# On the theory of organic superconducting materials

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We construct a theory of quasi-one-dimensional superconducting materials starting from a gapless model for weak tunneling of electrons between chains. We find for conservation of coherence (CCC) of Cooper or electron-hole  $2k_F$  pairs for interchain tunneling the conditions which are necessary for the formation of superconducting or dielectric states, respectively. The CCC depend on the symmetry of the crystal and on the external fields. Commensurability effects produce CCC for  $2k_F$  pairs. Essentially new effects are the occurrence of CCC for Cooper pairs when the equivalence of neighboring chains is violated and for  $2k_F$  pairs when the magnetic field is strong. These effects are caused by the mechanism, determined in this paper, of pair attraction in jump transfers under conditions of gradient phase shifts between the wave functions of electrons on different chains. The theory developed here enables us to describe the phase diagram of organic superconducting compounds (Bechgaard salts) in such a way that the sequences of electron states are mainly determined by the changes in the anion superstructure. We consider the thermodynamics of the superconducting phase.

#### **I. INTRODUCTION**

Recently the quasi-one-dimensional organic conducting compounds  $M_2X$ , where M is a TMTSF or a TMTTF molecule and X various monovalent anions (PF<sub>6</sub>, ClO<sub>4</sub>, Br, and so on) have been studied intensively. These materials display an extraordinarily rich set of electron states in conjunction with various kinds of structural ordering of the anions. The following are observed: normal and dielectric phases, a Peierls-type dielectric (with charge density waves-CDW), an antiferromagnetic dielectric (apparently with spin density waves-SDW), a paramagnetic dielectric phase without magnetic ordering, an unusual semimetal phase with an antiferromagnetic ordering arising only following superconductivity in strong magnetic fields and, finally, the superconducting phase itself (a singlet-SS-or, possibly, a triplet-TS-phase). The present state of the experimental data and of the theoretical ideas is reflected in review articles<sup>1-3</sup> and in the proceedings of recent conferences.4,5

The study of these materials was stimulated by their specific properties: superconductivity and intrinsic antiferromagnetic effects. At the same time old unsolved problems, typical for an entire class of organic metals, were also accentuated by this study. Among those problems are the competition between the band picture with lattice  $2k_F$ -deformations (Peierls effect) and the picture of strong interelectron interaction with Mott-Hubbard effects, the relation between quasi-one-dimensional and three-dimensional regimes, and many others. The interrelation between theoretical and experimental studies of organic conductors remains up to the present necessarily eclectic. Whereas the basic phenomena in other classes of quasi-one-dimensional compounds are qualitatively described on the basis of different variants of the Peierls-Fröhlich model, it has so far not been possible to formulate a general picture for the class of organic conductors. For instance, to get agreement between the theory of one-dimensional models with the observed properties (see Ref. 1), it has been proposed that a qualitative change of the basic electron-electron interactions take place when secondary parameters (pressure, replacement of selenium in TMTSF by sulphur in TMTTF, and the kind of anion X) are altered.

The band theory based upon a model of strongly anisotropic metal with open Fermi surfaces satisfactorily describes many properties.<sup>2,3</sup> One should mention especially the successful explanation<sup>2</sup> of the oscillations of the magneto-resistance in strong magnetic fields. However, there are several phenomena which this theory cannot explain as a matter of principle including, in particular, phenomena which are characteristic for the whole class of organic metals, such as the paramagnetic dielectric phase and the hightemperature  $2k_F$  anomaly. In the band theory there remain unexplained also the strong magnetic field dependences of the resistivity and of the tunneling and optical spectra (see Refs. 1 and 2 and also D. Jerome's paper in Ref. 5) at temperatures higher than the superconducting transition temperature by an order of magnitude.

The as yet unsolved contradictions between the different theories of organic conductors indicate that the usual set of data for a selected form of a single substance is insufficient to identify the model. We show in the present paper that a change in the structure of the anion subsystem exerts a unique and controlled influence on a subsystem of conducting molecular stacks. The symmetry of the anion subsystem in that case determines uniquely the electron state of the system.

As a result we can formulate a general model to describe at least a selected group of compounds. We assume that for the electron states there exists a general phase diagram whose details are mainly determined by a change in the symmetries of the crystal due to the anion ordering or to the effect of external fields.

The particular significance of the action of ion potentials on conducting chains in materials with a total charge transfer was formulated as an effect of weak twofold<sup>6</sup> commensurability for Peierls-type systems and as the effect of a weak single commensurability<sup>7</sup> for systems with dimerized monovalent or bivalent ions (see also the formulation of transitional models in Ref. 8). These effects were studied in experiments on platinum complexes as "non-Peierls superstructures".<sup>9</sup> An attempt to apply the idea of weak twofold commensurability to explain the properties of  $(TMTSF)_2X$ was undertaken at the very beginning of the study of these materials in Ref. 10 and developed in more detail in Ref. 11.

The structure of the present paper is the following one. We give the necessary information about the theory of onedimensional systems in Section 2. In Section 3 we study the structure of the perturbation-theory series with respect to interchain tunneling of electrons. For systems with a simple crystalline symmetry we shall distinguish two regimes, one of which leads to the band picture for an anisotropic Fermi liquid, and the other to an essentially one-dimensional regime characterized by the coherent tunneling of electron or electron-hole pairs. We shall consider in Section 4 the same problems for systems with a symmetry lowered by the effects of a weak twofold commensurability, incommensurability between neighboring chains, an external magnetic field, or internal slowly changing random potentials. We shall show that these effects reduce the coherence of either the exciton, or the magnon, or the Cooper pairs in the process of tunneling between the chains. This conclusion is the main methodical result of the present paper. We derive in Section 5 the Ginzburg-Landau functional for the superconducting phase in a system with incommensurability between neighboring chains and we find the form of the anomalous Green function near the transition point. We suggest in Section 6 an empirical classification of the observed states in M<sub>2</sub>X compounds according to the type of their lattice symmetry. We shall on the basis of the results of Sections 3 and 4 give a microscopic explanation of the phase diagram of the electron states for these materials. We shall also compare the results of the theory of Section 5 with experimental data about the thermodynamic properties and critical magnetic fields for superconductivity for  $M_2X$  compounds.

The main results of the present paper were briefly expounded in Ref. 12 and in conference proceedings.<sup>5</sup>

#### 2. CHOICE OF MODEL

We shall consider quasi-one-dimensional systems, assuming that the following two interactions are sufficiently weak: the integrals  $t_1$  of the interchain tunneling and the backward scattering amplitude  $g_1$  for electrons in different chains.<sup>1)</sup>

The interactions on a single chain and also, apparently, the three-dimensional long-range (Coulomb and deformation) forces do not have to be assumed to be small (as compared to the total bandwidth W) in the substances considered. We should therefore choose the most suitable description for the initial approximation:  $t_{\perp} = 0$ ,  $g_{\perp} = 0$ . The present-day picture of one-dimensional models is built up from the results of a whole number of approaches. These various points of view (see Ref. 15) are the summation of "parquet" diagrams for weak interactions,<sup>16,17</sup> the complete summation for models with long-range forces,<sup>18</sup> the strong attraction approximation,<sup>19</sup> the strong repulsion approximation,<sup>20</sup> and the retardation approximation.<sup>21</sup> A special place is occupied by the "bosonization" method<sup>22</sup> (see the review article, Ref. 23) which reproduces nearly the whole set of results of other approaches. When one makes a natural generalization of the type used in Ref. 19 and includes three-dimensional long-range forces,<sup>24</sup> the bosonization method gives us the most adequate approach to the systems considered.

The following basic results have been established for the low-temperature properties of the one-dimensional models:

1) A separation of the c and s channels connected with the excitations of the charge (c) and spin (s) degrees of freedom.

2) The acoustic nature of the c and s spectra or the formation of gaps in the s channel (in the case of an effective attraction)<sup>16,19,21,23,25</sup> and/or in the c channel (in the case of an effective repulsion for a half-filled band).<sup>17,20,23,25</sup> For instance, in the model of weakly interacting fermions, which has been named g-ology (see Ref. 25) the conditions for the formation of gaps have the form: in the spin channel  $g_1 < 0$ , in the charge channel  $|g_3| + 2g_2 - g_1 > 0$ . Here  $g_1, g_2, g_3$  are the backward, forward, and umklapp-including scattering amplitudes of the fermions.

3) The power-law behavior (at T = 0) of all or, when there are gaps present, several correlation functions.<sup>18–23</sup>

We introduce a complex coordinate  $z = x + iv_F \tau$  where x is the coordinate along the chain, and  $\tau$  the Matsubara time; we use a system of units in which  $\hbar = 1$ ,  $v_F = 1$ , a = 1,  $W \sim 1$ , where a is the period of the crystal along the chain and W the width of the conduction band. To simplify the problem we shall also assume that the speeds of ordinary and spin sounds are the same and equal to  $v_F$ . For what follows we need an expression for the two-particle correlation function of the one-dimensional electrons, in the form<sup>23</sup>

$$K_{\sigma,\sigma'}^{(0)}(z_1, z_2, z_3, z_4) = \langle \psi_{\sigma,+}(z_1) \psi_{\sigma',-}(z_2) \psi_{\sigma,+}^+(z_3) \psi_{\sigma',-}^+(z_4) \rangle_0$$
  
=  $K_{\rho}(z_1, z_2, z_3, z_4) K_{\sigma,\sigma'}^{(\bullet)}(z_1, z_2, z_3, z_4).$  (1)

The indexes  $\pm$  indicate here electrons with momenta close to  $\pm k_F$ ;  $\sigma$  and  $\sigma'$  are spin indexes; the index zero of the averaging sign of Eq. (1) indicates that it is taken neglecting coupling between the chains. We shall consider in our paper only such systems in which there is no gap in the *s* channel and no spin anisotropy. In that case  $K_{\sigma\sigma'}^{(s)}$  contains only slowly varying logarithmic functions.<sup>17,26</sup> When there is no gap in the *c* channel the function  $K_{\rho}$  has the form<sup>23,27</sup>

$$K_{\rho}^{(1)}(z_{1}, z_{2}, z_{3}, z_{4}) = \frac{\operatorname{const} \cdot \exp[i \arg(z_{1} - z_{3}) - i \arg(z_{2} - z_{4})]}{|s(z_{1} - z_{3})s(z_{2} - z_{4})|^{\eta_{F}}} \\ \times \left| \frac{s(z_{1} - z_{4})s(z_{2} - z_{3})}{s(z_{1} - z_{2})s(z_{3} - z_{4})} \right|^{\nu}, \qquad (2)$$
$$s(z) = \begin{cases} \operatorname{sh}(\pi T z)/\pi T, & |z| \ge 1, \\ \sim 1, & |z| \sim 1. \end{cases}$$

