Influence of electron hopping processes on a phase transition in a quasione-dimensional electron–phonon system

V. P. Lukin

A. A. Zhdanov State University, Leningrad
(Submitted 1 December 1979)
Zh. Eksp. Teor. Fiz. **78**, 2316–2331 (June 1980)

An investigation was made of the influence of the kinetic coupling on the behavior of a quasione-dimensional electron–phonon system in the energy range $\varepsilon_1 < \omega_0$. A diagrammatic analysis shows that the terms most important in the description of this system are those which govern the dependences on the kinetic coupling parameters. Summation of the leading terms of expansions by the renormalization group method gives equations which make it possible to study the gradual development of an instability in such a system. It is shown that the behavior of a quasione-dimensional system is governed by the influence of two factors: three-dimensional effects and one-dimensional fluctuations. In the selected model the greatest instability corresponds to a structural transition which produces a superstructure with a doubled transverse period. The dependence $T_p(\varepsilon_1)$ is determined in the range $\varepsilon_1 < \omega_0$. A superconducting transition is discussed briefly and the reasons for its suppression at low values of ε_1 are explained. The results obtained are compared with the experimental data.

PACS numbers: 74.10. + v, 63.20.Kr

1. INTRODUCTION

Allowance for the coupling between chains is most important in the case of a quasione-dimensional system. We can distinguish the kinetic coupling, due to electron hopping from chain to chain, and the potential coupling, due to the interaction between electrons in different chains. The influence of the potential coupling has been investigated sufficiently thoroughly in the example of a four-fermion model.[1,2] The influence of the kinetic coupling has been investigated only within the framework of one or another variant of the average field theory using the same model.[3-5] It has been assumed in these investigations that right up to temperatures $T = \varepsilon_1$, where ε_1 is the value of the first transverse resonance integral, the behavior of a system of this kind does not differ from that of a one-dimensional system and we can use purely one-dimensional solutions. In the range $T < \varepsilon_1$ it is assumed that the system exhibits "three-dimensional" behavior which can be described by the parquet or ladder approximations. A complete solution is found by matching the results of these two approximations at the boundary $T = \varepsilon_1$.

The validity of this approach is limited, on the one hand, by the condition of the validity of the ladder of parquet approximation in the three-dimensional range (at low values of ε_1 these approximations are clearly inapplicable). On the other hand, it is not quite clear whether it is possible to describe the behavior of a system at other temperatures by purely one-dimensional solutions. One of the tasks of the present study will be to settle this question in the case of an electron–phonon system. We shall show that at relatively high temperatures the behavior of a quasione-dimensional system is governed by two factors: three-dimensional effects, tending to establish correlations between electrons in different chains, and effects associated with one-dimensional fluctuations tending to destroy such correlations.

Cooling tends to enhance both effects. The degree of growth of one-dimensional fluctuations can be regarded as dependent on the unrenormalized coupling constant g_0. Thus, in the one-dimensional case, the lower the value of g_0, the lower the temperatures at which these fluctuations become significant or one can say also the lower the growth rate of such fluctuations. In the temperature range $T < \omega_0$ investigated below, where ω_0 is an energy of the order of the Debye value, the three-dimensional effects can be described by

$$\gamma_0 = \frac{3\varepsilon_1^2}{2(\pi^2\lambda^2+2\varepsilon_1^2)}\left(1+\ln\frac{\omega_0}{\lambda}\frac{\pi^2\lambda^2}{\pi^2\lambda^2+2\varepsilon_1^2}\right),$$

where λ is a normalization parameter defined below. Depending on the relationship between g_0 and γ_0, we can distinguish two cases.

In the first case, when $g_0 > \gamma_0$, the one-dimensional fluctuations increase at first faster and there is a range of temperatures in which these fluctuations predominate and where the behavior of the system is close to one-dimensional. In the second case, when $g_0 < \gamma_0$, the three-dimensional effects grow more rapidly and the one-dimensional fluctuations do not appear. Consequently, throughout the temperature range $T < \omega_0$ the system behaves as three-dimensional. At relatively high values of ε_1 ($\gamma_0 > 1/8$) the region of one-dimensional behavior of the system cannot be isolated for any value of g_0 and the situation resembles the second case.

In addition to this process, we shall consider also the influence of the kinetic coupling on the temperature of a phase transition at low values of ε_1 ($\varepsilon_1 < \omega_0$) when the average field approximation is inapplicable. In view of the special nature of the selected model, we shall concentrate our attention on a structural Peierls transition which predominates in this range of values of ε_1 and T and we shall discuss only briefly a superconducting transition. We shall solve these problems by identifying and summing the leading (major) terms of expan-

 0038-5646/80/061162-09$02.40

sions in perturbation theory. With this in mind we shall carry out a diagrammatic analysis which makes it possible to identify the features of the quasione-dimensional problem. We shall end by discussing the main conclusions and comparing the results obtained with the experimental data.

2. FORMULATION OF THE PROBLEM

We shall consider a quasione-dimensional electron-phonon system and confine our attention to the interaction of electrons with longitudinal acoustic phonons. We shall assume that the system is strongly anisotropic because of its crystal structure: chains are packed in a square lattice, the distance between the chains is b, and the distance between the atoms in a chain is a, where $b > a$. In the tight-binding approximation for a half-filled band the electron dispersion law $\varepsilon(\mathbf{k})$ can be written in the form

$$\varepsilon(\mathbf{k}) = -\varepsilon_0 \cos k_x a - \varepsilon_1(\cos k_x b + \cos k_y b) + O(\varepsilon_2), \quad (1)$$

where the z axis is directed along the chains and $O(\varepsilon_2)$ denotes the contribution of the electron jumps to the second-nearest sites; ε_2 is the value of the second transverse resonance integral. In the selected model the phonon spectrum $\omega(\mathbf{q})$ is also anisotropic and has the form

$$\omega^2(\mathbf{q}) = \omega_0^2 \sin^2 {}^1/_2 q_z a + \omega_1^2(\sin^2 {}^1/_2 q_x b + \sin^2 {}^1/_2 q_y b). \quad (2)$$

The Fermi energy is described by

$$\varepsilon(\mathbf{k}) = 0. \quad (3)$$

We shall assume that the following conditions are satisfied in the quasione-dimensional case

$$\varepsilon_2/\varepsilon_0 < \varepsilon_1/\varepsilon_0 \ll 1, \quad \omega_1/\omega_0 \ll 1. \quad (4)$$

We shall postulate that $\hbar = k_B = 1$. The matrix element of the electron–phonon interaction $v_0(\mathbf{q})$ can be represented in the form

$$v_0(\mathbf{q}) = \rho_0 \sin {}^1/_2 q_z a + \rho_1 f(q_x, q_y), \quad (5)$$

where ρ_0 and ρ_1 are, respectively, the longitudinal and transverse coupling constants; $f(q_x, q_y)$. If we determine the value of $v_0(\mathbf{q})$ in the Fröhlich approximation,[6] we find that ρ_1 is proportional to ω_1, but if the tight-binding approximation[7] is used (which is more correct in the present case), the value of ρ_1 is proportional to ε_1.

