \to -k_y$ and $l \to -l$. It is easy to verify that the derivative $df(k_y, l, \xi)/d\xi$ in (18) is likewise symmetric, if $f(k_y, l, \xi)$ is. Therefore the solutions of Eqs. (18) will also be symmetric in k_y and l. This means that at the transition point electron-hole pairs of four types will condense simultaneously with different combinations of signs of k_0 and l_0. The degeneracy in the sign of k_0 and l_0 is connected with the specific form of the Hamiltonian (1). It can be shown that if in expression (1) electron hops to farther stacks with $M = \pm 2$ are considered, then the symmetry of the initial conditions in (19) under the $l \to -l$ interchange is lost. The symmetry in k_y disappears when the structure of the electron hopping integrals is calculated accurately in a crystal with a triclinic cell. But, so as not to complicate the discussion, we will discuss only the simplest model (10), which has high symmetry in k_y and l.

The region of applicability of Eqs. (18) is limited from the small-τ side by the growth of critical fluctuations.[31,23] Using the results of Refs. 31, 23, and 32 we can evaluate the coefficients of the Ginzburg-Landau functional, and find that in the two-dimensional system discussed, the critical fluctuations are small under the condition

$$\tau \gg |g|^{1/2}. \tag{32}$$

Therefore, expression (22) applies in the region given by the inequalities (23) and (32). They are compatible if

$$|g| \ll 1. \tag{33}$$

Fulfillment of the inequality (33) is one of the necessary conditions for the applicability of the theory developed.

After the general analysis carried out in this section, the problem reduces to the following: what are the parameters k_0, l_0, ξ_c of the moving pole for the given initial conditions (19), in particular for the given magnetic field H? It is not possible to find in explicit form the exact solution of the system (18) of differential equations, although it is possible to make a set of exact statements, which are collected in Appendix B. These statements, however, do not help to answer the question set forth. Two methods have been used to solve the problem: perturbation theory for small λ (Sec. 4) and numerical solution of the system of Eqs. (18) (Sec. 5).

4. THE PERTURBATION THEORY

The system of Eqs. (18) does not contain any parameters, although the initial conditions (19) depend on the parameter λ. In this section we discuss the case of small λ. We

drop from expression (19) terms higher than second order in λ, carry out a Fourier transform in k_y and turn again to Eqs. (16). The initial conditions have the form

$$\Gamma(0,0,0)=g(1-\lambda^2),\ \Gamma(\pm1,0,0)=-g\lambda^2/2,$$
$$\Gamma(\pm1,\pm1,0)=g\lambda^2/4,\ \Gamma(0,\pm1,0)=g\lambda^2/2. \tag{34}$$

Expression (34) has a simple physical interpretation. In a strong magnetic field (for small λ) electrons and holes can pair up only on a given ($l=0$) or on neighboring ($l=\pm1$) Wannier stacks and can hop no farther than neighboring Wannier stacks: $\Gamma(m,l,0)=O(\lambda^4)$ for $|m|>1$, $|l|>1$ [see Eq. (13)].

The hierarchy of scales in the initial conditions (34) is preserved for evolution given by the Eqs. (16), for a certain range of ξ. Therefore for ξ not too large we can choose which small terms in Eqs. (16) to keep. We substitute (34) in (16) and discard on the right-hand side of (16) terms in λ of degree greater than two. Then these equations take the form

$$\begin{aligned} d\Gamma(0,0,\xi)/d\xi&=0,\\ d\Gamma(\pm1,0,\xi)/d\xi&=2\Gamma(0,0,\xi)\Gamma(\pm1,0,\xi),\\ d\Gamma(\pm1,\pm1,\xi)/d\xi&=-\Gamma(0,0,\xi)\Gamma(\pm1,\pm1,\xi). \end{aligned} \tag{35}$$

They have the solution

$$\begin{aligned} \Gamma(\pm1,0,\xi)&=-g\lambda^2\exp(2g\xi)/2,\\ \Gamma(\pm1,\pm1,\xi)&=g\lambda^2\exp(-g\xi)/4. \end{aligned} \tag{36}$$

It is obvious that, as in the purely one-dimensional case, the electron interaction amplitude on a single Wannier stack, $\Gamma(0,0,\xi)$, is not renormalized. With evolution in time ξ the hopping amplitude between neighboring Wannier stacks grows for a pair with $l=0$ (for $g>0$) or for a pair with $l=\pm l$ (for $g<0$). Growth continues as in (36) until ξ reaches a certain value ξ_1, for which the renormalized quantities $\Gamma(\pm1,0,\xi)$ or $\Gamma(\pm1,\pm1,\xi)$ are no longer comparable to $\Gamma(0,0,\xi)$: $\xi_1\approx\ln[2(3-\gamma)/\lambda^2]/\gamma|g|$, where $\gamma=2$ for $g>0$, and $\gamma=1$ for $g<0$. For $\xi>\xi_1$ we cannot use the equations above.

For a qualitative understanding of the further behavior of the system we can connect (36) directly with the moving-pole solution (22):

$$\begin{aligned} f(k_y,l,\xi)=&-|g|\lambda^2\exp(\gamma|g|\xi)\cos k_y\delta_{|l|,2-\gamma}\\ &\times[3-\gamma+(\xi-\xi_1)|g|\lambda^2\exp(\gamma|g|\xi)\cos k_y]^{-1}. \end{aligned} \tag{37}$$

We see that for either sign of g the pole in ξ is most rapidly reached at $k_y=\pi$. There $\xi_c-\xi_1\sim|g|^{-1}$ and

$$T_c\sim\Omega(B/\Omega)^{(3-\gamma)/|g|},\quad B\sim1. \tag{38}$$

From the analysis above we can draw the following conclusions. For both signs of the interaction g in strong magnetic fields (small λ) a CDW arises. For positive g it forms with parameters $l_0=0$, $k_0=\pi$, and for negative g, which corresponds to superconductivity, with parameters $l_0=\pm1$, $k_0=\pi$. Thus, for $g>0$ the electron-hole pairing occurs on a single Wannier stack, and for $g<0$, on neighboring Wannier stacks. In both cases the order parameter changes sign with a transition to the neighboring Wannier stack ($k_y=\pi$). The transition temperature is given by Eq. (38). In this formula the exponent is exact, and the expression raised to this power is determined to within a constant. The transition temperature decreases with increasing H. All these conclusions agree with the results in Refs. 25 and 26, which were obtained by perturbation theory in t, applied directly to the Hamiltonian in Eqs. (1) and (2).