The exponents  $\eta_F$  and  $\nu$  can be expressed in terms of the electron interaction constants for specific models. For instance, in g-ology (for the case when  $g_3 = 0$ ) we have

$$\eta_{F} = (2 + \gamma + \gamma^{-1})/4, \quad \nu = (\gamma - \gamma^{-1})/4, \gamma = \left[ \left( 1 - \frac{2g_{2} - g_{1}}{2\pi} \right) / \left( 1 + \frac{2g_{2} - g_{1}}{2\pi} \right) \right]^{\nu_{1}}.$$
(3)

In the general case when the amplitudes of the electronelectron interaction are not small and have a momentum and frequency dispersion, it is necessary to assume that  $\eta_F$  and  $\nu$ are arbitrary phenomenological constants characterizing the system considered. For non-interacting electrons

$$\eta_F = 1, \quad v = 0. \tag{4}$$

We also write down an expression for the single-particle Green function for the gapless case:

$$G_{\sigma,\pm}(z) = \langle \psi_{\sigma,\pm}(z) \psi_{\sigma,\pm}^{\dagger}(0) \rangle_{0} = \frac{\operatorname{const} \cdot \exp[\pm i(\arg z + \pi/2)]}{|s(z)|^{\operatorname{np}}}.$$
(5)

In the case of a gap in the charge channel in the region of most importance for what follows

$$\xi_{c} \ll |z_{1}-z_{4}|, \ |z_{3}-z_{2}| \ll |z_{1}-z_{3}| \approx |z_{2}-z_{4}| = |z|$$
(6)

we have the following expression<sup>24</sup>:

$$K_{\rho}^{(II)} = -\frac{\text{const} \cdot \exp(-|z_1 - z_4|/\xi_c - |z_2 - z_3|/\xi_c)}{|\xi_c|^{2\eta_F - 1} |s(z)|}, \quad (7)$$

where  $\xi_c \sim \Delta_c^{-1}$  is the correlation length,  $\Delta_c$  is the magnitude of the gap in the *c* channel, and const > 0.

We also consider a system with impurities which lead only to forward scattering. In that  $case^{28}$ 

$$K_{\rho}^{(III)}(z_{1}, z_{2}, z_{3}, z_{4}) = K_{\rho}^{(I)}(z_{1}, z_{2}, z_{3}, z_{4}) \exp\{-|x_{1}+x_{4}-x_{2}-x_{3}|/\xi_{imp}\}, \qquad (8)$$

where  $\xi_{imp}$  is the mean free path due to impurities.

As usual we introduce a set of order parameters<sup>10,25</sup>

$$O_{\rm CDW}(z) = \sum_{\sigma} \psi_{\sigma,+}^{+}(z) \psi_{\sigma,-}(z),$$

$$O_{\rm SDW}^{(j)}(z) = \sum_{\sigma,\sigma'} \psi_{\sigma,+}^{+}(z) \sigma_{\sigma,\sigma'}^{(j)} \psi_{\sigma',-}(z),$$

$$O_{\rm SS}(z) = \sum_{\sigma} \sigma \psi_{-\sigma,+}(z) \psi_{\sigma,-}(z),$$

$$O_{\rm TS}^{(j)}(z) = \sum_{\sigma,\sigma'} \sigma \psi_{-\sigma,+}(z) \sigma_{\sigma,\sigma'}^{(j)} \psi_{\sigma',-}(z),$$
(9)

where the  $\sigma_{\sigma,\sigma'}^{(j)}$  are the Pauli matrices. One can use Eq. (1) to obtain the correlation functions of these operators, by contracting appropriately pairs of points.

In the gapless case

$$K_{i}(z) = \langle O_{i}^{+}(z) O_{i}(0) \rangle_{0} = C_{i} (\ln |z|)^{e_{t}} |s(z)|^{-\eta_{t}}, \qquad (10)$$

where

$$i = \text{CDW}, \text{ SDW}: \eta_i = 2(\eta_F + \nu), \quad C_i < 0,$$
  

$$i = \text{SS}, \text{TS}: \eta_i = 2(\eta_F - \nu), \quad C_i > 0,$$
(11)

$$\varepsilon_i = \begin{cases} \frac{1}{2}, & i = \text{SDW}, \text{ TS}, \\ -\frac{3}{2}, & i = \text{CDW}, \text{ SS}. \end{cases}$$
(12)

The logarithmic factor in Eq. (10) is connected with the fact that there is no gap in the *s* channel.<sup>26</sup>

In the case of a gap in the c channel<sup>24</sup>

$$K_i(z) \propto \exp(-|z|/\xi_c), \quad |z| \gg \xi_c, \quad i=TS, SS.$$
 (13)

# 3. PHASE DIAGRAM OF SYSTEMS WITH A SIMPLE CRYSTAL SYMMETRY

We study in this section the effect of tunneling of electrons between chains on the properties of a quasi-one-dimensional system in the gapless regime. One usually assumes<sup>1,23</sup> that the phase diagram of a three-dimensional system with weakly coupled chains corresponds to the conventional phase diagram of a one-dimensional system determined when the various susceptibilities diverge:  $\chi_i^{(0)}(T) \rightarrow \infty$  as  $T \rightarrow 0$ . For the order parameters (9) we have according to (10)

$$\chi_{i}^{(0)}(T) = \int d^{2}z K_{i}(z) \propto T^{-\beta_{i}} + \text{const},$$

$$\beta_{i} = 2 - \eta_{i}, \quad \int d^{2}z = \int_{-\infty}^{+\infty} dx \int_{0}^{T-i} d\tau.$$
(14)

The divergence of  $\chi_i^{(0)}(T)$  occurs under the condition

$$\beta_i > 0. \tag{15}$$

We assume for the sake of simplicity that the chains are arranged in a rectangular lattice with periods b and c and are numbered by integer two-dimensional vectors  $\mathbf{m},\mathbf{n} = (n_b, n_c)$ . One expects that for suitable coupling between the chains

$$S_{\perp} = \sum_{i,\mathbf{m},\mathbf{n}} \int d^2 z \lambda_{\mathbf{m},\mathbf{n}}^{(i)} O_i^+(z,\mathbf{m}) O_i(z,\mathbf{n}), \quad \lambda_i = \sum_{\mathbf{m}} \lambda_{\mathbf{m},\mathbf{n}}^{(i)}, \quad (16)$$

characterized by the constants  $\lambda_i$ , the total susceptibility  $\chi_i(T)$  will diverge at a finite transition temperature  $T_c^{(i)}$ :

$$\chi_i(T) \approx \chi_i^{(0)} + \lambda_i(\chi_i^{(0)})^2 + \dots = [(\chi_i^{(0)})^{-1} - \lambda_i]^{-1}, \quad (17)$$

$$\chi_i(T_c^{(i)}) = \infty, \quad T_c^{(i)} \sim (\lambda_i)^{1/\beta_i}.$$
(18)

The last equality in (17) corresponds to the widely used (see, e.g., Refs. 1, 19) self-consistent field approximation in the interaction (16). The problem is that in all cases except i = CDW, the interaction (16) is not contained in the original action of the system. We show that condition (15) is a necessary but not sufficient condition for the susceptibility of the three-dimensional system to diverge at a finite temperature.

The coupling between the chains can be of three types. None of the constants  $\lambda_i$  is determined by the scattering with a small transfer of longitudinal momentum. It leaves all interchain correlators equal to zero<sup>24</sup> and retains for the single-chain ones the form (2), (10). The forward scattering by different chains assumes directly the form (16) for i = CDW and determines only this type of ordering (Ref. 24).<sup>21</sup> In the other cases i = SDW, SS, TS the parameters  $\lambda_i$  can arise only due to the tunneling of electrons between the chains, which is described by the action

$$S_{t} = \sum_{\sigma,\mathbf{m},\mathbf{n},\alpha} \int d^{2}z [t_{\mathbf{m}-\mathbf{n}} \psi_{\sigma,\alpha}^{+}(z,\mathbf{n}) \psi_{\sigma,\alpha}(z,\mathbf{m}) + \text{H.c.}], \quad (19)$$
$$t_{\perp}^{2} = \sum_{\mathbf{n}} t_{\mathbf{m}-\mathbf{n}}^{2}.$$

The index  $\alpha = \pm$  describes electrons with momenta  $\pm k_F$ .

We shall use perturbation theory to evaluate the effect of (19), developing in the standard way the series in powers of  $t_1$ . We consider the zeroth and first terms of the series in powers of  $t_1$  for one of the susceptibilities  $\chi_i$ . They are represented by the diagrams in Fig. 1a for i = SS, TS and in Fig. 1b for i = CDW, SDW. The shaded squares indicate two-particle correlation functions (1), the dashed lines the matrix elements  $t_{m-n}$  given in (19). In the case when there are no gaps either in the s or in the c channel, we get, using (2) and neglecting logarithmic and phase factors,

$$\chi_{i}(T) = \sum_{\mathbf{m}} \int d^{2}z \langle O_{i}^{+}(z, \mathbf{m}) O_{i}(0, \mathbf{n}) \rangle$$
  
= $\chi_{i}^{(0)}(T)$   
+ $\operatorname{const} t_{\perp}^{2} \int \frac{d^{2}z \, d^{2}u \, d^{2}v f_{i}(u, v)}{|s(u-v)|^{2r_{i}} |s(u)s(v)s(z-u)s(z-v)|^{n/2}},$   
 $2r_{i} = 2\eta_{F} - \eta_{i} = \begin{cases} 2v, & i = \mathrm{SS}, \mathrm{TS}, \\ -2v, & i = \mathrm{CDW}, \mathrm{SDW}. \end{cases}$  (20)

The function  $f_i(u,v)$  describes effects of a special crystal symmetry which are considered in the next section; in this section  $f_i(u,v) \equiv 1$  everywhere. Considering the series (20) we can distinguish two cases A and B differing in the convergence of the integral over u - v in (20) at the upper limit.