We shall be interested in how the kinetic coupling gives rise to an instability and a phase transition. With this in mind we shall investigate the behavior of the relevant Green functions depending on temperature and on the parameters ε_i $(i = 1, 2)$. The values of the external electron $\mathbf{k}$ and phonon $\mathbf{q}$ momenta will be selected to be such that the instability is strongest. In this model the electron spectrum has the property

$$\varepsilon(\mathbf{k}) = -\varepsilon(\mathbf{k}+\mathbf{Q}) + O(\varepsilon_2), \quad \mathbf{Q} = (\pi/a, \pi/b, \pi/b). \quad (6)$$

This is known to have the consequence that in the analysis of structural transitions the most singular terms correspond to $\mathbf{q} = \mathbf{Q}$ and the electron momenta should lie on the Fermi surface. In the case of a superconducting transition, when a study is made of an instability relative to electron pairing near the Fermi surface, the most singular terms are associated with the transfer of a phonon momentum $2\mathbf{k}_F$.

In the case of both transitions we shall be interested in the behavior of specific Green functions: the electron G and the vertex Γ functions in the case of a structural transition and the four-leg vertex Γ_4 in the case of a superconducting transition when the external electron momenta $\mathbf{k}$ lie on the Fermi surface. In view of the strong anisotropy of the problem, the relevant expressions depend strongly on the direction of the vector $\mathbf{k}_F$, particularly in the case of Γ_4 for a superconducting transition. Therefore, it is useful to average the expressions in question over the Fermi surface. We can thus assume that instabilities investigated in this way give rise to insulating or superconducting gaps on the whole Fermi surface, and the critical temperature thus found represents the temperature of a structural or a superconducting transition, respectively.

An investigation of the instability for any one specific direction $\mathbf{k}_F$ can be regarded as equivalent to the assumption of formation of a gap only near certain points on the Fermi surface. This situation cannot be regarded as a transition of the system to an insulating or a superconducting state; at best, the situation represents fluctuation-induced formation of such states. We shall employ the technique of the thermal Green functions.

We shall begin by analyzing a structural transition. In this case it is sufficient to investigate the behavior of the phonon Green function D at zero external frequencies $i\nu_n$, which again requires calculation of G and Γ. We shall assume that $\mathbf{k} = \mathbf{k}_F$ and $\mathbf{q} = \mathbf{Q}$. Moreover, in the final analysis we can also assume that the external electron frequencies $i\omega_n$ vanish. Subject to these conditions we obtain a symmetric theory in which all the quantities depend on one variable T. In the model employed the contribution of the potential coupling is proportional to the parameter ω_1^2/ω_0^2 or $\varepsilon_1^2/\omega_0^2$, depending on the selection of the constant ρ_1. The contribution of the kinetic coupling is proportional to the parameter ε_1^2/T^2. In the range of temperatures $T < \omega_0$ of interest to us we can assume that the contribution of the kinetic coupling predominates over the potential contribution. Therefore, we shall ignore the corrections due to the potential coupling assuming it to be small and, as in Refs. 3–5, we shall simply investigate the influence of the kinetic coupling.

3. ANALYSIS OF EXPANSIONS IN PERTURBATION THEORY

We shall investigate the diagrams for the functions D, G, and Γ in the $\mathbf{q} = \mathbf{Q}$ and $\mathbf{k} = \mathbf{k}_F$ cases. All the results obtained below apply to the temperature range $T < \omega_0$, — whereas shown earlier[8] — the logarithmic theory is applicable. We shall also ignore corrections of the order of $(\omega_0/\varepsilon_0)^2$, i.e., we shall ignore the contributions of the processes involving small transferred momenta which are unimportant in this case.[8] In the problem considered we shall separate, in contrast to the one-dimensional case, the class of ladder diagrams in which integration with the momenta contains only two electron energies. Consequently, these diagrams are less sensitive to the deviation of the spectrum from the one-di-

mensional form than the nonladder diagrams which contain at least one integration with respect to more than two electron energies.

We shall now consider the ladder diagram for Γ in Fig. 1a. Its contribution can be represented in the form

$$\rho_0\{g_0^2[\ln^2 A+2\Phi_0(\alpha_0^2)\ln A+\Phi_0^2(\alpha_0^2)]+O(g_0^2)\}, \quad (7)$$

where $g_0=\rho_0^2/\pi ab^2\varepsilon_0\omega_0$ denotes the dimensionless "bare" coupling constant, $A=\pi T/2\omega_0\gamma, \gamma=1.78$, and $\alpha_0=\varepsilon_2/2\pi T$. The function Φ_0 appears as a result of integration with respect to the transverse momenta and it is given by the following Mellin–Barnes integral[9]:

$$\Phi_0(z)=\frac{1}{2\pi i}\int_L \frac{\Gamma(-s)\Gamma(1+s)\Gamma^2(3/2+s)\zeta(2s+3,1/2)z^{s+1}}{\pi\Gamma^2(2+s)}ds, \quad (8)$$

where $\zeta(x,v)$ is the generalized zeta function. The function $\Phi_0(z)$ plays an important role in this problem and, therefore, we shall give expansions for this function

$$\left.\begin{aligned}\Phi_0(z)&=\sum_{n=0}^{\infty}\frac{(-1)^n z^{n+1}\Gamma^2(3/2+n)\zeta(2n+3,1/2)}{\pi\Gamma^2(2+n)}, \quad z<1,\\ \Phi_0(z)&=\ln 2\gamma z^{1/2}-\frac{2}{\pi^2 z^{1/2}}\sum_{n=0}^{\infty}\frac{(-z)^{-n}\Gamma^2(1/2+n)\zeta'(-2n,1/2)}{\Gamma^2(1+n)}, \quad z>1,\end{aligned}\right\} \quad (9)$$

where $\zeta'(x,v)$ is the derivative of the zeta function. It follows from Eqs. (7) and (9) that if $\alpha_0\gg 1$, the logarithmic terms are "truncated" at the value ε_2. An analysis of the ladder diagrams in higher orders shows that the influence of the kinetic coupling is described in all orders by the function $\Phi_0(\alpha_0^2)$. In this sense the diagrams considered here exhibit universal behavior.

We shall now discuss the nonladder diagram for Γ shown in Fig. 1b. Its contribution can be written in the form

$$\rho_0\{g_0^2[\ln^2 A+(\Phi_1(\alpha_1^2)+\Phi_0(\alpha_0^2))\ln A+\Phi_1(\alpha_1^2)\Phi_0(\alpha_0^2)]+O(g_0^2)\}, \quad (10)$$

where $\alpha_1=\varepsilon_1/2^{1/2}\pi T$. The function Φ_1 again appears as a result of integration with respect to transverse momenta allowing for averaging over the Fermi surface but in the case of Φ_1 we cannot find a representation of the (8) type and we can then describe this function by

$$\Phi_1(\alpha_1^2)=\int_0^{\infty}\frac{e^{-t/2}[J_0^4(2^{-1/2}\alpha_1 t)-1]}{1-e^{-t}}dt, \quad (11)$$

where J_0 is a Bessel function. It follows from Eq. (11) that

$$\Phi_1=\Phi_0(\alpha_1^2)+\varphi(\alpha_1^2), \quad (12)$$

where the function $\varphi(z)$ behaves as

$$\varphi=\begin{cases}z^2+O(z^4), & z\ll 1\\ z^{-1}+O(z^{-2}), & z\gg 1,\end{cases}$$

and we can assume that it describes small corrections

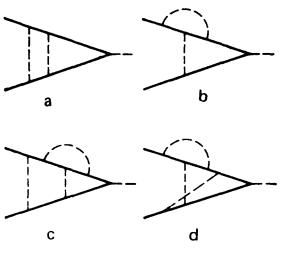

FIG. 1. Diagrams for the vertex function Γ.

to $\Phi_0(\alpha_1^2)$. We shall now assume that

$$\Phi_1(\alpha_1^2)\approx\Phi_0(\alpha_1^2). \quad (13)$$

We can see from Eqs. (7) and (10) that the behavior of the ladder and nonladder diagrams is different. For example, in the diagram in Fig. 1b the influence of the kinetic coupling is described mainly by the function $\Phi_1(\alpha_1^2)$, whose temperature dependence is governed by the parameter ε_1. Hence, as indicated by Eqs. (7) and (10), cooling reduces the contribution of the nonladder compared with the ladder diagrams and in the range $\alpha_1\gg 1$ there is a reduction in the degree of the principal logarithmic contribution of the nonladder diagrams. It should be noted that in this case the dependence on the direction of the vector $\mathbf{k}_F$ is governed mainly by the nonladder diagrams, but this dependence is very weak.