5. NUMERICAL SOLUTION

In the most interesting case, $\lambda\gtrsim1$, perturbation theory is inapplicable; therefore numerical methods were used. For numerical solution it is convenient to Fourier-transform (18) in the second argument and to exclude the coupling constant g from the critical conditions:

$$f(k_y,l,\xi)\to h(k_y,q_y,\zeta)/|g|,\quad \zeta=|g|\xi,\quad -\pi\leqslant q_y\leqslant\pi, \tag{39}$$

$$\frac{dh(k_y,q_y,\zeta)}{d\zeta}=\int_{-\pi}^{\pi}\frac{dp}{2\pi}[h(k_y,p,\zeta)h(k_y,q_y-p,\zeta)$$
$$-h(k_y+q_y-p,p,\zeta)h(k_y-p,q_y-p,\zeta)], \tag{40}$$

$$h(k_y,q_y,0)=\operatorname{sign}(g)J_0\left(V\cos\frac{k_y}{2}\sin\frac{q_y}{2}\right),\quad V=4\lambda=\frac{8tc}{ebvH}. \tag{41}$$

Since the function $h(k_y,q_y,\zeta)$ is symmetric in k_y and q_y (see Sec. 3) it was investigated only in the first quadrant of the Brillouin zone:

$$0\leqslant k_y\leqslant\pi,\quad 0\leqslant q_y\leqslant\pi. \tag{42}$$

In the region (42) a grid of 51×51 points was introduced, and Eqs. (40) were discretized on the points of the grid. The resulting system of 2601 ordinary differential equations were solved by the fourth-order Runge-Kutta method, with several values of the parameter V and both signs of g. The step in time ζ was 0.1. The functions $h(k_y,q_y,\zeta)$ of the variables k_y and q_y were represented in the k_y–q_y plane with the help of contour lines.

As an illustration, typical moments in the evolution are represented in Figs. 2–4 for the case $V=16$, $g<0$. In Fig. 2 the initial conditions $h(k_y,q_y,0)$ are represented; in Fig. 3 the initial derivative $dh(k_y,q_y,\zeta)/d\zeta|_{\zeta=0}$, that is, the right-hand side of (40), is calculated at $h(k_y,q_y,0)$. In Fig. 4, the function $h(k_y,q_y;3.5)$ is shown for $\zeta=3.5$, near ζ_c. The contours in these drawings are constructed in the following way. The maximum and minimum values are found for the represented function of two variables $R(k_y,q_y)$. For example, in Fig. 2, $R_{\max}=0.4$, $R_{\min}=-1$; in Fig. 4, $R_{\max}=19$, $R_{\min}=-23$. In an interval $(R_{\max}-R_{\min})/12$, 11 contours are produced. The direction of decrease is indicated by the cross-lines. Figure 4 shows conclusively that a singularity arises in the form of the l_0th harmonic of q_y for specified $k_y=k_0$, that is, in the form of the moving pole (22) (in Fig. 4, $l_0=3$, $k_0=0.38\pi$). It was especially verified that for $\zeta=3.5$, 3.6, that is, near the singularity, the shape of $h(k_y,q_y,\zeta)$ with q_y for fixed $k_y=k_0$ is nearly a cosine. Note that for $l_0=3$ it would have been natural to expect $k_0=\pi/3$. The modest deviation in the value found, $k_0=0.38\pi$, is associated with the errors due to the discrete approximation to Eqs. (40).

The behavior of the system near the singularity has the character of the moving pole (22) for all cases studied. Below, the parameters of the moving pole are cited as a function of V and $\operatorname{sign}(g)$:

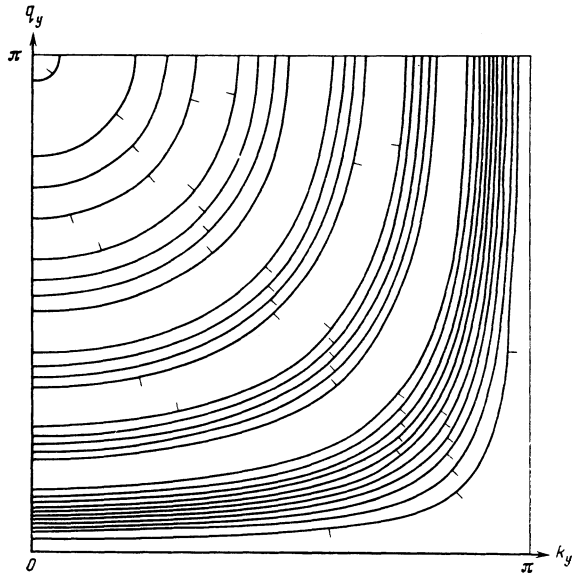

FIG. 2. The initial conditions of Eq. (41) for $V = 16$, $g < 0$.

V	0.5	2	10	0.5	2	4	7	10	13	16
sign (g)	+	+	+	−	−	−	−	−	−	−
k_0/π	1	1	1	1	1	0	0	0	0	0,38
l_0	0	0	0	1	1	0	1	2	0	3
ζ_c	1.3	0.8	0.6	2.6	1.8	2.8	3.8	3.4	3.3	3.6

The value of ζ_c here is the "time" at which the solution of the system (40) reached the singularity. It is related to the transition temperature by the formula

$$T_c = \Omega \exp(-\zeta_c/|g|). \tag{43}$$

A more detailed survey in V was not undertaken, due to the high cost in machine time. The same applies to large V, since in this case a decrease in grid mesh size is necessary due to the rapid oscillations in the initial conditions.

Consideration of the table above allows us to draw the following conclusions. The numerical solutions for $V = 0.5$ and 2 agree with the results of perturbation theory for $\lambda = V/4 \ll 1$ (Sec. 4). Furthermore, in the case $g > 0$ the same state with $l_0 = 0$, $k_0 = \pi$ is formed independent of magnetic field value. In agreement with (31), it has a corresponding wave vector $\mathbf{K} = (2k_F, \pm\pi)$; i.e., there is coupling with the complete nesting vector. Obviously, a CDW of this type forms even for $H = 0$; in the model (1) and (2) studied, there is complete nesting in the absence of a magnetic field. Therefore, for the given model in the case $g > 0$ it is in general impossible to speak of the magnetic field inducing a CDW. The CDW exists for $H = 0$ and continues to exist unchanged for any value of H. We note, however, that according to the table and Eq. (38), the transition temperature decreases as H increases: $T_c(H) \to 0$ for $H \to \infty$ ($V \to 0$).