A. Let the convergence of the integral over u - v in (20) at the upper limit be determined merely by the temperature cutoff  $\sim T^{-1}$ , i.e., let the following inequality hold:

$$2r_i = 2\eta_F - \eta_i < 2. \tag{21}$$

In that case the second term in (20) turns out for any *i* to be of order  $\varepsilon^2(T)T^{-\beta_i}$ , where

$$\varepsilon(T) \sim t_{\perp}/T^{\beta_{\mathbf{F}}} = (T_{3d}/T)^{\beta_{\mathbf{F}}}, \quad T_{3d} \sim t_{\perp}^{1/\beta_{\mathbf{F}}}, \quad \beta_{\mathbf{F}} = 2 - \eta_{\mathbf{F}}.$$
(22)

Similar estimates of the next terms in the series show that for any of the susceptibilities the series (20) has the form

$$\chi_i(T) = \chi_i^{(0)}(T) (1 + \varepsilon^2(T) + \varepsilon^4(T) + \ldots), \qquad (23)$$

i.e., the expansion is in powers of an undefined (*i*-independent) expansion parameter  $\varepsilon(T)$ . The hypothetical expansion (17) in powers of  $\chi_i^{(0)}(T)$  is thus not corroborated and, hence, the one-dimensional phase diagram is not reproduced at a finite temperature. Instead, at a temperature  $T \sim T_{3d}$  when  $\varepsilon(T) \sim 1$  and the series (23) diverges there occurs a transition to a three-dimensional behavior by electrons which have an open Fermi surface. When  $T \leq T_{3d}$  the conclusions of the band theory of metals are apparently applicable. Indeed, using Eq. (5) and a perturbation theory in  $t_{m-n}$  one can easily show that the series expansion for the single-



FIG. 1. Expansion of the susceptibility in powers of  $t_{\perp}$  for superconductivity (a) and for CDW, SDW (b).

particle Green function is also in powers of  $\varepsilon(T)$ . Hence it is clear that  $T_{3d}$  is nothing but the effective width of the singleparticle band for transverse motion renormalized using Eq. (22) to take interactions into account. We note that  $T_{3d} \sim t_1$ for free particles according to (22) and (4). In the case of weak interactions g, when  $\beta_F - 1 \propto g^2$ , the transition from the one- to the three-dimensional regime and the renormalization of the bandwidth were studied in detail in Ref. 14.

B. We consider the case when for any *i* the integral over u - v in (20) converges at some upper limit  $\xi$  such that  $\xi \leqslant T^{-1}$ . The range of integration variables  $|u - v| \sim \xi \leqslant |z| \sim T^{-1}$  is then the important one for the integral in (20) which is transformed into

$$t_{\perp}^{2} \int \frac{d^{2}(u-v)f_{i}(u,v)}{|s(u-v)|^{2r_{i}}} \int \frac{d^{2}z \, d^{2}u}{|s(u)s(z-u)|^{\eta_{i}}} \sim \lambda_{i} [\chi_{i}^{(0)}(T)]^{2},$$
(24)

$$\lambda_i \sim t_\perp^2 \xi^{2-2r_l}.$$

Considering similarly the ladder diagrams of higher order in  $t_1$  we see that the series (17) is reproduced with  $\lambda_i$  from (25) as the effective constant. We get from (18) and (25)

$$T_c^{(i)} \sim \xi^{-1} (T_{3d} \xi)^{2\beta_F/\beta_t}.$$
 (26)

For the self-consistency of the theory it is necessary to satisfy the condition

$$T_{c}^{(i)} \xi \ll 1,$$
 (27)

which is equivalent in view of (26) to the condition

$$T_{3d} \xi \ll 1. \tag{28}$$

When  $f_i(u,v) = \text{const}$ , the fast convergence of the integral over u - v in (20) can be guaranteed only by the inequality

$$2\eta_F - \eta_i - 2 > 0. \tag{29}$$

In that case  $\xi \sim 1$ , i.e., when jumping between the chains the electrons are bound into a pair of molecular size. Condition (29) is equivalent to the inequality  $2\beta_F < \beta_i$  from which it follows by virtue of (26), (28) that

$$T_c^{(i)} \gg T_{sd}.$$
 (30)

Equation (30) means that under condition (29) there is realized in the system a regime which can naturally be called quasi-one-dimensional in contrast to the band regime (case A): when the temperature is lowered the phase transition occurs before the band corrections to the single-particle Green function become important. Condition (29) is not satisfied for noninteracting electrons [see (4)] so that for the realization of the quasi-one-dimensional regime in a system with a simple crystal symmetry a strong electron-electron interaction is necessary (generally speaking, comparable with the bandwidth W).<sup>3)</sup>

We discuss the approximations made in reducing the power expansion (19) to the series (17). First, we selected only those diagrams in which both particles jumped to one and the same chain. This is valid because these diagrams have an expansion parameter  $t_{\perp}^2/T^{\beta_1}$  and diverge by virtue of the quasi-one-dimensionality condition (30) faster than diagrams with independent jumps for which the expansion parameter is  $\varepsilon(T)$  from (22). Second, we neglected corrections which arise when in the jumps a pair of particles turns up several times on a single chain. In that case one should use for that chain a multipoint one-dimensional correlator instead of (1), (2), or (10). One can show that taking these corrections into account is equivalent to considering the critical fluctuations of the order parameter. They are important only close to  $T_c$  and are not of special interest to us.

We note yet another point. The ordering for  $T < T_c$  can take place nonuniformly and have some transverse wave vector. If we assume that  $t_{m-n}$  is non-vanishing only for nearest neighbors, we must in the equation analogous to (17) for  $\chi_i(\mathbf{q}_\perp, T)$  introduce instead of (25) the quantity

$$\lambda(\mathbf{q}_{\perp}) \sim (t_b^2 \cos q_b b + t_c^2 \cos q_c c) \xi^{2\beta_F - \beta_l}, \qquad (31)$$

where  $\mathbf{q}_{i} = (q_{b}, q_{c})$  is the wave vector at right angles to the direction of the chains. Since according to (10), (11), (14)  $\chi_{i}^{(0)} > 0$  for i = SS and TS, and  $\chi_{i}^{(0)} < 0$  for i = CDW and SDW (we bear in mind that we are working in the Matsubara technique), it follows that the pole in (17) occurs, when we use (31), at  $\mathbf{q}_{i} = 0$  for superconductivity and at

$$\mathbf{q}_{\perp} = (\pi/b, \ \pi/c) \tag{32}$$

for dielectric transitions. The band theory with a cosine transverse dispersion law for the electrons leads to the same result. If, however, we take into account jumps between next-nearest neighbors, the ordering wave vector may differ from the value (32).

#### 4. PHASE DIAGRAM UNDER CONDITIONS OF SPECIAL CRYSTAL SYMMETRY OR UNDER THE ACTION OF EXTERNAL FIELDS

In this section we study how various actions, external to the electron subsystem, affect the coupling between the chains: 1) a crystalline field with wave vector  $4k_F$ ; 2) nonequivalence of neighboring chains; 3) a magnetic field perpendicular to the chains; 4) the presence of impurities from which forward scattering takes place. We show that all these actions lead, when well defined conditions are satisfied, to the behavior of the system corresponding to case B of section 3, although inequality (29) is not satisfied. The jumps of electron-hole pairs between chains become coherent in cases 1) and 3) and of Cooper pairs in cases 2) and 4).

#### 4.1. A system with a gap in the charge channel

We consider a system with one electron per elementary cell in a regime with a gap  $\Delta_c$  in the charge channel and no gap in the spin channel (see Section 2). As in Section 3, we use perturbation theory with respect to  $t_{\perp}$ . We consider the diagram of Fig. 1b for i = SDW, CDW. Assuming that  $\Delta_c \gg T$  and using (7) we get easily the following expression for the susceptibility:

$$\chi_{i}(T) \sim \frac{1}{T |\xi_{c}|^{2\eta - 1}} + \frac{t_{\perp}^{3}}{|\xi_{c}|^{2(2\eta - 1)}} \int d^{2}(u - v) \exp\left(-\frac{|u - v|}{\xi_{c}}\right) \\ \times \int \frac{d^{2}z \, d^{3}u}{|s(u)s(z - u)|} + \dots \sim \chi_{i}^{(0)} (T) [1 + \lambda_{c}\chi_{i}^{(0)} (T) + \dots],$$

$$\lambda_{c} \sim t_{\perp}^{2} |\xi_{c}|^{2}, \quad \chi_{i}^{(0)} (T) \sim 1/T |\xi_{c}|^{2\eta - 1}.$$
(33)
(34)

Equation (33) is analogous to Eq. (24) (neglecting a few differences in the indexes) and the next terms in the expansion in  $t_1$  reproduce the series (17). We see that the presence of a gap in the charge channel leads to the occurrence of a factor  $f_i(u-v) = \exp(-|u-v|/\xi_c)$  for i = SDW or CDW, which guarantees the convergence of the integral over u - v on the length  $\xi \sim \xi_c \sim \Delta_c^{-1} \ll T^{-1}$ . The situation considered thus corresponds to case B of Section 3. The gap in the charge channel guarantees the coherence of the jumps of the singlet and triplet electron-hole pairs and the quasione-dimensional regime of behavior. From Eq. (26) we get

$$T_c^{(i)} \sim \Delta_c (T_{sd}/\Delta_c)^{2\beta p}, \quad i=\text{CDW}, \text{SDW}.$$
 (35)

For self-consistency of (33) it is necessary to satisfy the condition

$$\Delta_{c} \gg T_{c}^{(i)}, \tag{36}$$

which by virtue of (35) is equivalent to the inequality

$$\Delta_c \gg T_{3d},\tag{37}$$

i.e., the gap  $\Delta_c$  must be appreciably larger than the transverse bandwidth.

Taking the logarithmic corrections (10), (12) into account shows that an SDW has a higher transition temperature than a CDW. As to superconductivity, it is clear from (13) that it is suppressed when there is a gap in the charge channel.

Similar results were obtained in Ref. 24 for the case of a gap  $\Delta_s$  in the spin channel. It was shown that the presence of  $\Delta_s$  leads to the coherence of the jump of singlet pairs, thus leading to Eqs. (33)–(35) for SS and CDW, but suppressing the TS and SDW.

#### 4.2. Systems with nonequivalent neighboring chains

We consider a system in which there is a crystalline field oscillating along the transverse **b** axis with a period 2b. Because of this the potential energies of neighboring chains will differ by some amount  $2\varkappa$ . The condition that the Fermi energy be constant leads to equilibrium Fermi momenta that alternate along the **b** axis alternating:

$$k_F^{(n)} = k_F + (-1)^{n_b} \varkappa. \tag{38}$$

If  $k_F = \pi/2a$ , i.e., the system was twofold commensurate when  $\varkappa = 0$ , the transition into the incommensurate state (38) occurs under the condition

$$\kappa \geq \Delta_c.$$
 (39)

The gap in the charge channel then vanishes.