These examples show that, in addition to the leading and secondary logarithms of the usual kind, we can identify in the perturbation-theory expansions also secondary logarithms with coefficients which are functions of the parameters ε_i^2/T^2. We shall call them the logarithms of the second kind. All the influence of the kinetic coupling discussed above is due to these terms. Therefore, it is important to find the structure of logarithms of the second kind. There is no need to consider the terms containing the function $\Phi_0(\alpha_0^2)$, i.e., terms of the type $g_0\Phi_0(\alpha_0^2)(g_0\ln A)$ etc., whose structure and allowance are trivial matters, but it is necessary to find the structure of terms of the $g_0\Phi_1(\alpha_1^2)(g_0\ln A)$ type generated by the nonladder diagrams.

With this in mind we shall consider briefly the diagrams for Γ in the fourth order. The addition of a "crossbar" to the diagram in Fig. 1b gives rise to diagrams of the kind shown in Fig. 1c, which are due to terms of the type $g_0\Phi_1(\alpha_1^2)(g_0\ln A)^2$ considered here. The addition of nonladder elements to Fig. 1b gives diagrams of the type shown in Fig. 1d, which also have terms of the $g_0F_2(\alpha_1^2)(g_0\ln A)^2$ type considered here, but the function F_2 is now different from Φ_1. The function F_2, like Φ_1, can be approximated as follows:

$$F_2(\alpha_1^2)\approx\Phi_0(4\alpha_1^2). \quad (14)$$

Comparing Eqs. (13) and (14), we can conclude that the higher-order diagrams generally contain, as the parameters of truncation at ε_1, larger quantities than the lower-order diagrams. This nonuniversal dependence on the parameter ε_1 plays an important role in the problem under discussion.

The contribution of terms of this kind due to all the fourth-order diagrams can thus be written in the form $g_0\Phi_2(\alpha_1^2)(g_0\ln A)^2$, where the function Φ_2 is expressed in terms of Φ_1 and F_2. An analysis of higher order shows that the addition of nonladder elements gives rise to diagrams containing functions $F_n(\alpha_1^2)$ which are different in each order so that the sum of the terms of this kind in each order also contains different functions $\Phi_n(\alpha_1^2)$ and these terms have the structure

$$g_0\Phi_n(\alpha_1^2)(g_0\ln A)^{n_1}. \quad (15)$$

The diagram 1d also gives rise to terms of the $g_0^2\Phi_1(\alpha_1^2)F_2(\alpha_1^2)(g_0\ln A)$ type, which behave approximately as $g_0^2\Phi_1^2(\alpha_1^2)(g_0\ln A)$. The structure of these terms is

similar to the structure of the terms discussed above:

$$g_0^2\Phi_n^2(\alpha_1^2)(g_0\ln A)^{n_1}. \quad (16)$$

We can easily see that there are terms of the $g_0^2\Phi_n(\alpha_1^2)(g_0\ln A)^{n_2}$ and similar types.

The examples given reveal the general structure of logarithms of the second kind. The terms containing the function $\Phi_0(\alpha_0^2)$, including cross terms of the $g_0\Phi_0(\alpha_0^2)\Phi_n(\alpha_1^2)(g_0\ln A)^{n_2}$ kind, can easily be included by introducing the variables

$$\tilde{\ln} A=\ln A+\Phi_0(\alpha_0^2), \quad \tilde{\Phi}_n=\Phi_n(\alpha_1^2)-\Phi_0(\alpha_0^2), \quad (17)$$

since the dependence on $\Phi_0(\alpha_0^2)$ is universal for all the diagrams.

The nature of the expansions for the function D is similar to Γ. The structure of the expansions of the function G depends on the ratio $|\omega|/T$, but since we are interested in the influence of temperature on the system, we shall go to the limit $|\omega|/T\to 0$ and to the same limit in the expansions of G. The logarithmic terms in the expression for G are given by the nonladder diagrams so that terms of the $g_0^2\tilde{\Phi}_1$ and similar type appear and these should be regarded as nonlogarithmic. Since in our problem the Green function $G_0(i\omega_n, k_F)$ is equal to $G_0=1/i\omega_n$, it is convenient to introduce the following dimensionless function

$$d=G_0^{-1}G, \quad (18)$$

and then go to the limit $|\omega|/T\to 0$. The nature of expansions for d is similar to the expansions described above.

We can thus see that the general structure of the perturbation theory expansions in the quasione-dimensional case at temperatures $T<\omega_0$ is

$$\begin{aligned}&(g_0\tilde{\ln} A)^n+g_0(g_0\tilde{\ln} A)^{n_1}+g_0\tilde{\Phi}_n(g_0\tilde{\ln} A)^{n_1}\\&\quad+g_0^2(g_0\tilde{\ln} A)^{n_2}+g_0^2\tilde{\Phi}_n^2(g_0\tilde{\ln} A)^{n_2}\\&+g_0^2\tilde{\Phi}_n(g_0\tilde{\ln} A)^{n_2}+\ldots+O(g_0^2\tilde{\Phi}_1)\quad\ldots,\end{aligned} \quad (19)$$

i.e., it can be represented as a series in powers of $g_0\tilde{\ln} A$ including regular corrections in respect of the coupling constant g_0 and also in respect of the kinetic coupling parameters described in terms of the function $\tilde{\Phi}_n$.

4. DERIVATION OF MAIN EQUATIONS

In solving the problems formulated above we shall be interested mainly in the range of values of ε_1 and T such that $\alpha_1<1$. In describing this range it is sufficient to include the first corrections in respect of the kinetic coupling, which are given by the terms $g_0\tilde{\Phi}_n(g_0\tilde{\ln} A)^n$ and which have to be added to the solution of the one-dimensional problem. In fact, in the range $\alpha_1<1$ these terms are leading among the logarithms of the second kind and the other terms [see Eqs. (9) and (19)] contain in each order an additional parameter which is small because of $\alpha_1^2\ll 1$ or because of $g_0<1$. We shall describe the one-dimensional system by including the first two terms in Eq. (19) which is known[8] to give the correct solution for this system but strictly speaking the approach is then approximate.