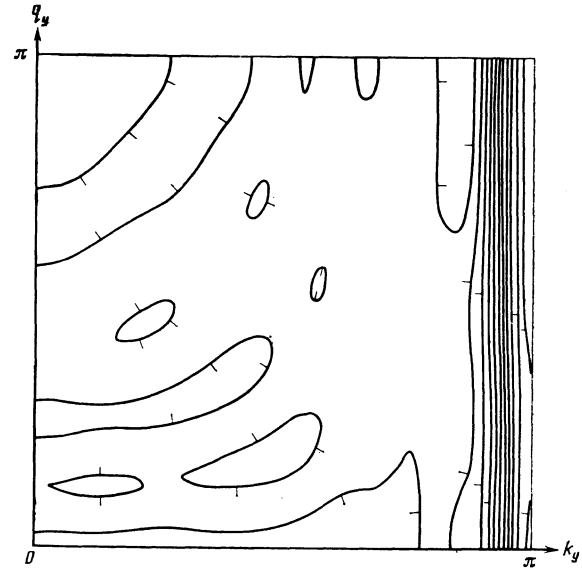

FIG. 3. The initial derivative (40) for $V = 16$, $\zeta = 0$.

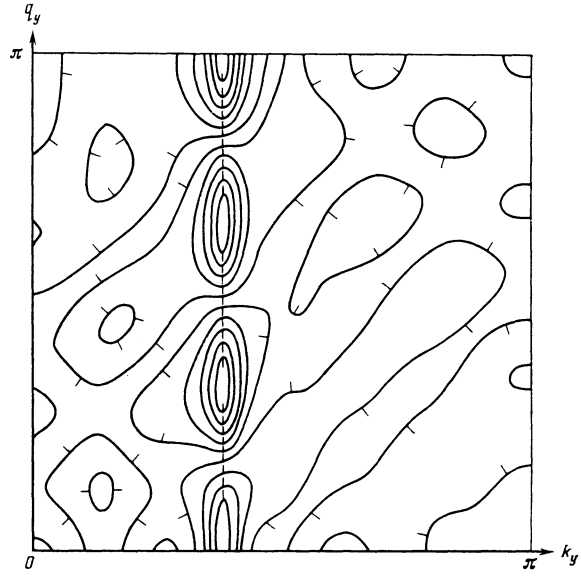

FIG. 4. The function $h(k_y, q_y; 3.5)$ obtained from evolution of the initial conditions of Fig. 2 in accordance with Eqs. (40).

In the $g < 0$ case for a zero magnetic field, superconductivity obviously exists. A sufficiently strong [satisfying condition (12)] magnetic field induces a CDW. As seen from the table, the type of CDW formed changes according to the magnitude of H; that is, a succession of phase transitions takes place as a function of magnetic field. Phases with nontrivial values of k_0, l_0 occur; for example, pairs can form not only on nearest neighbors ($l_0 = 0,1$) but farther apart ($l_0 = 2,3$). According to the table, the phase transitions occur approximately periodically with magnetic field although there is, evidently, not strict periodicity.

$$\Delta V \approx 3, \quad \Delta(1/H) \approx 1/H_0, \quad H_0 = 8tc/3ebv. \tag{44}$$

The transition temperature has a maximum for $V = 2$.

We now consider the question of the stability of the results when the initial conditions depend slightly from Eq. (41). These deviations can be, for instance, due to renormalization in the energy range (Ω, t) for $\Omega < t$, which we have neglected until now. Figures 2 and 3 are fairly typical pictures of the initial state for $V \geqslant 4$. We see that the initial derivative $dh(k_y, q_y, 0)/d\zeta$ (Fig. 3) has a sharp maximum for $k_y = \pi$, uniform in q_y. For $g > 0$ there is a similar maximum in the initial conditions $h(k_y, q_y, 0)$ (Fig. 2). Thus it is natural that for $g > 0$ there is always a final state with $k_0 = \pi$ and a zero harmonic in q_y, which corresponds to $l_0 = 0$. Small corrections scarcely change the type of final state.

For $g < 0$ the situation changes. The initial derivative has the sharp maximum formerly mentioned; however, $h(k_y, q_y, 0)$ now has a sharp minimum in this location due to the change in sign of g. The final state is determined by a

nontrivial interplay of small terms on a background of two large factors acting in opposing directions. Therefore small changes in the initial conditions for a change in V produce a change in the type of final state, which is reflected in the table. Deviations in the initial conditions from Eqs. (41) for $g<0$ can, evidently, change the types of final states in the table. They do not, however, change the fact that the succession of phase transitions occurs only for a sign of interaction corresponding to superconductivity, since this phenomenon is directly linked to the sensitivity of Eqs. (40) to initial conditions for $g<0$.

6. COMPARISON WITH OTHER MODELS

In this section we discuss the connection between the proposed theory and the mean-field theories, which are based on the ladder approximation.[2,15–21] In these theories only the Peierls diagrams are summed over, and Cooper diagrams are not accounted for. This corresponds to the removal of the second term on the right-hand side of Eqs. (18). For the model of Eqs. (1) and (2), summation over Peierls diagrams alone gives the following expression:

$$f(k_y,\ l,\ \xi)=gJ_l^2(2\lambda\cos(k_y/2))[1-gJ_l^2(2\lambda\cos(k_y/2))\xi]^{-1}, \tag{45}$$

which can be found by putting (19) in place of $C^{-1}(k_y, l)$ in (20) [see Eq. (45) and, for example, Eq. (15) in Ref. 17]. Having examined expression (45), we may draw the following conclusions. First, the pole in ξ in (45) exists only for $g>0$. Second, the singularity is reached most rapidly for $k_y=\pi, l=0$, T_c in this case being independent of H; that is, the sequence of phase transitions is absent. To avoid the reduction in H-dependence, modifications of the model were studied in Ref. 15. One of these was to take account of electron hops to further stacks with $M=\pm 2$ in the Hamiltonian (1). In this case magnetic field dependence is not lost for any k_y, l, and the sequence of phase transitions can be explained. In Ref. 15 another model was proposed, which was investigated in detail in Ref. 17. In it, it was proposed that g in Eq. (45) be not a constant, but a function of k_y, such that the pole is achieved most rapidly for $k_y=0$. The dependence of g on k_y can only be connected with the interaction (2) of electrons on different stacks, which in the present work we have taken to be negligible in comparison with interaction on a single stack.