We shall reckon the longitudinal momenta of the electrons in each chain from the equilibrium value (38); all onedimensional correlators will then, as before, be given by Eqs. (1), (2), (10). Changes occur only in the action (19) describing the jumps of electrons between chains:

$$S_{i} = \sum_{\alpha,\mathbf{m},\mathbf{n}} \int d^{2}z [t_{\mathbf{m}-\mathbf{n}} w_{\mathbf{m},\mathbf{n}}^{(\alpha)}(z) \psi_{\sigma,\alpha}^{\pm}(z,\mathbf{m}) \psi_{\sigma,\alpha}(z,\mathbf{n}) + \text{H.c.}], \quad (40)$$

$$w_{\mathbf{m},\mathbf{n}}^{(\alpha)}(z) = \begin{cases} \exp[-2i\alpha(-1)^{m_{b}} \times x] \equiv f_{\mathbf{m}}(x), & m_{b}-n_{b}=2k+1, \\ 1, & m_{b}-n_{b}=2k. \end{cases}$$

$$(41)$$

We use again perturbation theory with respect to  $t_{\perp}$ . We consider the diagrams of Fig. 1a for i = SS, TS. Using (2), (40), and (41) we find easily that the expressions corresponding to them reduce to (20) while for the jumps between non-equivalent chains  $(m_n - n_b \text{ odd})$ , for instance, between neighbors, we have

$$f_i(u, v) = \cos [2\kappa (x_u - x_v)], i = SS, TS.$$
 (42)

Here  $x_u = \operatorname{Re} u, x_v = \operatorname{Re} v$ . We shall assume that

$$\kappa \gg T$$
. (43)

The oscillating factor (42) then improves strongly the convergence of the integral over u - v in (20) in the region  $\kappa^{-1} \ll |u - v| \ll T^{-1}$ . For convergence it is now sufficient that the condition  $\nu > 0$  be satisfied. This is realized even for weak interactions [see (4)]. Indeed, the integral (24) over u - v can be evaluated exactly:

$$I = \int d^{2}z \frac{\cos 2\varkappa x}{|s(z)|^{2\nu}} = \frac{2}{(2\pi T)^{2-2\nu}} \left| \frac{\sin[\pi(\nu/2 - i\varkappa/2)]}{\sin \pi \nu} \right|^{2} \frac{|\Gamma(\nu/2 + i\varkappa/2)|^{4}}{\Gamma^{2}(\nu)}.$$
(44)

When condition (43) holds, it equals

$$I = \frac{a(v)}{x^{2-2v}}, \quad a(v) = \frac{2^{3-2v}\pi^2}{\sin^2 \pi v \Gamma^2(v)}, \quad (45)$$

which means convergence of the integral over distances  $\xi \sim \pi^{-1} \ll T^{-1}$ . Thus, if we sum diagrams with jumps between nonequivalent chains only, the behavior of the system considered corresponds to case B of Section 3. From Eqs. (26), (25) we get

$$T_{c}^{(i)} \sim (\lambda_{\rm SP})^{4/\beta_{t}} \sim \varkappa \left(\frac{T_{3d}}{\varkappa}\right)^{2\beta_{\rm F}/\beta_{t}}, \quad \lambda_{\rm SP} \sim \frac{t_{\perp}^{2}}{\varkappa^{2-2\nu}}, \quad i = \rm SS, TS,$$

$$(46)$$

where  $\lambda_{SP}$  is the effective Josephson coupling constant between chains.

For the self-consistency of the theory it is necessary that

a number of conditions are satisfied. First of all, it is necessary that conditions (21) and (15) for the exponents are satisfied

$$2 > v > 0, \quad \eta_i < 2, \quad i = SS, TS.$$
 (47)

These conditions are not stringent, since they are satisfied even for weak interactions [see (4)]. According to (3) they mean that there is an effective attraction in the charge channel. Second, the condition

$$\kappa \gg T_c$$
 (48)

is necessary, and guarantees the coherence of the jump of the electrons of a Cooper pair: in jumps they remain bound over distances  $\xi \sim \kappa^{-1}$ . By virtue of (46), condition (48) is equivalent to the inequality

$$\varkappa \gg T_{3d}, \tag{49}$$

i.e., the difference between the potential energies of the chains must be appreciably larger than the width of the transverse band at x = 0.

The evaluation of the single-particle Green function in the framework of the ladder approximation in  $t_{m-n}$  shows that when  $x \neq 0$  and under condition (49) the effective width of the single-particle band of transverse motion equals

$$T_{3d}^* \sim T_{3d}^2 / \varkappa \ll T_{3d}. \tag{50}$$

Yet one more condition for the applicability of the theory:

$$T_c \ge T_{3d}^* \tag{51}$$

guarantees the quasi-one-dimensional nature of the transition. It allows us to neglect diagrams with jumps of the electrons of a Cooper pair on different chains. It follows from (46), (50), (27) that condition (51) is equivalent to the inequality

$$\eta_i < \eta_F, \quad i = SS, \ TS. \tag{52}$$

We note that (52) is not satisfied for weakly interacting particles, so that for the applicability of our theory it is necessary to have sufficiently strong interactions although inequality (52) is weaker than (29).

There is an important difference between conditions (48), (49), and (51), (52). Condition (48) is necessary for the very existence of the effect that the electrons contract to a pair as they jump. However, condition (51) is a procedural restriction which allows us to obtain explicit formulae by selecting diagrams of a well-defined form. Apparently, inequality (51) is the condition for the applicability of the theory propounded here, but not the condition for the existence of the very effect of stimulation of superconductivity via nonequivalence of neighboring chains.

The inequalities to which our theory leads can be summarized as follows

$$\chi \gg T_{3d} \gg T_c \gg T_{3d}^*.$$
<sup>(53)</sup>

We note that both  $T_c$  and  $T^*_{3d}$  decrease with increasing  $\varkappa$ .

Due to the absence of a gap in the spin channel, the logarithmic corrections (10) and (12) lead to the triplet

superconductivity having a higher transition temperature than the singlet superconductivity.

We now consider the SDW and CDW channels. In this case we get instead of (42) for jumps between alternating chains the factor

$$f_i(u, v) = \cos \left[ 2\kappa \left( x_u + x_v \right) \right], \quad i = \text{CDW}, \text{SDW}, \quad (54)$$

which does not lead to convergence of the integral over u - v of to coherence of the jump of electron-hole pairs.

The difference between the Fermi momenta on neighboring chains leads thus to coherence of the jump of the electrons in a Cooper pair, to formation of an effective Josephson coupling between chains, and to transition into a superconducting state in the quasi-one-dimensional regime. In contrast to the models of quasi-one-dimensional superconductivity considered usually, in our theory there is no gap in the spin channel and the role of the coherence length of a Cooper pair is played by  $x^{-1}$ .

We note that different electron densities on neighboring chains can in principle be guaranteed not only through internal crystalline fields but also through an external electric field perpendicular to the chains, for instance, in field-effect transistor structures. This opens up a tempting possibility of controlling the superconductivity.

#### 4.3. Influence of a magnetic field

We consider the behavior of a quasi-one-dimensional system of equivalent chains ( $\kappa = 0$ ) in a gapless regime ( $\Delta_c = \Delta_s = 0$ ) in a relatively strong magnetic field *H* at right angles to the direction of the chains. Let, for instance, **H**||**c**. Performing on each chain a gauge transformation

$$\psi_{\sigma,\alpha}(z,\mathbf{n}) \rightarrow \psi_{\sigma,\alpha}(z,\mathbf{n}) \exp[iqn_b x], \quad q=(e/c) bH,$$

we see that changes occur only in the action (19) that describes the jumps. It will have the form (40) with

$$w_{\mathbf{m},\mathbf{n}}^{(\alpha)} = \exp\left[-iq\left(m_b - n_b\right)x\right]. \tag{55}$$

Studying the diagrams of Fig. 1b for the CDW and SDW channels we get Eq. (20) with

$$f_i(u, v) = \exp \left[-iq(m_b - n_b)(x_u - x_v)\right], i = CDW, SDW.$$
 (56)

For nearest neighbors this expression is analogous to Eq. (42) obtained for superconducting channels, with replacement of  $2\varkappa$  by q. The difference from the magnetic case is that all chains must be assumed to be nonequivalent. Using the same arguments as in the preceding subsection we confirm that the behavior of a system in a magnetic field corresponds to case B of Section 3 for i = CDW and SDW with a characteristic length  $\xi \sim q^{-1}$ . Of course, for this it is necessary that the conditions

$$-2 < v < 0, \quad \eta_i < 2, \quad i = \text{CDW SDW}$$
(57)

on the exponents are satisfied, which mean that there is an effective repulsion in the charge channel.

For the TS and SS channels in a magnetic field there appears a factor

$$f_i(u, v) = \exp [iq(m_b - n_b)(x_u + x_v)], i = SS, TS,$$

analogous to (54) and suppressing the superconductivity.

A magnetic field at right angles to the chains thus contracts into pairs; the electron hole jumps and induces a transition of the system into a state with SDW or CDW. Comparing this with the results of subsection 4.2 we see that there is a peculiar duality: electric vs magnetic field, superconducting vs electron-hole pairing.

For the applicability of our theory it is necessary that the condition  $q \ge T_c$ , which is equivalent to  $q \ge T_{3d}$ , be satisfied. The effect of stimulating SDW or CDW by a magnetic field was deduced earlier in Ref. 30 in the framework of band theory which is applicable when  $q \ll T_{3d}$ . This effect exists thus in a broad region of the parameter values of the problem.

We note that both from a theoretical and from an experimental point of view the case of a magnetic field against the background of a structure with alternating chains is of special interest.

## 4.4. Effects of scattering by impurities

We consider a system in which there are chemical-potential inhomogeneities which vary slowly along the chains, or impurities from which only forward scattering takes place. Using Eq. (8) we find that there are the following functions in Eq. (20):

$$f_i(u,v) = \begin{cases} \exp\left(-2|x_u - x_v|/\xi_{imp}\right), & i = \text{SS}, \text{TS}, \\ \exp\left(-2|x_u + x_v|/\xi_{imp}\right), & i = \text{CDW SDW}. \end{cases}$$
(58)

According to the theory of item B of Section 3 we find at once that there occur coherent jumps of Cooper pairs with an effective coherence length  $\xi \sim \xi_{imp}$ ,

$$T_{c}^{(i)} \sim \xi_{imp}^{-1} (T_{3d} \xi_{imf})^{2\beta_{F}/\beta_{l}}, \quad i = SS, TS.$$
 (59)

The necessary conditions for the existence of the effect are:

$$T_{3d}\xi_{imp} \ll 1, \quad 2 \ge \nu \ge 1, \quad \eta_i \le 2, \quad i = SS, TS.$$
 (60)

The second condition in (60) differs from the analogous condition in (47) of subsection 4.2 as the exponential cutoff is less effective than the oscillating one. This condition is necessary to guarantee the convergence at the upper limit at distances much less than  $T_c^{-1}$  of the integral (24) over  $d(\tau_u - \tau_v)$ . Impurities leading to forward scattering thus stimulate superconductivity but suppress [see (8)] SDW and CDW. Similar results were obtained in Ref. 31 but there the conditions for the applicability of the quasi-one-dimensional theory were not indicated.