Bearing in mind these points, we shall now sum the following terms:

$$(g_0\tilde{\ln} A)^n+g_0(g_0\tilde{\ln} A)^{n_1}+g_0\tilde{\Phi}_n(g_0\tilde{\ln} A)^{n_1}. \quad (20)$$

We can see from Eqs. (9) and (19) that the approximation (20) is valid also in the range $\alpha_1>1$ but it is incorrect in the range $\alpha_1\gg 1$, where terms $g_0\tilde{\Phi}_n(g_0\tilde{\ln} A)^{n_1}$ have to compete with terms of the (16) type, and where the nonlogarithmic terms become important. The condition of smallness of the terms subjected in each order, compared with those included, gives rise to the following restriction on T:

$$T\gg\varepsilon_1^2/\omega_0, \quad (21)$$

which determines the temperature range of the validity of the approximation (20). In the derivation of (21) we have omitted terms of the order of $(\varepsilon_2/\varepsilon_1)^2\ll 1$ and have imposed a stringent condition. The approximation (20) allows us to calculate the critical temperature T_p of a structural transition. The temperature T_p should satisfy the condition (21), which is true only for certain small values of ε_1. We shall show that the approximation (20) allows us to describe practically the whole range $\varepsilon_1<\omega_0$. In the summation of terms in Eq. (20) we shall use the renormalization group method following the general approach employed by the present author in an earlier paper.[8]

In the case under consideration we are dealing with a theory with four dimensional constants: ε_0, ω_0, ε_1, and ε_2. The values of ε_i then act as the parameters of the "infrared truncation" and, in contrast to the one-dimensional case, all the quantities in the theory depend on the dimensional constants of the problem in the range $T<\omega_0$. Consequently, we have here a theory with "masses" represented by the parameters ω_0 and ε_i. The general procedure for the derivation of the renormalization group equations[10] used earlier[8] allows us to sum all the terms, including logarithms of the second kind, by considering in the latter the functions $\tilde{\Phi}_n$ to be some functions of the mass variables.

We shall consider the renormalized Green functions d_R, D_R, and Γ_R related to the unrenormalized functions d, D, and Γ by the usual renormalization group transformation. We shall assume that the renormalized functions depend not only on T but also on the dimensionless renormalized coupling constant g_R and the dimensional constants ω_0, ε_0, and ε_i. Instead of the "bare" quantities ω_0, ε_0, and ε_1 we can introduce renormalization in the usual way[10] assuming that these quantities are equal to the values observed in the range under consideration.

Prigodin and Firsov[5] introduced multiplicative renormalization of ε_1. It should be noted that this procedure is possible and meaningful only if we can renormalize all the other quantities and functions in the theory independently of ε_1, but—as indicated by the above analysis—this is not possible in the problem under discussion. We shall consider the range of values of ε_1 and T of interest to us by selecting a normalization parameter λ satisfying the conditions

$$\lambda<\omega_0, \quad \varepsilon_1\leqslant\lambda, \quad T\leqslant\lambda, \quad (22)$$

which are selected so as to remain within the logarithmic theory framework. Repeating all the procedures of the earlier investigation,[8] we obtain the following relationship between the constants g_R and g_0 correct to within terms of the order of g_0^3:

$$g_R=g_0\{1-2g_0\widetilde{\ln}\,v+4g_0\eta+4g_0^2\widetilde{\ln}^2 v+4g_0^2\widetilde{\ln}\,v +16g_0^2\eta^2-16g_0^2\eta\widetilde{\ln}\,v-3g_0^2\Phi_1\widetilde{\ln}\,v\}, \tag{23}$$

where

$$\left.\begin{aligned}&\Phi_1=\Phi_1(\delta_1^2),\quad \Phi_0=\Phi_0(\delta_0^2),\quad \delta_1=\varepsilon_1/2^{1/2}\pi\lambda,\\ &\delta_0=\varepsilon_2/2\pi\lambda,\quad v=\lambda/\omega_0,\quad \eta=\ln(\varepsilon_0/\omega_0).\end{aligned}\right\} \tag{24}$$

The last term in Eq. (23) is due to logarithms of the second kind, and the functions Φ_1 and Φ_0 depend on the mass variables δ_1 and δ_0.

In the symmetric theory under discussion the behavior of the Green functions is governed by the behavior of the invariant coupling constant $\tilde{g}_R$. The equation for $\tilde{g}_R(t, \varepsilon_i/\lambda, \omega_0/\lambda)$, where $t=\ln(\lambda/T)$ is of the form (see Ref. 8)

$$d\tilde{g}_R/dt=\beta(\tilde{g}_R, \tilde{\varepsilon}_i(t)/\lambda, \tilde{\omega}_0(t)/\lambda) \tag{25}$$

subject to the boundary condition $\tilde{g}_R(0)=g_R$. The function $\beta(g_R, \varepsilon_i/\lambda, \omega_0/\lambda)$ is[1)]

$$\beta=2sg_R^2-4f(\varepsilon_i/\lambda, w_0/\lambda)g_R^3, \tag{26}$$

where

$$\left.\begin{aligned}&s=1+\Phi_0'(\delta_0^2),\\ &f=s-{}^3/_4\Phi_1'\widetilde{\ln}\,v-{}^3/_4\Phi_1 s.\end{aligned}\right\} \tag{27}$$

In Eq. (27), we have introduced

$$\tilde{\Phi}_1'=\lambda\frac{\partial}{\partial\lambda}\tilde{\Phi}_1. \tag{28}$$

The effective parameters of the problem $\tilde{\varepsilon}_i(t)$ and $\tilde{\omega}(t)$ are[8]

$$\tilde{\varepsilon}_i(t)=\varepsilon_i e^t,\quad \tilde{\omega}_0(t)=\omega_0 e^t. \tag{29}$$

The influence of the kinetic coupling in Eq. (25) is described by the function $f(t)=f[\tilde{\varepsilon}_i(t)/\lambda, \tilde{\omega}_0(t)/\lambda]$. Equation (25) shows how an instability develops in a system. Cooling increases the parameters $\tilde{\varepsilon}_i$ and $\tilde{\omega}_0$ and reduces the function $f(t)$, which vanishes as some temperature $T=T_0$ and then changes sign. The change of sign of the coefficient in front of g_R^3 means that $\tilde{g}_R$ begins to grow rapidly and becomes singular at some temperature $T=T_p$. The occurrence of this singularity can be regarded as an indication of an instability in the system and of a phase transition at $T_p=T$. Since an analytic solution of Eq. (25) is not generally possible, we shall give the results of the solution of Eq. (25) and supplement them whenever possible by analytic reasoning. It is convenient to divide the whole investigated temperature range into two intervals: $T\geqslant T_0$ and $T\leqslant T_0$.

We shall first consider the interval $T\geqslant T_0$, which allows us to study the influence of the three-dimensional effects and of the one-dimensional fluctuations.

5. INTERVAL $T\geqslant T_0$

In an investigation of a structural transition we can simplify Eq. (27) by dropping the function $\Phi_0(\delta_0^2)$ because of its smallness throughout this interval; the resultant error is then of the order of $(\varepsilon_2/\varepsilon_1)^2\ll 1$. It is not convenient to use expansions (9) in numerical solution of Eq. (25) because such expansions diverge at $z=1$. An analysis of these expansions shows that the function $\Phi_0(z)$ can be approximated as follows:

$$\Phi_0(z)={}^1/_2\ln(1+4z). \tag{30}$$

The formula (30) describes well the behavior of $\Phi_0(z)$ in the $z<1$ case, since for $z=1/4$ it follows from Eq. (9) that $\Phi_0(1/4)=0.355$ and it is clear from Eq. (30) that $\Phi_0(1/4)=0.346$. In the range $z\gg 1$, the asymptotes of Eqs. (9) and (30) are practically identical, so that the approximation (30) is sufficiently good in the interval of interest to us.