It is clear, from the analysis in the preceding sections, that in the model of Eqs. (1) and (2) neglect of the Cooper diagrams is justified only near the transition point when the system enters the moving pole regime. The existence of the pole itself for $g<0$ is guaranteed by the inclusion of the Cooper diagrams in the earlier stages of evolution. This means that in Eq. (20), in place of $C^{-1}(k_y, l)$, it is necessary to insert, not the initial conditions as in (45), but a renormalized amplitude differing strongly from (19). It is remarkable that with the Cooper pathway accounted for an explanation of the sequence of phase transitions and its connection with superconductivity can be obtained by using the extremely simplified model (1), (2) without additional complication assumptions. It is interesting that, in agreement with the table, for $g<0$ a CDW actually arises with $k_y=0$ in a broad range of values of V. The method developed in the present work allows clarification of the reason for this phenomenon (the renormalization of the interaction amplitude) in the region of its existence ($2<V<16$).

7. THE ROLE OF THE SPINS

Until now we have looked at spinless fermions. When spins are accounted for the Hamiltonian of the model (1), (2) is modified in the following way. In Eq. (1) it is necessary to add summation over the spin indices and the Zeeman term:

$$\hat{H}_s=-\mu_B H\sum_{N,\alpha,\sigma}\int dx\sigma\hat{\psi}^+(x,N,\alpha,\sigma)\hat{\psi}(x,N,\alpha,\sigma), \tag{46}$$

where $\sigma=\pm$ is the spin index. The interaction Hamiltonian (2) will have the form

$$\hat{H}_{int}=\sum_{N,\sigma_1,\sigma_2,\sigma_3,\sigma_4}\int dx\, G(\sigma_1,\sigma_2,\sigma_3,\sigma_4)\hat{\psi}^+(x,N,+,\sigma_1)$$

$$\times\hat{\psi}^+(x,N,-,\sigma_2)\hat{\psi}(x,N,-,\sigma_3)\hat{\psi}(x,N,+,\sigma_4), \tag{47}$$

$$G(\sigma_1,\ \sigma_2,\ \sigma_3,\ \sigma_4)=(-g_1\delta_{\sigma_1,\sigma_3}\delta_{\sigma_2,\sigma_4}+g_2\delta_{\sigma_1,\sigma_4}\delta_{\sigma_2,\sigma_3})2\pi\hbar v. \tag{48}$$

We introduce new variables $\hat{\psi}'(x, N, \alpha, \sigma)$ so that the Zeeman term can be included in $\hat{H}_0$:

$$\hat{\psi}(x,\ N,\ \alpha,\ \sigma)=\hat{\psi}'(x,\ N,\ \alpha,\ \sigma)\exp[i\alpha\sigma q_s x],\ q_s=\mu_B H/\hbar v. \tag{49}$$

In the $\hat{\psi}'$-representation the Hamiltonian H_0 has the previous form (1) (except for the summation over spin indices). The interaction Hamiltonian $\hat{H}_{\text{int}}$ has the form (47), where the scattering amplitudes are equal to

$$\begin{aligned}G_a&=G(+,+,+,+)=G(-,-,-,-)=(g_2-g_1)2\pi\hbar v,\\ G_b&=G(+,-,-,+)=G(-,+,+,-)=g_2 2\pi\hbar v,\\ G_c&=G(+,-,+,-)=G(-,+,-,+)\\ &=-g_1 2\pi\hbar v\exp(-4iq_s x).\end{aligned} \tag{50}$$

Since $\hat{H}_0$ is of the form (1), it is possible to transform to the basis (6). In this representation the interaction Hamiltonian H_{int} will be of the form (8), (9) with the spin structure of (47) and (50). Since the interaction G_c of Eq. (50) has an oscillatory coefficient it does not conserve the longitudinal momentum k_x in Eq. (8). Thus the logarithmic divergence of this vertex is cut off at an energy $\sim 4\Omega_s=4\hbar v q_s=4\mu_B H$. For $T\ll 4\Omega_s$ this vertex can be neglected. We shall show that in the $(TMTSF)_2X$ compounds the Zeeman energy cutoff $4\Omega_s$ and the orbital $\Omega=ebHv/c$ of (10) are of the same order of magnitude and must therefore be considered simultaneously. In fact, using the standard formula $v=a_0 t_a/\sqrt{2}\hbar$ and inserting the parameters for the $(TMTSF)_2X$ compounds $t_a=0.25$ eV, $a_0=7.3$ A and $b=7.7$ A, we get

$$4\Omega_s/H=2.7\ \text{K/T},\quad \Omega/H=1.8\ \text{K/T}. \tag{51}$$

Thus, in the energy region

$$T\ll 4\Omega_s,\ \Omega \tag{52}$$

it is only necessary to take account of the scattering amplitudes G_a and G_b. When account is taken of the selection rules described the interaction Hamiltonian (13) will have the form

$$\hat{H}_{int}=-\sum_{n,m,l}\sum_{i=\text{I}}^{\text{IV}}G_i(m,l)\hat{O}_i^+(x,n+m,l)\hat{O}_i(x,n,l), \tag{53}$$

where

$$\hat{O}_{\rm I}(x,n,l)=\hat{a}'^{+}(x,n+l,-,+)\hat{a}'(x,n,+,+),$$
$$\hat{O}_{\rm II}(x,n,l)=\hat{a}'^{+}(x,n+l,-,-)\hat{a}'(x,n,+,-),$$
$$\hat{O}_{\rm III}(\ldots)=\hat{a}'^{+}(\ldots,-)\hat{a}'(\ldots,+),$$
$$\hat{O}_{\rm IV}(\ldots)=\hat{a}'^{+}(\ldots,+)\hat{a}'(\ldots,-). \qquad (54)$$

To find the RG equations for the vertices $G_i(n,l,\xi)/2\pi\hbar v$, we must put on the lines of Fig. 1 spin indices, in all the possible ways consistent with the constraints on the spin structure of the vertices. It is found that the RG equations for the vertices $\Gamma_i(n,l,\xi)$ with different i are independent and have the form (16) for each i = I, II, III, IV. The lack of cross-terms in i in the RG equations is connected, aside from the Zeeman splitting, with the fact that in the Hamiltonian (53) there are no terms of the type $\hat{O}_{\rm III}+\hat{O}_{\rm IV}$ and $\hat{O}_{\rm IV}+\hat{O}_{\rm III}$. Such terms are permitted by the momentum conservation law. However, they are absent in (47) due to the spin conservation rule, and do not arise in the renormalization process.