We consider the system described in subsection 4.2 for the case when there is disorder in the crystalline fields, so that  $\langle \varkappa \rangle = 0$ . One must average Eq. (42) over the spatial fluctuations of  $\varkappa$ . We assume that the anions which produce the crystal field are completely disordered. Performing the averaging with a Gaussian weight we return to Eqs. (58) with

$$\xi_{imp} \sim 1/a \varkappa_0^2, \tag{61}$$

where a is the distance between the anions and coincides with the lattice constant, and  $x_0$  is the potential produced by a single anion. Disordered crystal fields thus stimulate superconductivity in the same way as ordered ones.

#### 5. SUPERCONDUCTING PHASE IN A SYSTEM WITH NONEQUIVALENT CHAINS

In this section we consider the superconducting state described in subsection 4.2 near the transition temperature.<sup>4)</sup> To simplify the exposition we drop the spin indexes, i.e., the entire derivation is for spinless fermions.

To derive the Ginzburg-Landau functional we add to the action of the system a term with a generalized field  $h(z_1,z_2,\mathbf{n})$ , which produces Cooper pairs:

$$S_{h} = \sum_{n} \int d^{2}z_{1} d^{2}z_{2} \{h(z_{1}, z_{2}, \mathbf{n}) \psi_{+}^{+}(z_{1}, \mathbf{n}) \psi_{-}^{+}(z_{2}, \mathbf{n}) + \text{H.c.}\}.$$
(62)

The first term in the expansion of the free energy in powers of h has the form

$$\frac{\mathscr{F}\{h\} - \mathscr{F}\{0\}}{T} \approx \frac{\mathscr{F}^{(1)}}{T} = -\frac{1}{2} \sum_{\mathbf{m}, \mathbf{n}} \int d^2 z_1 d^2 z_2 d^2 z_3 d^2 z_4$$
$$\times h^{\bullet}(z_1, z_2, \mathbf{m}) h(z_3, z_4, \mathbf{n}) K_{\mathbf{m}, \mathbf{n}}(z_1, z_2, z_3, z_4), \quad (63)$$

where the correlation function is

$$K_{\mathbf{m},\mathbf{n}}(z_1, z_2, z_3, z_4) = \langle \psi_+(z_1, \mathbf{m})\psi_-(z_2, \mathbf{m})\psi_+^+(z_3, \mathbf{n})\psi_+^+(z_4, \mathbf{n})\rangle.$$
(64)

The mean value is evaluated here for h = 0, but  $t_{\perp} \neq 0$ .

We change to the conjugated potential  $\Phi(F)$ :

$$\Phi = \mathscr{F} + T \sum_{\mathbf{n}} \int d^2 z_1 \, d^2 z_2 h^*(z_1, z_2, \mathbf{n}) F_{\mathbf{n}}(z_1, z_2).$$
(65)

The connection between h and F is given by the formula

$$F_{\mathbf{n}}(z_{1}, z_{2}) = -\frac{\delta \mathcal{F}}{T \delta h^{*}(z_{1}, z_{2}, \mathbf{n})} = \langle \psi_{+}(z_{1}, \mathbf{n})\psi_{-}(z_{2}, \mathbf{n}) \rangle$$
$$= \sum_{\mathbf{m}} \int d^{2}z_{3} d^{2}z_{4} h(z_{3}, z_{4}, \mathbf{m}) K_{\mathbf{m}, \mathbf{n}}(z_{1}, z_{2}, z_{3}, z_{4}) + O(h^{3}). \quad (66)$$

The first term in the expansion of  $\Phi(F)$  in powers of F has the form

$$\frac{\Phi^{(1)}}{T} = \frac{1}{2} \sum_{\mathbf{m},\mathbf{n}} \int d^2 z_1 \, d^2 z_2 \, d^2 z_3 \, d^2 z_4 F_{\mathbf{m}}^{\bullet}(z_1, z_2) K_{\mathbf{m},\mathbf{n}}^{-1}(z_1, z_2, z_3, z_4) \\ \times F_{\mathbf{n}}(z_3, z_4), \qquad (67)$$

where  $K^{-1}$  is the kernel which is the inverse of (7).

The operator K satisfies in the ladder approximation the following equation which corresponds to a summation of diagrams of the kind shown in Fig. 1a:

$$K_{n, m}(z_{1}, z_{2}, z_{3}, z_{4}) = \delta_{n, m} K_{0}(z_{1}, z_{2}, z_{3}, z_{4}) + \sum_{\delta} \int d^{2}z' d^{2}z'' K_{0}(z_{1}, z_{2}, z', z'') \times K_{n+\delta, m}(z', z'', z_{3}, z_{4}) \cdot t_{\delta}^{2} w_{n, n+\delta}(z'-z'').$$
(68)

Here,  $K_0$  is given by Eqs. (1) and (2); w by Eq. (41); the  $\delta$  are two-dimensional vectors which connect nonequivalent chains. In deriving (68) we selected only diagrams with jumps between alternating chains, in as much as according to the conclusions of Sections 3 and 4 jumps between equiva-

lent chains lead to indefinite corrections of order  $\varepsilon(T)$  from (22).

We find the eigenfunctions  $\varphi$  and eigenvalues  $\lambda^{-1}$  of the operator K, which are defined as follows

$$\sum_{\mathbf{m}} \int K_{\mathbf{n},\mathbf{m}}(z_{1}, z_{2}, z_{3}, z_{4}) \varphi_{\mathbf{m}}(z_{3}, z_{4}) d^{2} z_{3} d^{2} z_{4} = \lambda^{-1} \varphi_{\mathbf{n}}(z_{1}, z_{2}).$$
(69)

Substituting (69) into (68) we get

$$\varphi_{\mathbf{n}}(z_{1}, z_{2}) = \lambda \int d^{2}z_{3} d^{2}z_{4}K_{0}(z_{1}, z_{2}, z_{3}, z_{4}) \varphi_{\mathbf{n}}(z_{3}, z_{4}) + \sum_{\delta} \int d^{2}z_{3} d^{2}z_{4}K_{0}(z_{1}, z_{2}, z_{3}, z_{4}) t_{\delta}^{2}f_{\mathbf{n}}(z_{3} - z_{4}) \varphi_{\mathbf{n}+\delta}(z_{3} - z_{4}).$$
(70)

We introduce new variables:

$$R_1 = (z_1 + z_2)/2, \quad r_1 = z_1 - z_2, \quad R_2 = (z_3 + z_4)/2, \quad r_2 = z_3 - z_4.$$
(71)

Using Eq. (2) for  $K_0$  we can rewrite Eq. (70) in the form

$$\varphi_{\mathbf{n}}(R_{\mathbf{1}}, r_{\mathbf{1}}) = \int d^{2}R_{2} d^{2}r_{2} \frac{\Gamma(R_{1} - R_{2}, r_{1}, r_{2})}{|s(r_{1})s(r_{2})|^{\mathbf{v}}} \times \left[\lambda\varphi_{\mathbf{n}}(R_{2}, r_{2}) + \sum_{\delta} t_{\delta}^{2}f_{\mathbf{n}}(r_{2})\varphi_{\mathbf{n}+\delta}(r_{2})\right], \quad (72)$$

where

$$\Gamma(R, r_{1}, r_{2}) = \left| s\left(R + \frac{r_{1} + r_{2}}{2}\right) s\left(R - \frac{r_{1} + r_{2}}{2}\right) \right|^{\nu} \left| s\left(R + \frac{r_{1} - r_{2}}{2}\right) \times s\left(R - \frac{r_{1} - r_{2}}{2}\right) \right|^{-\eta_{r}}.$$
(73)

We introduce a new variable

$$Y_{n}(R, r) = \varphi_{n}(R, r) |s(r)|^{\nu}.$$
(74)

Fourier-transforming with respect to R in (72) using the definition

$$f(Q,r) = \int d^2R f(R,r) \exp[-iq_{\parallel}x + i\omega_n\tau], \quad Q = (\omega_n, q_{\parallel}), \quad (75)$$
  
we get

 $Y_{n+\delta}(Q, r_2) | s(r_2) |^{-2v}$ 

$$Y_{n}(Q, r_{1}) = \sum_{\mathbf{A}} t_{\delta}^{2} \int d^{2}r_{2}f_{n}(r_{2})$$

$$\times \Gamma(Q, r_{1}, r_{2}) + \lambda(Q) \int d^{2}r_{2}Y_{n}(Q, r_{2}) |s(r_{2})|^{-2\nu} \Gamma(Q, r_{1}, r_{2}).$$
(76)

Using (41) and the condition  $\nu > 0$  the first integral in (76) converges at distances  $|r_2| \sim \pi^{-1}$ , i.e.,  $|r_2| \ll |Q|^{-1}$  for characteristic  $|Q| \sim T_c$ . Hence, we can in that term put  $\Gamma(Q, r_1, r_2) \approx \Gamma(Q, r_1, 0)$  up to terms of order  $T/\pi \ll 1$ .