When Eq. (30) is used, the function $f(t)$ becomes

$$f(t)=1-\frac{3}{4}\frac{4\delta_1^2e^{2t}}{1+4\delta_1^2e^{2t}}\left(\ln\frac{\omega_0}{\lambda}+t\right)-\frac{3}{8}\ln(1+4\delta_1^2e^{2t}). \tag{31}$$

It follows from Eq. (31) that the temperature T_0 is

$$T_0\approx\frac{\varepsilon_1}{2^{1/2}\pi}\left[\frac{3}{2}\ln B-\frac{11}{4}+\left(\left(\frac{3}{2}\ln B-\frac{11}{4}\right)^2+\frac{3}{2}\right)^{1/2}\right]^{1/2}. \tag{32}$$

In Eq. (32) and later we shall use the notation $B=2^{1/2}\pi\omega_0/\varepsilon_1$.

In the investigation of Eq. (25) it is convenient to replace $\tilde{g}_R(t)$ with a function $u(t)$ defined by

$$\tilde{g}_R=u(t)/f(t). \tag{33}$$

The function $u(t)$ obeys

$$\left.\begin{aligned}&f(t)\,du/dt=2u^2-4u^3+f'(t)\,u,\\ &u(0)=u_0=g_Rf(0),\end{aligned}\right\} \tag{34}$$

where $f'=\partial f/\partial t$. The point $t=t_0=\ln(\lambda/T_0)$ is a zero of the function $u(t)$. According to the general theory,[11] the behavior of the solutions of Eq. (34) depends on the relationship between u_0 and $|f'(0)|=2\gamma_0$.

If $\gamma_0<1/8$, we have to distinguish two cases:

$$\left.\begin{aligned}&1)\ u_0>u_2,\quad 2)\ u_0<u_2,\\ &u_2={}^1/_4-{}^1/_4(1-8\gamma_0)^{1/2},\quad u_0<1.\end{aligned}\right\} \tag{35}$$

In the former case the integral curves (34) rise in the interval $0\leqslant t\leqslant t_1$, where the value of t_1 is defined as that t for which the right-hand side of (34) has no real zeros. The value of t_1 corresponds to the temperature

$$T_1\approx\frac{\varepsilon_1}{2^{1/2}\pi}[12\ln B-8+((12\ln B-8)^2+12)^{1/2}]^{1/2},\quad \ln B>5. \tag{36}$$

Then, in the interval $t_1<t\leqslant t_0$ the integral curves decrease to zero. In the second case, we find that throughout the interval $0\leqslant t\leqslant t_0$ the integral curves (34) decrease from u_0 to zero.

In the interval $0\leqslant t\leqslant t_1$ the function $f(t)$ varies slightly from $f(0)$ to $f(0)-1/8$, which allows us to find the approximate solution of Eq. (34) by linearization of $f(t)$ with respect to t: $f(t)\approx f(0)-2\gamma_0 t$.

In this approximation (assuming that $u_0>u_2$), we find that, to within terms of the order of $(u_2/u_0)^2\ll 1$, Eq. (34) yields

$$\left.\begin{aligned}&\frac{1}{u_1}\ln\left|\frac{u_0(u_1-u)}{u(u_1-u_0)}\right|-\frac{1}{u_0}+\frac{1}{u}=\tau,\\ &\tau=\frac{(1-8\gamma_0)^{1/2}}{\gamma_0}\ln\left|1-\frac{2\gamma_0}{f(0)}t\right|\qquad u_1=\frac{1}{4}+\frac{1}{4}(1-8\gamma_0)^{1/2}.\end{aligned}\right\} \tag{37}$$

The first expression in Eq. (37) resembles the one-dimensional solution and, according to Eq. (33), the behavior of $\tilde{g}_R$ in the interval $T \geqslant T_1$ is practically the same as in the one-dimensional case. This is illustrated by the curves in Fig. 2 obtained by numerical solution of Eq. (25) for various values of $\ln B$; the continuous curves correspond to the case $g_R = 0.1$ and the dashed curves to $g_R = 0.3$.

We shall assume that $\ln(\omega_0/\lambda) = 2$, so that the conditions (22) are satisfied with the necessary rigor. The values of $\ln B$ and the positions of the points t_0 and t_1 of the curves are shown in Fig. 2. We can see that in the limit of small values of ε_1 the influence of the one-dimensional fluctuations is so strong that the low-temperature behavior of the system is almost independent of the value of g_R and, since the latter is related to g_0 by Eq. (23), we can speak of a weak dependence on the unrenormalized coupling constant (Fig. 2a). On increase in ε_1 the influence of these fluctuations and the size of the region where they predominate decrease and the behavior of the system depends increasingly on g_0 (see Fig. 2b). Thus, only in the case of a sufficiently strong interaction (and when $\gamma_0 < 1/8$) can we identify a region of one-dimensional behavior of the system whose limit is the temperature T_1. For $t_1 < t \leqslant t_0$, the function $u(t)$ decreases but more slowly than $f(t)$ so that $\tilde{g}_R$ begins to rise significantly (Fig. 2). This behavior can naturally be attributed to the fact that the three-dimensional effects begin to predominate in this region.

If $u_0 < u_2$, the application of the same approximation yields the following expression from Eq. (34)

$$u \exp\left[\frac{u-u_0}{\gamma_0}\right] = u_0\left(1 - \frac{2\gamma_0}{f(0)}t\right). \tag{38}$$

It is clear from Eqs. (33) and (38) that in the range $0 < t < t_1$ the function $u(t)$ decreases and $\tilde{g}_R$ changes slightly relative to its limiting value. This means that for a weak interaction the three-dimensional effects begin to rise faster. In this case the system behaves right from the beginning as three-dimensional and it is greatly affected by the value of g_0. This case is of no physical interest when ε_1 is small since the constant g_R should be exponentially small.

In the case of ε_1 satisfying the condition

$$\varepsilon_1 > \frac{\pi\lambda}{10^{1/2}}\left[\left(\left(2+3\ln\frac{\omega_0}{\lambda}\right)^2+5\right)^{1/2} - \left(2+3\ln\frac{\omega_0}{\lambda}\right)\right]^{1/2} \tag{39}$$

the function $u(t)$ decreases in the interval $0 \leqslant t \leqslant t_0$ irrespective of the value of u_0. In other words, if $\gamma_0 > 1/8$, the three-dimensional effects predominate in the system. For the selected parameters of the problem we can assume that this situation appears when $\ln B = 4$, and $t_1 = 0.015$.

6. INTERVAL $T \leqslant T_0$

The value of $\tilde{g}_R$ rises rapidly at temperatures $T < T_0$ and it has a singularity at $T = T_p$. We can assume that an instability appears in the system at these temperatures. The growth of this instability is demonstrated in Fig. 2 for various values of ε_1.

Numerical solution of Eq. (25) allows us to determine the value of T_p as a function of the parameters ε_1, ω_0, g_R or g_0. As mentioned earlier, the approximation (20) allows us to calculate T_p only in the case of small values of ε_1. Such calculations indicate that for $\ln B = 4$ and $g_R = 0.3$ the condition T_p governing the limit of validity of Eq. (21) is not satisfied sufficiently rigorously and it is disobeyed for $\ln B = 4$ and $g_R = 0.1$. We can thus assume that the approximation (20) makes it possible to determine T_p in the case

$$\ln B \geqslant 4. \tag{40}$$

The value of $\varepsilon_1 = \lambda$ corresponds to $\ln B = 3.5$ so that the approximation (20) allows us to calculate T_p throughout the range of values of ε_1 set by the conditions (22).