The initial conditions for Eqs. (16) have the form (17), where in place of G we must put, according to (50) and (54), G_a for i = I, II and G_b for i = III, IV. In the expression (50), for g_1 and g_2 we must take the values $g_1(0)=g_1(\xi)|_{\xi=0}$ and $g_2(0)=g_2(\xi)|_{\xi=0}$ appropriate to the energy Ω. [We recall that $\xi=\ln(\Omega/T)$.] They can be found from the starting vertices $g_1(-\ln(\varepsilon_0/\Omega))$, $g_2(-\ln(\varepsilon_0/\Omega))$ determined on the molecular scale ε_0, with the aid of renormalization in the energy interval (Ω,ε_0). The RG equations in this interval have the purely one-dimensional form[1)]:[30]

$$dg_1(\xi)/d\xi=-2g_1^2(\xi),\quad d[g_1(\xi)-2g_2(\xi)]/d\xi=0. \qquad (55)$$

According to Refs. 25 and 33, in the compounds considered[2)]

$$g_1(\xi)>0,\quad 2g_2(\xi)-g_1(\xi)<0. \qquad (56)$$

Due to Eqs. (55) and (56), $g_1(\xi)$ dies off as ξ increases; thus the renormalized value $g_1(0)>0$ is small, and $g_2(0)<0$. Putting these inequalities into (50), we see that

$$G_a<0,\quad G_b<0,\quad |G_a|>|G_b|. \qquad (57)$$

So, when the Zeeman energy is accounted for in the spin case, two types of electron-hole instabilities are possible: pairing with parallel spins (order parameters $Y^{(\rm I)}=\langle\hat{O}_{\rm I}\rangle$ and $Y^{(\rm II)}=\langle\hat{O}_{\rm II}\rangle$) and with antiparallel spins (order parameters $T^{(\rm III)}=\langle\hat{O}_{\rm III}\rangle$ and $Y^{(\rm IV)}=\langle\hat{O}_{\rm IV}\rangle$). The RG equations for each type of pairing are independent and agree with Eqs. (16) for spinless fermions when in the initial conditions (17) of G is replaced by G_a or G_b respectively. Since $G_a<0$ and $G_b<0$, the sequence of phase transitions with magnetic field described in Sec. 5 can be observed for both types of ordering. However, since $|G_a|>|G_b|$, pairing with parallel spins occurs at a higher temperature.

Let us calculate the modulation of charge density ρ and spin $\mathbf{s}$ corresponding to the different order parameters:

$$\begin{pmatrix}\rho(x,N)\\ \mathbf{s}(x,N)\end{pmatrix}=\sum_{\alpha,\sigma,\sigma'}\begin{pmatrix}\delta_{\sigma,\sigma'}\\ \tau_{\sigma,\sigma'}\end{pmatrix}\langle\hat{\psi}^{+}(x,N,-\alpha,\sigma)\hat{\psi}(x,N,\alpha,\sigma')\rangle\exp(2i\alpha k_F x), \qquad (58)$$

where $\tau_{\sigma,\sigma'}$ are the Pauli matrices. Returning in (54) to the original operators $\hat{\psi}$ of (49) and using Eq. (28), it is not difficult to find that for pairing with parallel spins

$$\left.\begin{matrix}\rho(x,N)\\ s_z(x,N)\end{matrix}\right\}=\{Y^{(\rm I)}_{k_0,l_0}\exp[i(2k_F+l_0q+2q_s)x+ik_0N]$$
$$\pm Y^{(\rm II)}_{k_0,l_0}\exp[i(2k_F+l_0q-2q_s)x$$
$$+ik_0N]\}F(k_0,l_0,\lambda)+\text{comp. conj.},\qquad s_x=s_y=0, \qquad (59)$$

where $F(k_0,l_0,\lambda)$ is given by Eq. (29). Thus, in this case a modulation of both charge and spin arises. Both spin and charge are modulated along the stack (the x-axis) with two different spatial frequencies, differing in $4q_s=4\mu_B H/\hbar v$. We see that pairing with parallel spins is associated with features of both a CDW and an SDW. This would make it possible to measure the wave vector of the charge modulation with the aid of x-ray or unpolarized neutron scattering. From an experimental point of view, this is easier than measuring the wave vector of a spin modulation. A characteristic feature of this wave should be the line doublet, the distance between the x-components of which grows in proportion to H within the boundaries of one region of the phase diagram with fixed k_0 and l_0. Moreover, the spin modulation will give rise to an inhomogeneity of the local magnetic field, leading to an inhomogeneous broadening of the NMR linewidth. This very effect is used in experimental investigations to identify SDW formation in a magnetic field.[3)]

Since the difference in G_a and G_b is not great, due to the small magnitude of $g_1(0)$, it cannot be ruled out that ordering with antiparallel spins may be favorable for some reason. In this case

$$\begin{pmatrix}s_x(x,N)\\ s_y(x,N)\end{pmatrix}=\begin{pmatrix}1\\ i\end{pmatrix}(Y^{(\rm III)}_{k_0,l_0}\pm Y^{(\rm IV)}_{k_0,l_0})\exp[i(2k_F+l_0q)x$$
$$+ik_0N]F(k_0,l_0,\lambda)+\text{comp. conj.},\qquad \rho=s_z=0. \qquad (60)$$

We see that charge modulation is absent, and the spin vector lies in the plane perpendicular to H.

