# Thermodynamic and magnetic properties of quasi-one-dimensional systems in the coexistence phase of the charge-density wave and superconductivity



1990 J. Phys.: Condens. Matter 2 2699

(http://iopscience.iop.org/0953-8984/2/11/013)

J. Phys.: Condens. Matter 2 (1990) 2699–2711. Printed in the UK

# Thermodynamic and magnetic properties of quasi-one-dimensional systems in the coexistence phase of the charge-density wave and superconductivity

V M Vackalyuk, M E Palistrant and I V Padure
Institute of Applied Physics, 277028 Kishinev, USSR

Received 19 January 1989, in final form 26 July 1989

**Abstract.** The effects of deviation from the half-filling of the conduction band ($\mu \neq 0$) and magnetic field on the coexistence of superconductivity (SC) and the charge-density wave (CDW) in a quasi-one-dimensional system are investigated. The behaviour of the superconducting order parameter $\Delta_s$ and dielectric order parameter $\Delta_P$ as functions of temperature essentially depends on the theory parameters $p = T_{s0}/T_{P0}$, $\mu$ and the external magnetic field $H_0$. In particular, it is possible to increase the superconducting transition temperature $T_s$ as the magnetic field grows. The spin magnetic susceptibility and penetration depth are calculated in the mixed SC+CDW phase and it is shown that their temperature dependences essentially differ from the BCS theory both qualitatively and quantitatively.

## 1. Introduction

There has been long and thorough research, both experimentally and theoretically, of those substances which exhibit owing to the peculiarities of their crystal lattice a strong anisotropy of electroconductivity and it allows one to treat them as quasi-one-dimensional materials.

Such substances are, in particular, the organic conductors and chain compounds [1–5]. They are interesting, first of all, because of their unusual properties. While they behave as metals at high temperatures, they undergo a transition to the dielectric state of the charge-density wave (CDW) and spin-density wave (SDW) at low temperatures. The transitions to these states occur while 'nesting' is present, when there are congruent parts on the Fermi surface which could be matched by a parallel transfer of the vector $\boldsymbol{Q}$.

Because there is always 'nesting' in a one-dimensional system, in a strongly anisotropic nearly one-dimensional system transitions to CDW and SDW states are possible at $Q \simeq 2K_F$. The question about which of these transitions will occur is determined by the condition in [6, 7], i.e. by the relation between the parameters $g_Q$ of the electron–phonon interaction and the magnitude $V(Q)$ of the Coulomb interaction. When $g_Q > N(0)V(Q)$ a transition to the CDW state occurs. Periodic stationary shifts of the electrons with the wavevector $\boldsymbol{Q}$ appear and on the congruent parts of the Fermi surface a dielectric gap appears. When $g_Q < N(0)V(Q)$ the system passes into a magnetically ordered SDW state. In this case the periodic effective exchange magnetic field acts on the electrons and on the congruent part of the Fermi surface a dielectric gap will also appear. In accordance with this a Peierls transition is observed, for instance, in the chain compounds $TaS_3$, $NbS_3$, $K_{0.3}MoO_3$ [8–10] and also in organic compounds such as tetracyanoquinodimethane (TCNQ) [1, 11]. A transition to the SDW state occurs in rare-earth molybdenum sulphides $(RE)_{1.2}Mo_6S_8$ (RE ≡ Tb, Dy, Er) [5], and in the organic conductors $(TMTSF)_2X$ (X ≡ $PF_6$, $AsF_6$, $SbF_6$) [6, 7].

In several theoretical papers in which the Peierls instability is considered [12–17] the investigations are carried out within the mean-field approximation. When doing this, only the case of one-dimensional systems with a half-filled conduction band ($\mu = 0$, where $\mu$ is the Fermi energy as measured from the middle of a conduction band) is considered. In such systems a wave of shifts and the CDW connected with the latter with the wavevector $Q = 2K_F = \pi/d$ ($d$ is the lattice constant) develop. Meanwhile on the Fermi surface a dielectric gap appears.

An investigation beyond the framework of the mean-field approximation is carried out in [18], where the fluctuations in the framework of the Ginsburg–Landau statistical approximation are taken into account. This theory is valid when $2K_F \neq \pi/d$. It is concluded that only when $T < \frac{1}{4}T_P$ ($T_P$ is the temperature of the Peierls transition in the mean-field approximation) does a Peierls superlattice appears in the system and the density of states is near that obtained within the mean-field approximation.

A detailed review of papers covering the Peierls instability in quasi-one-dimensional systems with a half-filled band is given in [11]. In this review, in particular, the role of the Coulomb interaction of electrons in a Peierls transition is discussed as well as the role of commensurability and incommensurability, of fluctuation and so on.

The influence of the deviation from the half-filling of the band $\mu$ on various properties of one-dimensional conductors was first considered in [19]. It was indicated that in the mean-field approximation, when the Umklapp processes (the periodicity of the lattice) are not taken into account, the wavevector of the CDW $Q = 2K_F$ for any $\mu$, as in the case of the jellium model [13]. Taking into account the Umklapp processes at $\mu < \mu_c = 1.056$ $T_{P0}$, where $T_{P0}$ is the temperature of the Peierls transition at $\mu = 0$, does not alter the overall picture, i.e. a CDW with the wavevector $Q = 2K_F$ is established in the system. However, at $\mu > \mu_c$ taking into account the Umklapp processes gives rise to a stable CDW state only at $Q \neq 2K_F$. In this case a CDW with a wavevector $Q = 2K_F + q$, $q \ll K_F$ appears. Then the dielectric gap appears not exactly on the Fermi level (depending on whether $Q \neq 2K_F$) and one has a state with free carriers under the Fermi surface, which could form Cooper pairs.