The results of such calculations are plotted in Fig. 3. We can see that in the limit of small ε_1 ($\ln B \gg 1$) the finite renormalization of $\tilde{g}_R$ makes the temperature T_p weakly dependent on the "bare" coupling constant g_0 and the values of T_p lie in the range $\alpha_1 < 1$. The shift of the values of T_p in the range $\alpha_1 < 1$ in the $\ln B \gg 1$ case is due to the fact that the total contribution of all the terms is then important and the contributions of different diagrams are known to depend in a different way on the parameter ε_1. On increase in ε_1 the behavior of T_p shows an increasingly strong dependence of g_0 and the values of T_p approach the limit of the region $\alpha_1 = 1$ and go over to $\alpha_1 > 1$.

An analytic expression for T_p can be found in the limit of small values of ε_1 if $\ln B \gg 1$. It then follows from Eq. (31) that the function $f(t)$ rises almost exponentially in the range $t > t_0$ and we have $\tilde{g}_R(t_0) > 1/2$ (Fig. 2a). This means that throughout most of the range considered, with the exception of a small region near t_0, the second term on the right of the right-hand side of Eq.

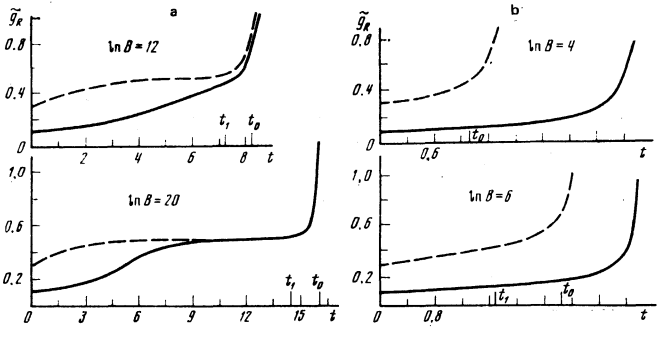

FIG. 2. Behavior of the function $\tilde{g}_R(t)$ for various values of $\ln B$ and g_R.

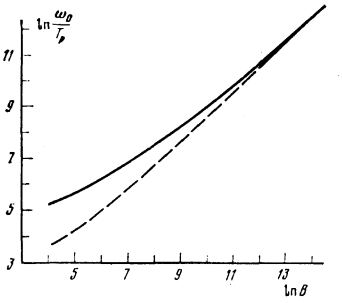

FIG. 3. Dependence of the critical temperature T_p on the parameter ε_1 for $g_R = 0.3$ and $g_R = 0.1$.

(25) is greater than the first. Therefore, in this limit we can describe the range $t > t_0$ by the equation

$$d\tilde{g}_R/dt = -4f(t)g_R^3. \quad (41)$$

Solution of Eq. (41) gives the following equation for the determination of T_p:

$$1 = \tilde{g}_R^2(t_0)\left[3\ln\frac{\omega_0}{T_p}\ln\left(1+\frac{2\varepsilon_1^2}{\pi^2 T_p^2}\right)+4+8\ln\frac{T_0}{T_p}\right]. \quad (42)$$

If $\ln B \gg 1$, the values of T_p lie in the range defined by $2\varepsilon_1^2/\pi^2 T_p^2 \ll 1$ and we can find T_p by expanding $\ln(1+\pi^2 T_p^2)$ as a series in powers of $2\varepsilon_1^2/\pi^2 T_p^2$. We shall consider only the first term of the expansion, which is valid in the adopted limit and which gives

$$T_p = \frac{\tilde{g}_R(t_0)}{[1+6\tilde{g}_R^2(t_0)]^{1/6}}\frac{\varepsilon_1}{2^{1/6}\pi}\left(\frac{36}{5}\ln B\right)^{1/6}. \quad (43)$$

We can obtain $\tilde{g}_R(t_0)$ using the curves in Fig. 2. The formula (43) is in good agreement with the results of calculations for the range $\ln B > 12$.

It is clear from Fig. 2a that in the limit $\ln B \gg 1$ an instability grows very rapidly in the system. This is due to the rapid growth of the effects of the kinetic coupling and also due to the effective renormalization of the coupling constant in the interval $T > T_0$. These two factors can be regarded as reflecting the influence of the one-dimensional approximation and they enhance the critical fluctuations. The approach employed, like any other method based on perturbation theory, is inapplicable in a certain range ΔT_p near T_p, where the critical fluctuations are strong. We can assume that if this region is narrow, $\Delta T_p/T_p \ll 1$, the error is small. In the limit of small values of ε_1 the region $T_0 - T_p$ where an instability appears is narrow: $(T_0 - T_p)/T_p \approx 0.14$ for $\ln B = 20$ and, since the region where the approximation is invalid is less than $T_0 - T_p$, we can assume that in this case we have $\Delta T_p/T_p \ll 1$ and Eq. (43) describes correctly (in the qualitative sense) the limit of small values of ε_1.

The case of small ε_1, when T_p lies within the range $\alpha_1 < 1$, is discussed in Ref. 3. The problem is solved in Ref. 3 in the first approximation of the renormalization group, which naturally results in a strong dependence of T_p on the "bare" coupling constants. It should be noted that this approximation is generally inapplicable in the case of small ε_1 and this accounts for the result obtained in Ref. 3.

An analytic expression for T_p can also be obtained in the range $\ln B \geq 4$. It follows from Eq. (31) that in this case the function $f(t)$ varies quite slowly for $t > t_0$; when ε_1 increases, the law of variation of $f(t)$ in this region approaches linearity. Then, in the range $t > t_0$ we can use the expansion of $f(t)$ in powers of $t - t_0$, and it can be limited to the first term, i.e., we can assume that

$$f(t) \approx -2(t - t_0). \quad (44)$$

Solving Eq. (34) subject to Eq. (44), we obtain the following expression for T_p:

$$T_p = T_0 \exp\left[-\frac{1}{2^{1/6}\chi\tilde{g}_R(t_0)}\right], \quad (45)$$

where $\chi = \exp(7^{-1/2}\tan^{-1}7^{1/2}) \approx 1.58$. The formula (45) is in good agreement with the results of calculations in the range $\ln B \gtrsim 4$.

7. SUPERCONDUCTING TRANSITION

As mentioned earlier, we shall discuss only briefly a superconducting transition. With this in mind we shall consider the behavior of the vertex Γ_4. This vertex is a function of three four-momenta $\mathbf{p}_1 + \mathbf{p}_2, \mathbf{p}_1 - \mathbf{p}_3$, $\mathbf{p}_1 - \mathbf{p}_4$, where $\mathbf{p} = (\mathbf{k}, i\omega_n)$, and it describes two channels: Cooper $\mathbf{p}_1 + \mathbf{p}_2$ (S channel) and Peierls $\mathbf{p}_1 - \mathbf{p}_3$ (P channel). In the quasione-dimensional case the instabilities correspond to different transferred momenta $2\mathbf{k}_F$ and $\mathbf{Q}$ and in analyzing them (for example the analysis based on the behavior of the vertex Γ_4) we need to investigate the vertex for various external momenta ($\pm\mathbf{k}_F$ and $\pm\mathbf{Q}/2$).