It is now clear from (76) and (73) that  $Y_n(r)$  is an even function of r, so that the first integral in (76) contains only a symmetric part

$$f(r) = \frac{1}{2} [f_n(r) + f_n(-r)] = \cos 2\varkappa x, \qquad (77)$$

which is independent of **n**. Fourier-transforming with respect to **n** we get

$$Y(Q, \mathbf{q}_{\perp}, r_{1})$$
  
= $t^{2}(\mathbf{q}_{\perp}) \Gamma(Q, r_{1}, 0) \int d^{2}r_{2}f(r_{2}) Y(Q, \mathbf{q}_{\perp}, r_{2}) |s(r_{2})|^{-2\nu}$   
+ $\lambda(Q, \mathbf{q}_{\perp}) \int d^{2}r_{2}Y(Q, \mathbf{q}_{\perp}, r_{2}) |s(r_{2})|^{-2\nu} \Gamma(Q, r_{1}, r_{2}).$  (78)

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Close to  $T_c$  the eigenvalues  $\lambda$  are small so that the eigenfunctions Y can be looked for by iterating Eq. (78) with respect to  $\lambda$ :

$$Y(Q, \mathbf{q}_{\perp}, r_{1}) \approx C(Q, \mathbf{q}_{\perp}) \left[ t^{2}(\mathbf{q}_{\perp}) \Gamma(Q, r_{1}, 0) + t^{2}(\mathbf{q}_{\perp}) \lambda(Q, \mathbf{q}_{\perp}) \int d^{2}r_{2}\Gamma(Q, r_{1}, r_{2}) \Gamma(Q, r_{2}, 0) \left| s(r_{2}) \right|^{-2\nu}.$$
 (79)

We find the self-consistency condition for the constant C by substituting (79) into (78). To first order in  $\lambda$  it is sufficient to consider only the first term on the right-hand side of (78) and we get

$$\lambda(Q, \mathbf{q}_{\perp}) = [1 - t^{2}(\mathbf{q}_{\perp}) \Gamma(Q, 0, 0) I] / [t^{2}(\mathbf{q}_{\perp}) I \S d^{2} r \Gamma(Q, 0, r) \\ \times \Gamma(Q, r, 0) |s(r)|^{-2v}], \qquad (80)$$

where *I* is given by Eq. (45). Clearly  $\Gamma(Q,0,0) \equiv \Gamma(Q)$  is the generalized susceptibility of the one-dimensional system. Close to  $T_c$  small values of the momentum  $q_{\parallel} \ll T_c$ ,  $\omega_n = 0$  are important. In that case we get from (73)

$$\Gamma(Q)^{\bullet} \sim T_{c}^{\eta-2} \left( 1 - \frac{C_{1}q_{\parallel}^{2}}{T_{c}^{2}} \right),$$

$$C_{1} = \frac{1}{(4\pi)^{2}} \left[ \psi'\left(\frac{\eta}{4}\right) - \psi'\left(1 - \frac{\eta}{4}\right) \right],$$
(81)

where  $\psi'(\sigma)$  is the trigamma function and  $\eta = 2(\eta_F - \nu)$ . Estimating the integrals in Eq. (80) we get

$$\lambda(\mathbf{q}) = C_2 T_c^{4-2\tau_F} \left[ \frac{T - T_c}{T_c} + \frac{C_1 q_{\parallel}^2}{T_c^2} + \frac{t_{\perp}^2 - t^2(\mathbf{q}_{\perp})}{t_{\perp}^2} \right], \quad C_2 \sim 1.$$
(82)

We find the form of the anomalous Green function  $F_n(z_1,z_2)$ . To do this we expand it in terms of the eigenfunctions  $\varphi$  of the operator  $K^{-1}$  of (69) using (74). Close to  $T_c$  we can neglect in Eq. (79) the second term on the right-hand side and neglect the  $r_1$ -dependence in the first term when  $|r_1| \ll T_c^{-1}$ . Hence

$$F_{\mathbf{n}}(z_1, z_2) = |s(r)|^{-v} Y_{\mathbf{n}}(R), \quad r = z_1 - z_2, \quad R = (z_1 + z_2)/2,$$
(83)

where the function  $Y_n(R)$  [the inverse Fourier-transform of the function in (79)] plays the role of the wave function of the center of mass of the electron pair. Its modulus is determined by the next terms of the expansion (67). We draw attention to the fact that the anomalous Green function (83) at small distances has a power-law dependence on the relative distance between the electrons. Substituting (83) into (67) we get

$$\Phi \{Y\} - \Phi \{0\} = B \sum_{\mathbf{q}} \lambda(\mathbf{q}) |Y(\mathbf{q})|^2,$$

$$B = \int \frac{d^2r}{|s(r)|^{2\nu}} = \frac{b(\nu)}{T_c^2}, \quad b(\nu) = \frac{1}{(2\pi)^{2-2\nu}} \frac{\Gamma^4(\nu/2)}{\Gamma^2(\nu)} \operatorname{ctg} \frac{\pi\nu}{2}.$$
(84)

We now find the next term in the expansion of the free energy in powers of h:

$$\mathcal{F}^{(2)}{h} = -\frac{1}{4!} \sum_{\mathbf{k} \mathbf{l} \mathbf{m} \mathbf{n}} \int \prod_{i=1}^{4} d^{2}z_{i} d^{2}z_{i}' h^{*}(z_{1}, z_{1}', \mathbf{k}) h^{*}(z_{2}, z_{2}', \mathbf{l})$$

$$\times h(z_{3}, z_{3}', \mathbf{m}) h(z_{4}, z_{4}', \mathbf{n}) L_{\mathbf{k}, \mathbf{l}, \mathbf{m}, \mathbf{n}}(\{z_{i}, z_{i}'\}), \qquad (85)$$

$$L_{\mathbf{k},1,\mathbf{m},\mathbf{n}}(\{z_{i},z_{i}'\}) = \langle \psi_{+}(z_{1},\mathbf{k})\psi_{-}(z_{1}',\mathbf{k})\psi_{+}(z_{2},\mathbf{l})\psi_{-}(z_{2}',\mathbf{l})$$

$$\times \psi_{+}^{+}(z_{3},\mathbf{m})\psi_{-}^{+}(z_{3}',\mathbf{m})\psi_{+}^{+}(z_{4},\mathbf{n})\psi_{-}^{+}(z_{4}',\mathbf{n})\rangle - \langle \psi_{+}(z_{1},\mathbf{k})$$

$$\times \psi_{-}(z_{1}',\mathbf{k})\psi_{+}^{+}(z_{3},\mathbf{m})\psi_{-}^{+}(z_{3}',\mathbf{m})\rangle$$

$$\times \langle \psi_{+}(z_{2},\mathbf{l})\psi_{-}(z_{2}',\mathbf{l})\psi_{+}^{+}(z_{4},\mathbf{n})$$

$$\times \psi_{-}^{+}(z_{4}',\mathbf{n})\rangle - \langle \psi_{+}(z_{1},\mathbf{k})\psi_{-}(z_{1}',\mathbf{k})\psi_{+}^{+}(z_{4},\mathbf{n})\psi_{-}^{+}(z_{4}',\mathbf{n})\rangle$$

 $\times \langle \psi_+(z_2, \mathbf{l}) \psi_-(z_2', \mathbf{l}) \psi_+^+(z_3, \mathbf{m}) \psi_-^+(z_3', \mathbf{m}) \rangle.$ 

(86)

Here all averages are evaluated for h = 0. We shall evaluate Eq. (86) also using perturbation theory in  $t_{\perp}$ . The summation is over all trajectories of the meandering two electron pairs in the two-dimensional system of chains. If these two trajectories do not intersect, i.e., if the two particle pairs do not land on the same chain, expression (86) vanishes. We consider trajectories with only a single intersection on the chain **p**. Using (66), Eq. (85) takes in this case the form

$$\frac{\mathcal{F}^{(2)}}{T} = \frac{1}{4!} \sum_{klmnp\delta_{i}} \int \prod_{j=1}^{8} d^{2}z_{j} d^{2}z_{j}' \left(\prod_{i=1}^{4} t_{\delta_{i}}^{2}\right) \\
\times h^{*} (z_{5}, z_{5}', \mathbf{m}) h^{*} (z_{6}, z_{6}', \mathbf{l}) \\
\times h (z_{7}, z_{7}', \mathbf{m}) h (z_{8}, z_{8}', \mathbf{n}) \left[\prod_{i=1}^{2} f_{\mathbf{p}}^{*} (z_{i} - z_{i}')\right] \left[\prod_{i=3}^{4} f_{\mathbf{p}} (z_{i} - z_{i}')\right] \\
\times K_{\mathbf{k}, \mathbf{p}+\delta_{1}} (z_{5}, z_{5}', z_{1}, z_{1}') K_{\mathbf{l}, \mathbf{p}+\delta_{2}} (z_{6}, z_{6}', z_{7}, z_{7}') \\
\times K_{\mathbf{p}+\delta_{3}, \mathbf{m}} (z_{3}, z_{3}', z_{7}, z_{7}') \\
\times K_{\mathbf{p}+\delta_{4}, \mathbf{n}} (z_{4}, z_{4}', z_{8}, z_{8}') L_{0} (\{z_{i}, z_{i}'\}) \\
= \frac{1}{4!} \sum_{\mathbf{p}\delta_{i}} \int \prod_{i=1}^{4} d^{2}z_{i} d^{2}z_{i}' f(z_{i} - z_{i}') \\
\times t^{2}_{\delta_{i}} F_{\mathbf{p}+\delta_{1}} (z_{1}, z_{1}') \\
\times F_{\mathbf{p}+\delta_{2}} (z_{2}, z_{2}') F_{\mathbf{p}+\delta_{3}}^{*} (z_{3}, z_{3}') F_{\mathbf{p}+\delta_{4}}^{*} (z_{4}, z_{4}') L_{0} (\{z_{i}, z_{i}'\}), (87)$$

where

$$L_0(\{z_i, z_i'\}) = -L_{\mathbf{p}, \mathbf{p}, \mathbf{p}, \mathbf{p}}(\{z_i, z_i'\}).$$
(88)

Expression (88) is the correlator (86) of eight electron operators pertaining to a single chain. We can evaluate it using the bosonization method. In the region  $|z_i - z'_i| \ll |z_i - z_j|, i \neq j$ , which is important for what follows, it has the form

$$L_{0}(\{z_{i}, z_{i}'\}) = \left(\prod_{i=1}^{n} |s(z_{i} - z_{i}')|^{-\nu}\right) \Lambda(\{z_{i}\}), \quad (89)$$

where

$$\Lambda(\{z_i\}) = |s(z_1-z_3)s(z_2-z_4)|^{-\eta} + |s(z_1-z_4)s(z_2-z_3)|^{-\eta}$$
(90)
$$- \left| \frac{s(z_1-z_2)s(z_3-z_4)}{s(z_1-z_3)s(z_2-z_4)s(z_1-z_4)s(z_2-z_3)} \right|^{\eta}.$$

Substituting expressions (83) and (89) into (87) and assuming  $Y_n(x)$  to be a slowly varying function we get

$$\Phi^{(2)}\{Y\} = D \sum_{n} \int dx |Y_{n}(x)|^{4},$$
  
$$D = \frac{1}{4!} (t_{\perp}^{2}I)^{4} \int \left(\prod_{i=1}^{3} d^{2}z_{i}\right) \Lambda(\{z_{i}\}) \sim T_{c}^{2-2\eta}.$$
 (91)