8. CONCLUSIONS

In the present work we have analyzed the model (1), (2) of a layered quasi-one-dimensional metal in a magnetic field **H** perpendicular to the layer. It has been shown that the behavior of the system depends strongly on the sign of the interaction g. For $g>0$ and $H=0$ a CDW with a fully nested wave vector forms. As H increases, the type of CDW does not change; the transition temperature decreases and tends to zero as $H\to\infty$ according to Eq. (38). For $g<0$, the system exhibits superconductivity for $H=0$. A sufficiently strong magnetic field [fulfilling condition (12)] induces a CDW. As H increases, a series of phase transitions occurs in the system between different types of CDW. The type of CDW is determined by its wave vector, the longitudinal component of which takes on the quantized values given by Eq. (31). The dependence of the type of CDW on magnetic field is presented in the table. In accordance with Eq. (44), the transitions occur approximately periodically in $1/H$. For $H\geqslant 4tc/ebv$ a CDW is established with electron-hole pairing on neighboring ($l_0=\pm 1$) Wannier stacks. For further increase in H the type of CDW does not change, and the transition temperature tends to zero for $H\to\infty$ (Eq. 38). The re-

gion of applicability of the theory is limited by the condition $|g| \ll 1$ (Eq. 33).

The generalization of model (1), (2) for fermions with spin has also been investigated. In this model two types of electron-hole pairings are possible: with parallel and antiparallel spins. In the first case a modulation of spin and charge arises along the stack with two different spatial frequencies differing by $4\mu_B H/\hbar v$. In the second case only a spin modulation with a single frequency occurs. When Zeeman splitting is accounted for, both types of instability are described by the same parquet equations as the instability in the spinless-fermion model of Eqs. (1), (2). With a choice of signs of the microscopic constants appropriate to the $(TMTSF)_2X$ compounds, parallel-spin pairing occurs at higher temperatures.

We now discuss the connection of the proposed theory with experiment. We note again that in all three materials in which the sequence of phase transitions is observed [$X = PF_6$ (Refs. 3, 11, 12); $X = ClO_4$ (Ref. 1); $X = ReO_4$ (Ref. 7)] a superconducting state exists for zero magnetic field. These facts are in complete agreement with the conclusions of our theory. We also note that the negative slope of the $T_c(H)$ curve predicted by the theory [Eq. (38)] for large H has been observed for $H \sim 25$ T in resistivity measurements.[34] According to the theory developed above, this means that in fields $H > 25$ T the compound $(TMTSF)_2ClO_4$ goes into the metallic phase. It would be interesting to experimentally verify this assertion with the aid of appropriate methods, for instance by NMR. For a final verification of the theory it is necessary to carry out measurements of the H-dependence of the SDW wave vector and compare with the results of the table in Sec. 5. Comparing Eq. (44) with the experimental value $H_0 = 76$ T for $(TMTSF)_2PF_6$ (Ref. 4) and using the values of v and b cited in Sec. 7, we find $t = t_a/58 = 4.3$ meV.

In contrast to $(TMTSF)_2PF_6$, in $(TMTSF)_2ClO_4$ (Refs. 7, 35, 36) and $(TMTSF)_2ReO_4$ (Ref. 7) there are, besides the sequence of phase transitions (the so-called slow oscillations), also small oscillations in the magnetoresistance. They are periodic in H^{-1} with a high frequency H_f and are called the "fast oscillations": $\Delta(1/H) = 1/H_f$. The theory discussed in this article describes the slow oscillations. To explain the second type of oscillations we need to introduce an additional physical parameter into the model. Brazovskiĭ and the author proposed a theory in Ref. 26 according to which the fast oscillations arise due to a difference in the energy $\varkappa$ of neighboring stacks.[3)] This difference is linked to the doubling of the crystalline lattice period of $(TMTSF)_2ClO_4$ in the direction perpendicular to the stacks due to ordering of the ClO_4 anions (see details in Refs. 37 and 25). According to the theory,[25] which explains the insulating, superconducting and magnetic aspects of the $(TMTSF)_2X$ compounds from a unified viewpoint, the inequality $\varkappa \gg t$ applies. Therefore the energy spectrum is split into two sub-bands with transverse width $4t^2/\varkappa$. The theory discussed in the present article applies to electron-hole pairing in the same sub-band, if we replace the transfer integral t in Eq. (1) by an effective value:

$$t^* = t^2/\varkappa, \quad b^* = 2b. \tag{61}$$

The fast oscillations arise because of a small interband interaction. A detailed analysis of this model will be discussed in a separate article. We will only give the values of the experimental parameters here. From Eqs. (44) and (61) we find that the frequency of the slow oscillations is equal to $H_s \approx 4t^2 c/3\varkappa ebv$; according to Ref. 26, $H_f = \varkappa c/2ebv$. Substituting in these formulas the experimental values for $(TMTSF)_2ClO_4$ (Ref. 8), $H_s \approx 23$ T and $H_f = 275$ T, and using the values of v and b cited in Sec. 7, we find $\varkappa = 83$ meV, $t = 15$ meV, $t^* = 2.6$ meV and $\varkappa/t = 5.7$.

Let us examine whether the conditions of applicability of the theory in Eqs. (12) and (33) are satisfied in real materials. The observed phenomena lie in the range $H \sim 4$–10 T. These fields correspond, according to Eq. (51), to characteristic energies $\Omega \sim 7$–18 K. The transition temperatures are 1 K for superconductivity and 1.4 K for the SDW in a magnetic field. Obviously condition (12) is fulfilled, although $\ln(\Omega/T)$ is not too large. This means that the interactions in the system are not very small. One may expect, however, that the theory discussed here for small $|g|$ will remain qualitatively valid for large $|g|$.

In this work we have not investigated the influence of the hopping amplitude $t_\parallel = t_c$ along the magnetic field on the system's behavior. In Ref. 17, t_c is used to find H_{thr} (see the Introduction). Within the parquet approach, taking account of $t_\parallel$ leads to the separation for $\omega < t_\parallel$ of the Peierls and Cooper channels.[29] In the region $\omega < t_\parallel$ they can be considered independent. The limiting case of large transfer along the magnetic field was discussed in Ref. 38, where only Cooper diagrams were summed. It was shown that at low temperatures superconductivity is not destroyed, no matter how large the magnetic field. Such a situation can in principle be observed experimentally when the magnetic field is directed along the **b**-axis.

The author thanks S. A. Brazovskiĭ for the continuing interest in this work and numerous discussions; L. N. Shchur for help in computational work; and L. P. Gor'kov, I. E. Dzyaloshinskiĭ, A. G. Lebed', V. L. Pokrovskiĭ and D. E. Khmel'nitskiĭ for useful discussions.