We shall now see how a superconducting transition is suppressed at low values of ε_1. We shall do this by considering the behavior of Γ_4 in the $\mathbf{k}_1 = \mathbf{k}_2 = -\mathbf{k}_3 = \mathbf{k}_F$ case. The transferred momentum $\mathbf{k}_1 - \mathbf{k}_3$ in the P channel is then equal to $2\mathbf{k}_F$ and the behavior of Γ_4 depends strongly on the direction of the vector $\mathbf{k}_F$. Since the vector $2\mathbf{k}_F$ generally does not satisfy the condition (6) (in the selected model this condition corresponds to a specific value of $\mathbf{Q}$) and we are interested in the vertex Γ_4 averaged over the Fermi surface, we find that the averaging truncates strongly the contributions of the ladder diagrams to the P channel and the temperature dependence is now governed by the parameter ε_1; however, there is no truncation of the contributions of the ladder diagrams to the S channel. Consequently, the mutual renormalization of the P and S channels becomes considerably weakened and this suppresses a superconducting transition compared with a structural one.

We shall estimate the temperature of a superconducting transition T_s by considering the behavior of Γ_{4R} in terms of the symmetric theory which we can assume to be approximately valid in the limit of small values of ε_1 when T_s lies in the range $\alpha_1 < 1$. In this limit the deviation from the one-dimensional problem is slight and we can assume that in the case under consideration the processes with large transferred momenta play the decisive role. Assuming that $i\omega_{n_1} + i\omega_{n_2} = i\omega_{n_3} - i\omega_{n_4} = i\nu_m = 0$, we obtain the following equation for $\tilde{\Gamma}_{4R} = \Gamma_{4R}/\pi a b^2 \varepsilon_0$ (see Ref. 8):

$$\left(\frac{\partial}{\partial t} + \beta\frac{\partial}{\partial g_{R_1}} - \omega_0\frac{\partial}{\partial\omega_0} - \varepsilon_1\frac{\partial}{\partial\varepsilon_1} - 2\gamma_G\right)\tilde{\Gamma}_{4R} = 0, \quad (46)$$

where the quantity γ_G is defined in Ref. 8.

In analyzing a superconducting transition we have to know the renormalized coupling constant defined at the normalization point $q = 2k_F, \lambda = T$ which can be done easily by investigating the diagrams for Γ_4. The value of this constant is denoted by g_{R_1} in Eq. (46). The constant g_{R_1} corresponds to the invariant coupling constant $\tilde{g}_{R_1}$. The limiting value of $\Gamma_{4R}(\lambda)$ can be taken to be the value calculated from perturbation theory.

It should be noted that Eq. (46) is valid for the part symmetric in respect of spins and for the antisymmetric part. It follows from Eq. (46) that the positions of the singularities $\tilde{\Gamma}_{4R}$ and $\tilde{g}_{R_1}$ coincide in the symmetric theory. The equation for $\tilde{g}_{R_1}$ is the same as Eq. (25) subject to the substitutions

$$\Phi_0(\delta_0^2)\to\Phi_0(\delta_1^2),\quad \Phi_1(\delta_1^2)\to\Phi_1(\delta_2^2),\quad \delta_2=\varepsilon_1/\pi\lambda. \tag{47}$$

Allowing for the approximation (30), we find that the equation for $\tilde{g}_{R_1}$ and the expression $f(t)$ retain their original form if we make the substitution $t \to t = \ln[\pi\lambda/(2\varepsilon_1^2+\pi^2T^2)^{1/2}]$. An investigation of the latter can give the value of T_s. A comparison of the equations for $\tilde{g}_R$ and $\tilde{g}_{R_1}$ shows that $T_\rho > T_s$. Thus, in the limit of low values of ε_1, we obtain

$$T_s=\frac{\tilde{g}_{R_1}(t_0)}{(1+6\tilde{g}_{R_1}^2(t_0))^{1/4}}\frac{\varepsilon_1}{2^{1/2}\pi}\left(\frac{36}{5}\ln B-4\right)^{1/2}, \tag{48}$$

where $\tilde{g}_{R_1}(t_0)$ can be determined with the aid of the curves in Fig. 2.

The above conditions are valid if $\ln B \gg 1$, but on increase in ε_1 we have to use the asymmetric theory regarding the quantities $i\omega_{n_1}+i\omega_{n_2}$ and $i\omega_{n_1}-i\omega_{n_2}$ as independent variables; moreover, we have to allow for the contributions of the processes in which the transferred momentum is small.

8. CONCLUSIONS

Our analysis shows that in describing a quasione-dimensional system it is most important to allow for the terms governing the dependence on the kinetic coupling parameters. These are the terms responsible for the change in the behavior of the system from one- to three-dimensional at low temperatures. In contrast to other investigations,[3-5] the problem is solved above by identifying and summing (within the logarithmic theory framework) of the leading terms of this type. The equations obtained in this way describe the behavior of the system in the range defined by $T < \omega_0$ and $\varepsilon_1 < \omega_0$. An investigation of these equations shows that the matching procedure used in Refs. 3–5 is not quite correct.

In the adopted model a one-electron spectrum has the property described by Eq. (6) in the case of a finite number of the vectors Q. This is true of a number of crystals when the one-electron spectrum can be described in the tight-binding approximation. In this case a structural transition is suppressed by the hopping of electrons to the second-nearest sites, which are characterized by the parameter $\varepsilon_2 < \varepsilon_1$. For this reason the strongest instability of systems of this kind corresponds to a structural transition which produces a superstructure with a doubled transverse period. We can assume that in such systems the nature of three-dimensional ordering of charge density waves is goverend primarily by the kinetic coupling processes. The critical temperature T_ρ in the region $\varepsilon_1 < \omega_0$ increases on increase in ε_1, but Fig. 3 shows that T_ρ has a tendency to approach a maximum which we can assume to lie in the region $\varepsilon_1 > \omega_0$.

In an analysis of a superconducting transition we have to allow for the fact that the possibility of the appearance of a Cooper instability is goverened by the whole three-dimensional Fermi surface so that in the quasi-one-dimensional case we have to average over this surface. The result of averaging is generally a reduction in the effects of mutual influence of the Cooper and Peierls channels in a superconducting transition compared with, for example, a structural transition in the range of small values of ε_1. This is one of the reasons for the suppression of a superconducting transition in quasione-dimensional systems with a strong anisotropy. The nature of the selected model is such that a superconductivity is not expected even for relatively high values of ε_1.

In this sense a more favorable situation is encountered in those systems whose one-electron spectrum does not have the property described by Eq. (6). The results of the present work are sufficient to conclude that a structural transition in such systems is suppressed, for example, for $\ln B \sim 5$ if $g_R = 0.3$ and for $\ln B \sim 8$ if $G_R = 0.1$ so that a superconducting state becomes possible. In the earlier investigations[3-5] it has been established, within the framework of the adopted approximations, that in this case the dependence $T_s(\varepsilon_1)$ should have a maximum at $\varepsilon_1 \sim \omega_0$. It should be noted than an increase in T_s in a quasione-dimensional system, compared with the three-dimensional case, is possible only because of the more effective renormalization of the coupling constants, but the influence of this factor is ignored in Refs. 3–5 and this is why the effects of the mutual influence of the S and P channels have been overestimated. On the whole, an analysis of the dependence $T_s(\varepsilon_1)$ for the electron–hole system in this case and also outside the range limited by the conditions (22) requires separate study.