We now perform in (91) and (84) the substitution

$$\Psi_{\mathbf{n}}(x) = [C_2 b(\mathbf{v})]^{\frac{1}{2}} T_c^{1-\eta_F} Y_{\mathbf{n}}(x),$$

after which we find finally

$$\Phi \{\Psi\} = \sum_{\mathbf{q}} |\Psi(\mathbf{q})|^{2} \left( \frac{T - T_{c}}{T_{c}} + \xi_{a}^{2} q_{\parallel}^{2} + \frac{t_{\perp}^{2} - t^{2}(\mathbf{q}_{\perp})}{t_{\perp}^{2}} \right) + \frac{C_{s}}{T_{c}^{2}} \sum_{\mathbf{n}} \int dx |\Psi_{\mathbf{n}}(x)|^{4}, \quad \xi_{a}^{2} = \frac{C_{1}}{T_{c}^{2}}, \quad C_{s} \sim 1.$$
(92)

The Ginzburg-Landau type functional (92) was derived by us assuming rare intersections of Cooper pair trajectories on a single chain. We got the first term in the zeroth approximation and the second one in first order in such intersections. Taking a larger number of intersections into account is equivalent to considering critical fluctuations. It is clear that the neglect of critical fluctuations can quantitatively be justified only for models with a large number Z of interacting chains. As usual in phase transition theory, Eq. (92) is a qualitatively correct extrapolation to the region  $Z \sim 1$ . An additional complication arises from the fact that the materials of interest to us are not only quasi-one-dimensional, but also quasi-two-dimensional, i.e.,  $t^{2}(\mathbf{q}_{\perp})$  depends weakly on one of the components of  $\mathbf{q}_{\perp}$ . In that case we must consider (92) as the approximate functional of the problem for the phase transition in a lamellar superconductor. The specific nature of such phase transitions is discussed in Refs. 33 and 34 although the final results for the vicinity of the phase transition point are not known.

## 6. APPLICATION OF THE THEORY TO ORGANIC SUPERCONDUCTING COMPOUNDS

#### 6.1. Phase diagram

We consider the phase diagram of the  $(TMTSF)_2X$  and (TMTTF)<sub>2</sub>X compounds, which can have highly diverse forms (see the Introduction). The key to its interpretation is, in our opinion, given by a study of the types of ordering of the anions (see the review papers 2 and 3) occurring at a temperature  $T_{ao}$  and characterized by superstructure wave vectors  $\mathbf{Q} = (Q_a, Q_b, Q_c)$  measured in terms of the initial inverse lattice vectors. The types of ordering are apparently determined by the Coulomb interaction of the anions, their chemical properties, and other factors, which we assume given.<sup>5)</sup> We show that the electron states of the compounds considered can naturally be classified according to the anion superstructure wave vector. In the list given below we are dealing only with the behavior at atmospheric pressure, since x-ray structural measurements under pressure have not been made at sufficiently low temperatures.<sup>35</sup>

1.  $\mathbf{Q}_1 = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ . Almost all compounds with nonspherically symmetric anions belong to this type of ordering. It is characterized by the fact that the first component of the vector  $\mathbf{Q}_1$  equals  $2k_F$ , so that the potential produced by the anions opens a gap on the Fermi surface causing transition of the substance into a dielectric state. The phase diagram takes the form of a metal-dielectric transition at the temperature  $T_{ao}$ , and is a trivial effect that follows both from the quasione-dimensional and the band pictures. A special case are the compounds with  $X = NO_3$  where  $Q'_1 = (\frac{1}{2}, 0, 0)$  rather than  $Q_1$  is realized. Here  $(TMTSF)_2NO_3$  changes into another, also metallic, state which persists all the way to dielectric transition at T = 12 K. Such a behavior forces us to assume that the anion displacement amplitude is anomalously small.

2.  $\mathbf{Q}_2 = (0, \frac{1}{2}, \frac{1}{2})$ . The main property of this structure is the nonequivalence of the TMTTF molecules which are neighbors along the longitudinal *a* axis. It is realized in only one compound, (TMTTF)<sub>2</sub>SCN ( $T_{ao} = 160$  K). The phase diagram is<sup>36</sup>:  $T > T_{ao}$ —metal,  $T_{ao} > T > T_N = 7$  K—paramagnetic dielectric,  $T_N > T$ —antiferromagnetic. In the paramagnetic-dielectric phase the substance has a conductivity activation energy  $\Delta_c \sim 10^3$  K while at the same time the magnetic susceptibility retains its metallic nature.

3.  $\mathbf{Q}_3 = (0, \frac{1}{2}, 0)$ . The main property of this structure<sup>37</sup> is the alternation of the crystalline fields on neighboring molecular stacks (along the *b* axis). The only example is (TMTSF)<sub>2</sub>ClO<sub>4</sub> in the *R* phase (relaxed state)  $T_{ao} = 24$  K. The phase diagram is: a metal-superconductor transition at  $T_c \approx 1.3$  K. In strong magnetic fields (H > 50 kOe) a specific phase with a magnetic ordering is realized.<sup>1</sup>

4.  $\mathbf{Q}_4 = (0,0,0)$ . This is an undeformed structure which is retained, when the temperature is lowered, by all compounds with spherically symmetric anions. An important property of this structure is the alternation of distances between the TMTSF molecules along the *a* axis. Assuming the anions to be monovalent, we see that in the cases 2 and 4 the crystal structure is such that there must occur umklapp processes by a vector  $4k_F$  when two electrons collide. When the temperature is lowered these compounds go through the following phases: metal-paramagnetic dielectric-antiferromagnetic (presumably SDW).<sup>6)</sup> An intermediate phase is observed in TMTTF salts where  $T_{MI} = 200$  K,  $T_N \approx 10$  K,  $\Delta_c \approx 600$  K.<sup>39</sup> On the other hand, in TMTSF salts the temperatures of these transitions are practically the same:  $T_{MI} \approx T_N \approx 10$  to 20 K.<sup>1</sup> To this class may also belong  $(TMTSF)_2ClO_4$  in the Q phase (quenched state). This phase is obtained by fast cooling when the anions remain in the disordered state, so that on average they produce a potential with the vector  $\mathbf{Q}_{4}$ .

We now attempt an interpretation of the phase transitions described above from the point of view of the theory developed in the preceding sections. The existence of a paramagnetic dielectric phase in cases 2 and 4 indicates the splitting up of the spin and charge channels which is most adequately described using the bosonization method. In that case it is necessary to assume that there is no gap in the spin channel which is also one of the reasons for the SDW dominating over the CDW (see Section 4). In the framework of the g-ology model (see Section 2) this means that  $g_1 > 0$ . We note that our ideas differ from the ideas developed in Ref. 1, where essentially the presence of a pseudo-gap in the spin channel was assumed. As to the charge channel, it is necessary to assume that the umklapp amplitude is sufficiently large and guarantees the presence of a gap  $\Delta_c$  in the charge channel. In the framework of g-ology this means that  $|g_3| + 2g_2 - g_1 > 0$ . The presence of the gap  $\Delta_c$  guarantees dielectric behavior at  $T < T_{MI}$  and also, in accordance with the results of subsection 4.1, coherence of the jump of magnon pairs and three-dimensional SDW ordering at a temperature  $T_N < \Delta_c$ . From this point of view there is only a quantitative difference between the superstructures  $Q_4$  and  $Q_2$ . In case 2 the additional dimerization of the molecules in the stack leads, apparently, to an appreciable increase in  $g_3$ as compared to case 4.

A weakness of the proposed interpretation is that the paramagnetic dielectric phase is not clearly observed in the TMTSF salts. From the point of view of the theory of subsection 4.1, these compounds must be on the borderline of the applicability of the quasi-one-dimensional theory  $\Delta_c \sim T_{3d} \sim T_N \approx 10$  to 20 K. Nonetheless, the qualitative role of the weak two-dimensional commensurability remains, since the SDW phase vanishes upon transition of (TMTSF)<sub>2</sub>ClO<sub>4</sub> into the incommensurable state (the *R* phase) produced by an anion ordering of the type Q<sub>3</sub> considered below.<sup>40</sup>

Of most interest is the structure  $Q_3$ . In that case the alternation of crystal fields in the transverse b direction leads, for a sufficiently small transverse bandwidth, to an alternation in the electron densities on neighboring chains. Because of this the values of the Fermi momentum (38) alternate. As a result, firstly, the commensurability of the wave vector of the dimerized anion potential and of the Fermi momenta  $k_{F}^{(n)}$  on each chain is violated. If condition (39) is satisfied, the gap in the charge channel vanishes as a result of the transition to an incommensurate phase and does not guarantee a large coherent jump of magnons (see subsection 4.1). The vanishing, not explained by the band theory, of the instability to the formation of SDW in the incommensurate phase, indicates that this effect is essentially quasi-one-dimensional. Secondly, the difference of  $k_F^{(n)}$  on neighboring chains leads, as we described in subsection 4.2, to a coherent jump of Cooper pairs and, thus, also to superconductivity.

As we discussed in subsection 4.2, for our theory of superconductivity to be valid when the structure  $Q_3$  is present, it is necessary that a number of conditions are satisfied. Condition (47) in the *g*-ological model means that

$$2g_2-g_1>0,$$
 (93)

i.e., there is an effective attraction in the charge channel. As to the energy scales of the problem, we have for them Eq. (53). According to experimental data,  $T_c \approx 1$  K. If we use for estimates (see below) the optical data  $2\pi \approx 40$  K,  $T_{3d} \approx 10$  K from the transition temperature of commensurate SDW (see above), and  $T_{3d}^*$  from Eq. (50), we find that inequality (53) is satisfied as to order of magnitude. The estimates made for the transverse bandwidth do not agree with those generally accepted in the band picture<sup>2,3</sup> but do not contradict any direct measurements whatever. Another possibility is that the region where the effect exists is broader than the region where the quasi-one-dimensional theory is applicable, so that one can forgo some of the inequalities (53). As we discussed in subsection 4.2, to contract the electrons when they jump one needs only satisfy the condition  $x \gg T_c$  which is certainly satisfied in the compounds considered. In such a case inequality (52) also drops out; strong interactions are required to satisfy that one. However, this possibility needs to be studied further.

The effects of SDW restoration in strong magnetic fields also have a unique character when there is structure of the type  $Q_3$  present. These effects, especially the oscillatory behavior, require a more detailed study than the analysis of the simplified model with  $\varkappa = 0$ ,  $g_3 = 0$  in subsection 4.3. Here we mention merely that the period of the oscillations of the magnetoresistivity can be determined by the condition  $Hbl = 2\phi_0/n$ , where *n* is an integer,  $\phi_0$  is a flux quantum,  $l = \hbar v_F/\varkappa$  is the complete period of the structure along the chain with (38) taken into account. One can show that when a magnetic field and the structure  $Q_3$  are present at the same time, SDW exist even when condition (93) is satisfied, i.e., in the case of an effective attraction.