APPENDIX A

In this appendix Eqs. (18) are solved without the first term on the right-hand side. It is convenient to do a Fourier transform in the second argument and go to Eqs. (40). We perform a charge of arguments:

$$h(k, q, \xi) = L(k+g, k-q, \xi). \tag{A1}$$

Then Eqs. (40), without the first term on the right-hand side, will have the form

$$dL(k_1, k_2, \xi)/d\xi = -\int_{-\pi}^{\pi} \frac{dk}{2\pi} L(k_1, k, \xi) L(k, k_2, \xi). \tag{A2}$$

We now expand the integral kernel $L(k_1, k_2, \xi)$ in its eigenfunctions:

$$\int_{-\pi}^{\pi} \frac{dk}{2\pi} L(k_1, k_2, \xi) \varphi_n(k_2, \xi) = \lambda_n(\xi) \varphi_n(k_1, \xi), \tag{A3}$$

$$L(k_1, k_2, \xi) = \sum_n \lambda_n(\xi) \varphi_n(k_1, \xi) \varphi_n(k_2, \xi). \tag{A4}$$

The spectrum of Eq. (A3) is necessarily discrete, the inte-

gration having been carried out in a finite interval. Substituting (A4) in (A2), we get

$$\frac{d}{d\xi}\sum_n \lambda_n(\xi)\varphi_n(k_1,\xi)\varphi_n(k_2,\xi)$$

$$=-\sum_n \lambda_n^2(\xi)\varphi_n(k_1,\xi)\varphi_n(k_2,\xi). \quad (A5)$$

Equations (A5) have a solution of the following form: only the eigenvalues $\lambda_n(\xi)$, but not the eigenfunctions $\varphi_n(k, \xi)=\varphi_n(k)$, depend on ξ:

$$d\lambda_n(\xi)/d\xi=-\lambda_n^2(\xi),\ \lambda_n(\xi)=(\Lambda_n^{-1}+\xi)^{-1}, \quad (A6)$$

$$L(k_1,k_2,\xi)=\sum_n \varphi_n(k_1)\varphi_n(k_2)(\Lambda_n^{-1}+\xi)^{-1}. \quad (A7)$$

The parameters Λ_n and the eigenfunctions $\varphi_n(k)$ must be found from Eqs. (A3) with the initial kernel $L(k_1, k_2, 0)$, which, according to (41) and (A1) has the form

$$L(k_1,k_2,0)=gJ_0(2\lambda[\sin(k_1/2)-\sin(k_2/2)]). \quad (A8)$$

For $g<0$ we expect that at least some of the eigenvalues will have $\Lambda_n<0$. Then in (A7) we will have a singularity in ξ, which is determined by the negative eigenvalue Λ_0 with the largest absolute value. Near the singularity

$$L(k_1,k_2,\xi)\approx-\varphi_0(k_1)\varphi_0(k_2)/\tau,\quad \tau=|\Lambda_0|-\xi. \quad (A9)$$

In contrast with Eq. (22), in the denominator of (A9) there is no dependence on the continuous parameters k_1, or k_2, therefore such a solution is called a "stationary pole." By performing the inverse transformation in k_1 and k_2 we get the expression (24).

APPENDIX B

In this appendix a set of exact expressions relevant to the system of Eqs. (18) is collected. We introduce the two-dimensional vector $\rho=(k_y, l)$ and the vector product of $\rho_1=(k_1, l)$ and $\rho_2=(k_2, l)$:

$$[\rho_1\rho_2]\equiv k_1l_2-k_2l_1,\qquad \sum_\rho \equiv \sum_l \int_{-\pi}^{\pi}\frac{dk_y}{2\pi}.$$

Then Eqs. (18) can be written in the form

$$df(\rho,\xi)/d\xi=f^2(\rho,\xi)-\sum_{\rho_1,\rho_2} f(\rho_1,\xi)f(\rho_2,\xi)$$

$$\times\exp\{i[\rho(\rho_2-\rho_1)]-i[\rho_1\rho_2]\}. \quad (B1)$$

1. The system (B1) of differential equations has the integral of motion

$$I(\xi)=\sum_\rho f(\rho,\xi),\qquad dI(\xi)/d\xi=0. \quad (B2)$$

The expression (B2) was used to monitor the accuracy of the numerical solution of Eqs. (B1) (Sec. 5). In the final stages of evolution the deviation of $I(\xi)$ from the initial value $I(0)$ was less than 10%.

2. The system (B1) can be rewritten in the form of equations of dissipative dynamics:

$$\frac{df(\rho,\xi)}{d\xi}=\frac{1}{3}\frac{\delta S}{\delta f(\rho,\xi)}, \quad (B3)$$

where the functional S has the form

$$S=\sum_\rho f^3(\rho,\xi)-\sum_{\rho_1\rho_2\rho_3}\exp\{-i([\rho_1\rho_2]+[\rho_2\rho_3]$$

$$+[\rho_3\rho_1])\}f(\rho_1,\xi)f(\rho_2,\xi)f(\rho_3,\xi). \quad (B4)$$

Due to Eq. (B3) the functional S grows monotonically with evolution time:

$$\frac{dS}{d\xi}=\sum_\rho\frac{df(\rho,\xi)}{d\xi}\frac{\delta S}{\delta f(\rho,\xi)}=\frac{1}{3}\sum_\rho\left(\frac{\delta S}{\delta f(\rho,\xi)}\right)^2\geqslant 0. \quad (B5)$$

The existence of such a function for the RG equations of two-dimensional field-theory models was proven in a general form by Zamolodchikov.[39]

3. Let us examine the functional

$$R=\sum_\rho f^2(\rho,\xi)\geqslant 0. \quad (B6)$$

It is easy to verify that, in accordance with (B1), (B4), and (B5),

$$\frac{dR}{d\xi}=2\sum_\rho f(\rho,\xi)\frac{df(\rho,\xi)}{d\xi}=2S,\qquad \frac{d^2R}{d\xi^2}\geqslant 0. \quad (B7)$$

[1)] As in Sec. 2, we will neglect renormalization in the energy interval (Ω, t) for $\Omega<t$, assuming condition (11) to be satisfied.

[2)] Formula (93) of Ref. 25 contains a misprint. In the expression mentioned it is necessary to take the opposite sign of the inequality.