Among the large number of quasione-dimensional compounds the most suitable materials for comparison are planar square complexes of transition metals among which the salt designated as KCP has been investigated most thoroughly: its formula is $K_2Pt(CN)_4Br_{0.3}\cdot 3H_2O$ (Refs. 12, 13). The structure of such compounds agrees with the adopted model and their one-electron spectra can be assumed to have the form (1) with predominance of the electron–phonon interaction.[12,13] In these compounds the band population differs from 1/2 but the results can be applied if the vector Q of Eq. (6) is replaced with the vector $2k_F, \pi/b, \pi/b$) without a significant change in the other parameters. As pointed out above, crystals of this kind should exhibit a superstructure with a doubled transverse period. In fact, below 120 °K the salt KCP exhibits a tendency to form such a superstructure but below 40 °K a stabilization takes place and further three-dimensional order is not established.[12,13] This is due to an internal disorder of KCP crystals associated with the random distribution of the Br ions.[13]

This approach allows us to determine T_ρ for KCP-type crystals. The degree of anisotropy of KCP is known from the measurements of σ along chains $\sigma_\parallel$ and at right-angles to the chains $\sigma_\perp$: $\sigma_\perp/\sigma_\parallel \sim 4\cdot 10^{-4}$ at $T = 20$ °K and $\sigma_\perp/\sigma_\parallel \sim 2\cdot 10^{-5}$ at $T = 300$ °K (Ref. 13). Using the KCP parameters $\varepsilon_0 \sim 1.5$ eV, $\omega_0 \sim 10^{-2}$ eV, $g_R \sim 0.5$ (Ref. 13) and assuming that $\sigma_\perp/\sigma_\parallel \sim (\varepsilon_1/\varepsilon_0)^2$, we find $\ln B = 0.4$ and $\ln B = 1.9$ for the two values of the anisotropy quoted above. For these values of ε_1 the conditions (22) are not obeyed and, strictly speaking, the nonlogarithmic terms should be used in the determination of T_ρ. However, in a qualitative estimate we can calculate T_ρ

in the adopted logarithmic approximation if we assume that $\lambda = \omega_0$. Such a calculation gives $T_p \approx 78$ °K for $\ln B = 0.4$ and $T_p \approx 33$ °K for $\ln B = 1.9$. Allowance for the internal disorder suggests that at temperatures 33–78 °K there should be no phase transition in KCP but the compounds should exhibit maximum (antiphase) correlation between charge density waves in different chains. These estimates are in good agreement with the experimental results. The selected model is inapplicable to compounds of the TTF-TCNQ type which also exhibit a structural instability because these compounds have a complex structure: there are two kinds of conducting chain and the transverse directions are inequivalent.[13]

We can thus assume that the properties of systems of this kind are related to a structural transition which is affected (as is true of KCP) by other factors such as the internal disorder, etc.

The author is grateful to L.N. Lipatov for valuable discussions of a number of topics and to Yu. A. Firsov for comments on the work reported above, and also to G.I. Podol'skaya for her help in numerical calculations.

[1)] It should be noted that in the earlier investigation[8] the contribution of the diagram 1c was not doubled. The second coefficient of the function β in the normalization Ref. 8 should be 16.

[1]L. P. Gor'kov and I. E. Dzyaloshinskiĭ, Zh. Eksp. Teor. Fiz. **67**, 397 (1974) [Sov. Phys. JETP **40**, 198 (1975)].
[2]L. Mihaly and J. Solyom, J. Low Temp. Phys. **24**, 579 (1976).
[3]Y. Suzumura and H. Fukuyama, J. Low Temp. Phys. **31**, 273 (1978).
[4]A. I. Larkin and J. Sak, Phys. Rev. B **18**, 6053 (1978).
[5]V. N. Prigodin and Yu. A. Firsov, Zh. Eksp. Teor. Fiz. **76**, 1602 (1979) [Sov. Phys. JETP **49**, 808 (1979)].
[6]H. Frohlich, Proc. R. Sco. London Ser. A **223**, 296 (1954). [Russ. Transl. in: Teoriya sverkhprovodimosti (Theory of Superconductivity), IIL, M. 1960].
[7]T. K. Mitra, J. Phys. C **2**, 52 (1969).
[8]V. P. Lukin, Zh. Eksp. Teor. Fiz. **74**, 1093 (1978) [Sov. Phys. JETP **47**, 574 (1978)].
[9]A. Erdélyi (ed.), Higher Transcendental Functions (California Institute of Technology H. Bateman MS Project), 3 vols., McGraw-Hill, New York (1953, 1955) [Russ. Transl. Nauka, M. 1973].
[10]N. N. Bogolyubov and D. V. Shirkov, Vvedenie v teoriyu kvantovannykh poleĭ, Nauka, M., 1976 (Introduction to the Theory of Quantized Fields, Interscience, New York, 1959).
[11]E. L. Ince, Ordinary Differential Equations, Longmans, New York (1927) [Russ. Transl. ONTI, Kharkov, 1939].
[12]L. N. Bulaevskiĭ, Usp. Fiz. Nauk **115**, 263 (1975) [Sov. Phys. Usp. **18**, 131 (1975)].
[13]V. L. Ginzburg and D. A. Kirzhnits (eds.), Problema vysokotemperaturnoĭ sverkhprovodimosti (Problem of High-Temperature Superconductivity), Nauka, M., 1977, Chap. 7.

Translated by A. Tybulewicz

Study of phase transitions in $(TSeT)_2Cl$ under pressure at low temperatures

V. N. Laukhin and I. F. Shchegolev

Institute of Chemical Physics, Academy of Sciences, USSR
(Submitted 12 November 1979)
Zh. Eksp. Teor. Fiz. **78**, 2332–2336 (June 1980)

The effect of high hydrostatic pressure on the phase transitions in the $(TSeT)_2Cl$ complex is studied at temperatures ranging from room to helium. The first-order phase transition which occurs under a pressure of 5 kbar at room temperature continues to exist at all temperatures down to helium temperature. The temperature of the metal-semimetal phase transition decreases with pressure. However it is not possible to suppress this transition completely since the initial metallic phase goes over either to the semimetal state (at $P < 4$ kbar) or to the high-pressure phase (at $P > 4$ kbar). The T-P state diagram of the complex is plotted.

PACS numbers: 64.70.Kb, 71.30. + h

Among all the presently known organic compounds of the quasi-one-dimensional type which are metallic at high temperatures, perhaps one of the most interesting is the tetraselenotetracene chloride complex $(TSeT)_2Cl$, the structure and basic properties of which were described earlier.[1,2] This complex, having metallic conductivity at high temperatures, undergoes in the region of 19 K a second order phase transition from the metallic state to a semimetal state whose conductivity is close to the room-temperature conductivity of the high-temperature phase.[3] Furthermore, under a pressure of 5 kbar and at room temperature, this compound undergoes a first-order phase transition to a new metallic state, which remains stable down to helium temperatures. The residual resistivity of the new metallic phase at temperatures below 10 K is 1.1×10^{-5} ohm-cm (Ref. 4).

To clarify the nature of this transformation the authors studied its characteristics at low temperatures. We were particularly interested by the possibility of maintaining the high-pressure phase in a metastable state at normal pressure. Moreover, it was of independent interest to investigate the possibility of suppressing the metal-semimetal phase transition and maintain the initial low-pressure metallic phase at

 0038-5646/80/061170-04$02.40