We showed in subsection 4.4 that a disordered anion potential also stimulates superconductivity, so that the problem arises why (TMTSF)<sub>2</sub>ClO<sub>4</sub> is not superconducting in the Q phase. However, this mechanism is less effective than the formation of the  $Q_3$  structure. From the estimates using Eqs. (61), (39) and taking the values of x and  $\Delta_c$  given above into account, we find easily that  $\xi_{imp} \sim W x^{-2}$  $> \xi_c \sim \Delta_c^{-1} > x^{-1}$  so that a substance in the Q phase is in the commensurate dielectric phase whereas in the R phase the commensurability is lost. We note that according to the band theory nonmagnetic disorder must strongly suppress SDW but not affect the superconducting transition temperature; this is in complete contradiction to the Q and R phases of (TMTSF)<sub>2</sub>ClO<sub>4</sub>.

The presence of a superstructure of the  $Q_3$ -type has been finally established only for the compound  $(TMTSF)_2ClO_4$ . For the compounds  $(TMTSF)_2ReO_4^{41}$ and  $(TMTSF)_2FSO_3^{43}$  it has been ascertained that at a certain pressure the type of anion ordering changes, and at the same time superconductivity appears. The type of the new structure has not yet been elucidated. Our assumption is that a structural transition of the type  $Q_3$  occurs in these and all other compounds where superconductivity is observed only under pressure.

The results of the present paper may turn out to be useful also for an interpretation of the properties of the quasione-dimensional conductors  $MX_3$  (M = Nb, Ta; X = S, Se) in which CDW and superconductivity compete. Under well defined conditions superconductivity is observed in TaSe<sub>3</sub>, NbSe<sub>3</sub>, and NbS<sub>3</sub><sup>43</sup> while in all these substances there are two or three (in NbSe<sub>3</sub>) different kinds of chains.<sup>44</sup> Thanks to the development of CDW the quantities  $2k_F^{(n)}$  have been measured experimentally in these substances; for instance, in NbSe<sub>3</sub>  $x = 0.02 k_F$ .<sup>44</sup> In NbSe<sub>3</sub> a selective effect of each of the structural instabilities on the NMR signal of the Nb atoms which are positioned on different kinds of chains was established,<sup>45</sup> which indicates the validity of the inequality  $\varkappa \langle T_{3d} \rangle$  assumed in subsection 4.2. An important distinction of the MX<sub>3</sub> compounds is the presence of a gap in the spin channel. In that case the effects of the interchain nonequivalence are not the only but rather additional superconductivity mechanisms. The transitional region from CDW to superconductivity corresponds probably to the theory of Ref. 46. It is interesting that it has recently been shown for a new class of organic superconducting compounds<sup>47</sup> (BEDT-TTF)<sub>2</sub>I<sub>3</sub> that the superconducting transition precedes the structural transition into the incommensurate phase.<sup>48</sup> On the basis of the data and the theory given in Section 4 we conclude that incommensurability is a necessary condition for the superconducting transition.

#### 6.2. Superconducting properties

In this subsection we compare the results of Section 5 with the observed properties of the superconducting phase of Bechgaard salts. To study the Ginzburg-Landau functional (62) we must specify the form of  $t^2(\mathbf{q}_1)$ . It is natural to assume that in the compounds considered the jump amplitude is maximal between nearest neighbors along the **b** axis. There is also a small jump amplitude along the vector **c** but these transitions take place between equivalent chains and can be neglected. However, it is clear from the structure of the compound (see, e.g., Ref. 3) that the amplitude for jumps along the vector  $\mathbf{b} + \mathbf{c}$  may be of the same amplitude; those occur between alternating chains. In the strong coupling approximation we then get

$$t^{2}(\mathbf{q}_{\perp}) = 2[t_{b}^{2} \cos q_{b} b + t_{c}^{2} \cos (q_{b} b + q_{c} c)].$$
(94)

Expanding expression (94) for small  $q_b$  and  $q_c$ , and neglecting cross terms under the condition  $t_b \ge t_c$ , we get the following expression for the functional (62):

$$\Phi \{\Psi\} = \sum_{\mathbf{q}} |\Psi(\mathbf{q})|^{2} \left( \frac{T - T_{c}}{T_{c}} + \xi_{a}^{2} q_{\parallel}^{2} + \xi_{b}^{2} q_{b}^{2} + \xi_{c}^{2} q_{c}^{2} \right)$$
  
+  $\frac{C_{3}}{T^{2}} \sum_{\mathbf{n}} \int dx |\Psi_{\mathbf{n}}(x)|^{4}, \ \xi_{a}^{2} = C_{1}/T_{c}^{2}, \quad \xi_{b}^{2} = b^{2}/2,$   
 $\xi_{c}^{2} = c^{2} t_{c}^{2}/2 t_{b}^{2}.$ (95)

One can easily determine from the form of the functional (95) that fluctuation effects must be large. The experimental information about critical fluctuations is ambiguous. On the other hand, according to calorimetric measurements the width of the transition is small:  $\tau \approx 4\%$ .<sup>49</sup> On the other hand, according to resistivity measurements it is appreciably larger: several tens of per cents.<sup>50</sup> One deduces easily from Eq. (95) that the jump in the heat capacity is  $\Delta C \sim T_c$ , i.e., in dimensional units  $\Delta C/C_n \sim 1$ , where  $C_n$  is the heat capacity of the normal state at  $T = T_c$ , which qualitatively agrees with the experimental data.<sup>49</sup>

We now evaluate the upper critical fields of the superconductivity. It is well known that it follows from the Ginzburg-Landau theory for an anisotropic superconductor that

$$H_{c2}^{(i)\prime} \equiv T_c \frac{dH_{c2}^{(i)}}{dT} \Big|_{T_c} = \frac{\phi_0}{2\pi\xi_i\xi_k}, \quad \phi_0 = \frac{\pi\hbar c}{e}, \quad i\neq j\neq k,$$
(96)

where i,j,k indicate the **a**,**b**,**c** axes. To get an estimate we take in Eq. (81)  $\eta = 1$  and use the data of Ref. 49 for the density of states. Using (95) we get in dimensional units

$$H_{c2}^{(e)\prime} = \frac{1}{2\pi} \left(\frac{2}{C_1}\right)^{\frac{1}{2}} \frac{\phi_0}{ab} \frac{T_c a}{\hbar v_F} \approx 8 \text{ kOe}.$$
(97)

The estimate (97) agrees in order of magnitude with the experimental value 1 kOe.<sup>51</sup> Further we get from Eq. (96)

$$H_{c2}^{(b)\prime} = (t_b/t_c) H_{c2}^{(c)\prime}.$$

Starting from the experimental value<sup>51</sup>  $H_{c2}^{(b)'}/H_{c2}^{(c)'} = 16$  one must take  $t_b/t_c = 16$ . Using that value we get from (96)

$$H_{c2}^{(a)} = \frac{\phi_0}{\pi bc} \frac{t_b}{t_c} \approx 6.10^4 \text{ kOe} .$$
 (98)

The value (98) does not agree at all with the experimental value 47 kOe.<sup>51</sup> The functional (95) thus gives the correct order of magnitude for  $H_{c2}^{(c)}$  and, for a reasonable value of the fitting parameter  $t_b/t_c$ , for  $H_{c2}^{(b)}$ , but is in complete disagreement with the experimental value for  $H_{c2}^{(a)}$ . The reason for this disagreement may be the appreciable quasi-one-dimensionality of these systems which was not taking into account by us when deriving (95). Because  $t_c \ll t_b$  the relative fluctuations in the order parameter in different planes are much larger than in a single plane. The Ginzburg-Landau theory (95) with fluctuations neglected can thus give results which are correct as to order of magnitude only for motion in the *ab* plane, i.e., for a magnetic field along the **c** axis.

We note that the Josephson coupling between chains using the mechanism described in subsection 4.2 manifests itself in fact when  $T_{ao} \gg T_c$ . The presence of such a coupling explains those effects which in Ref. 1 were ascribed to the presence of a superconducting pseudo-gap: the large magnetoresistance and the temperature dependence of the resistivity (see the theory in Ref. 52). At the same time there are no anomalies in the heat capacity of the system which would show up if there were a pseudo-gap present. The pseudo-gap in the optical spectra of the compounds considered with an energy  $\omega_0 = 3.8 \text{ meV}$  can also be ascribed<sup>2</sup> by the direct transitions of electrons between two subbands having the same superstructure  $\mathbf{Q}_3$ :  $\omega_0 = 2\varkappa$ . In that case the sensitivity of the optical absorption to the magnetic field is explained by the fact that it is connected with electron transport between different chains, and the matrix element of the transport depends on the magnetic field.

<sup>&</sup>lt;sup>1)</sup>Systems with small  $t_1$ , but strong  $g_1$ , were studied in Ref. 13. In that case as a rule the CDW instability must develop at relatively high temperatures which does not correspond to the observed effects in the materials which are of interest to us. The case of weak electron-electron interac<sub>7</sub> tions for intermediate (see Section 3) values of  $t_1$  was considered in Ref. 14.

<sup>&</sup>lt;sup>2)</sup>It was shown in Ref. 29 that, generally speaking, there exists also an interaction (16) for i = SDW. It is given by backward scattering processes with an inversion of the electron spin on different lattices, i.e., by relativistic effects: dipole and spin-orbit interactions. For this reason  $\lambda_{SDW}$  is relativistically small and, as compared to tunneling effects, can be neglected.

<sup>&</sup>lt;sup>3)</sup>We note that for yet stronger interactions the condition  $\eta_F > 2$  may be satisfied from which it follows [see (22)] that  $T_{3d} = 0$ , i.e., the band regime is not satisfied under any conditions. We shall not consider that case, assuming everywhere that  $\eta_F < 2$ .

- <sup>4)</sup>This problem was considered in Ref. 32 for the case of a gap in the *s* channel. Our results differ from the results of Ref. 32.
- <sup>5)</sup>A model describing the competition of different kinds of anion ordering was proposed in Ref. 53.
- <sup>6)</sup>An exception are the compounds  $(TMTTF)_2 PF_6^{38}$  and, possibly,  $(TMTTF)_2 A_5 F_6^{5}$ , in which CDW at low temperatures rather than SDW are observed.
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