[3)] In Ref. 17 the fast oscillations are connected with the transfer of electrons between stacks within a layer, and the slow oscillations with transfer between layers (along the **c**-axis).

[1] D. Jerome and H. J. Schulz, Adv. Phys. **31**, 239 (1982).
[2] L. P. Gor'kov, Usp. Fiz. Nauk **144**, 380 (1984) [Sov. Phys. Usp. **27**, 809 (1985)].
[3] T. Takahashi, D. Jerome, and K. Bechgaard, J. de Phys. **45**, 945 (1984).
[4] J. F. Kwak, J. E. Schirber, R. L. Greene, and E. M. Engler, Phys. Rev. Lett. **46**, 1296 (1981).
[5] K. Kajimura, H. Tokumoto, M. Tokumoto *et al.*, Sol. St. Comm. **44**, 1573 (1982).
[6] G. Greuzet, J. R. Cooper, F. Greuzet *et al.*, J. de Phys. Lett. **46**, L1133 (1985).
[7] H. Schwenk, S. S. P. Parkin, R. Schumaker *et al.*, Phys. Rev. Lett. **56**, 667 (1986).
[8] P. M. Chaikin, M. Y. Choi, J. F. Kwak *et al.*, Phys. Rev. Lett. **51**, 2333 (1983).
[9] M. Ribault, D. Jerome, J. Tuchendler *et al.*, J. de Phys. Lett. **44**, L953 (1983).
[10] M. Ribault, J. R. Cooper, D. Jerome *et al.*, J. de Phys. Lett. **45**, L935 (1984).
[11] J. F. Kwak, J. E. Schirber, P. M. Chaikin *et al.*, Phys. Rev. Lett. **56**, 972 (1986).
[12] B. Piveteau, L. Brossard, F. Creuzet *et al.*, J. Phys. C **19**, 4483 (1986).
[13] M. J. Naughton, J. S. Brooks, L. Y. Chiang *et al.*, Phys. Rev. Lett. **55**, 969 (1985).
[14] F. Pesty, P. Garoche, and K. Bechgaard, Phys. Rev. Lett. **55**, 2495 (1985).
[15] L.P. Gor'kov and A. G. Lebed', J. de Phys. Lett. **45**, L433 (1984).
[16] L. P. Gor'kov and A. G. Lebed', Mol. Cryst. Liq. Cryst. **119**, 73 (1985).
[17] A. G. Lebed', Zh. Eksp. Teor. Fiz. **89**, 1034 (1985) [Sov. Phys. JETP **62**, 595 (1985)].
[18] A. G. Lebed', Pis'ma Zh. Eksp. Teor. Fiz. **43**, 137 (1986) [JETP Lett. **43**, 174 (1986)].
[19] M. Heritier, G. Montambaux, and P. Lederer, J. de Phys. Lett. **45**, L943 (1984) and **46**, L831 (1985); Phys. Rev. Lett. **55**, 2078 (1985); J. Phys. C **19**, L293 (1986).
[20] P. M. Chaikin, Phys. Rev. B **31**, 4770 (1985).
[21] D. Poilblanc, M. Heritier, G. Montambaux, and P. Lederer, J. Phys. C **19**, L321 (1986); K. Maki, Phys. Rev. B **33**, 4826 (1986).
[22] Yu. A. Bychkov, L. P. Gor'kov, and I. E. Dzyaloshinskiĭ, Zh. Eksp. Teor. Fiz. **50**, 738 (1966) [Sov. Phys. JETP **23**, 489 (1966)].

[23]L. P. Gor'kov and I. E. Dzyaloshinskiĭ, Zh. Eksp. Teor. Fiz. **67**, 397 (1974) [Sov. Phys. JETP **40**, 198 (1975)].
[24]S. A. Brazovskiĭ, Zh. Eksp. Teor. Fiz. **61**, 2401 (1971) [Sov. Phys. JETP **34**, 1286 (1972)].
[25]S. A. Brazovskiĭ and V. M. Yakovenko, Zh. Eksp. Teor. Fiz. **89**, 2318 (1985) [Sov. Phys. JETP **62**, 1340 (1985)].
[26]S. A. Brazovskiĭ and V. M. Yakovenko, Pis'ma Zh. Eksp. Teor. Fiz. **43**, 102 (1986) [JETP Lett. **43**, 134 (1986)].
[27]S. P. Obukhov, Zh. Eksp. Teor. Fiz. **72**, 1051 (1977) [Sov. Phys. JETP **45**, 550 (1977)].
[28]Yu. A. Firsov, V. N. Prigodin, and C. Seidel, Phys. Rep. **126**, 245 (1985).
[29]V. N. Prigodin and Yu. A. Firsov, Zh. Eksp. Teor. Fiz. **76**, 736 (1979) [Sov. Phys. JETP **49**, 369 (1979)].
[30]I. E. Dzyaloshinskiĭ and A. I. Larkin, Zh. Eksp. Teor. Fiz. **61**, 791 (1971) [Sov. Phys. JETP **34**, 422 (1972)].
[31]S. A. Brazovskiĭ, doctoral dissertation in physical-material sciences, Chernogolovka: L. D. Landau Institute of Theoretical Physics, 1972.
[32]N. Menyhard, J. Phys. C **11**, 2209 (1978).
[33]C. Seidel and V. N. Prigodin, J. de Phys. Lett. **44**, L403 (1983).
[34]T. Osada, N. Miura, and G. Saito, Sol. St. Comm. **60**, 441 (1986).
[35]H. Bando, K. Oshima, M. Suzuki *et al.*, J. Phys. Soc. Jpn. **51**, 2711 (1982).
[36]J. P. Ulmet, A. Khmou, P. Auban, and L. Bachere, Sol. St. Comm. **58**, 753 (1986).
[37]R. Moret, J. P. Pouget, R. Comes, and K. Bechgaard, J. de Phys. **46**, 1521 (1985).
[38]A. G. Lebed', Pis'ma Zh. Eksp. Teor. Fiz. **44**, 89 (1986) [JETP Lett. **44**, 114 (1986)].
[39]A. B. Zamolodchikov, Pis'ma Zh. Eksp. Teor. Fiz. **43**, 565 (1986) [JETP Lett. **43**, 730 (1986)].

Translated by I. A. Howard