In strictly one-dimensional systems the long-range ordering is attenuated by growing fluctuations near the transition temperature [18, 20]. However, the results of the theoretical papers [13, 17, 19] can be applied to describe the properties of quasi-one-dimensional systems. The three-dimensional lattice with an evidently expressed anisotropy is meant here, when the electrons may move only along a single direction. In such systems the fluctuations may be strongly suppressed and display themselves only in a narrow interval of temperatures near $T_P$. There are no doubts about the validity of the application of the quasi-one-dimensional model for the description of properties of strongly anisotropic systems at $T < T_P$ when the fluctuations are insignificant. Thus, in $K_{0.3}MoO_3$ the fluctuations vanish below $T = 0.9\ T_P$ [10, 21].

As to the transition temperature $T_P$, it seems that it may differ from that determined within the framework of more accurate calculations when the interactions of linear chains and fluctuations are quantitatively taken into account.

The CDW in quasi-one-dimensional conductors with $\mu \neq 0$ turns out to be unstable with respect to the Cooper pairs. The question of the coexistence of superconductivity

(SC) and CDW in these systems has been investigated in [22]. This was limited to the case of weak superconductivity on the background of the CDW state and proved that the conditions for the coexistence of SC and CDW strongly depend on the peculiarities of the excitation spectrum of the dielectric phase and appear only at $\mu \neq 0$. With increase in $\mu$ ($\mu > \mu_c \ll W$, where $W$ is the half-width of the band) a transition to the CDW state occurs with $Q = 2K_F + q$ ($q \ll K_F$) and the quasi-one-dimensional system passes to a qualitatively new state, when ordering occurs to the dielectric type, yet without the gap in the excitation spectrum. This circumstance gives rise to some interesting peculiarities in the behaviour of the magnetic susceptibility as a function of temperature in the SDW or CDW state [23].

Because the condition $\mu \neq 0$ in real systems is rather probable, it is of interest to investigate more thoroughly the influence of $\mu$ on the low-temperature properties of quasi-one-dimensional systems as well as on the coexistence of SC and CDW. Our paper is dedicated to this matter and to the investigation of the influence of the magnetic field on the mixed SC + CDW phase. The investigations are carried out in the mean-field approximation. The work in [24, 25] may serve as a justification of this; in [24, 25] it was shown that the behaviour of a quasi-one-dimensional system with two parameters of long-range order (SC and CDW) in the mean-field approximation is qualitatively consistent with the treatment on the basis of the static approximation of Ginsburg and Landau, allowing one to take into account the fluctuations.

In the following the system of equations for two order parameters—the superconducting order parameter $\Delta_s$ and the dielectric order parameter $\Delta_P$—determining the state of the system in the magnetic field $H_0$ is obtained, the difference $\delta F = F(\Delta_s, \Delta_P, H_0) - F(0, \Delta_P, H_0)$ in the free energies is calculated, the wavevector $\boldsymbol{Q}$ of the CDW is optimally determined for the given $\mu$, $H_0$, the magnetic susceptibility and the penetration depth of the magnetic field in the mixed SC + CDW phase, and the temperature dependence of the above-mentioned magnitudes at various values of the theory parameters is investigated.

## 2. The Hamiltonian of the system and the main equations

We start with a Frolich-like Hamiltonian [22] to which the Hamiltonian of the electron–magnetic field interaction is added. This Hamiltonian in the mean-field approximation may be reduced to this form

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\mathrm{CDW}} + \mathcal{H}_{\mathrm{BCS}} + \mathcal{H}_{H0} \tag{1}$$

where

$$\mathcal{H}_0 = \sum_{\boldsymbol{K},\alpha} (\varepsilon_{\boldsymbol{K}} - \mu) a^+_{\boldsymbol{K},\alpha} a_{\boldsymbol{K},\alpha}$$

$$\mathcal{H}_{\mathrm{BCS}} = -\sum_{\boldsymbol{K}} \Delta_s (a^+_{\boldsymbol{K}\uparrow} a^+_{-\boldsymbol{K}\uparrow} + a_{-\boldsymbol{K}\downarrow} a_{\boldsymbol{K}\uparrow})$$

$$\mathcal{H}_{\mathrm{CDW}} = -\sum_{\boldsymbol{K},\alpha} \Delta_P (a^+_{\boldsymbol{K}-\boldsymbol{Q},\alpha} a_{\boldsymbol{K},\alpha} + a^+_{\boldsymbol{K},\alpha} a_{\boldsymbol{K}-\boldsymbol{Q},\alpha})$$

$$\mathcal{H}_{H_0} = -\sum_{\kappa,\alpha,\beta} H_0 (\sigma^z)_{\alpha,\beta} a^+_{\boldsymbol{K},\alpha} a_{\boldsymbol{K},\beta}.$$

Here $\mathcal{H}_0$ is the kinetic energy of the conductive electrons; $\mathcal{H}_{\mathrm{BCS}}$ and $\mathcal{H}_{\mathrm{CDW}}$ are the operators responsible for the SC and the Peierls instability, respectively; $\mathcal{H}_{H_0}$ is the interaction of electrons with the external magnetic field; $a^{+}_{K,\alpha}$ and $a_{K,\alpha}$ are creation and annihilation operators, respectively; $\hat{\sigma}$ is the Pauli matrix.

The superconducting order parameter $\Delta_s$ and the dielectric order parameter $\Delta_P$ are determined by the relations

$$\Delta_s = g_s T \sum_{K} \sum_{\omega_n} F^{\downarrow\uparrow}_{-K,K}(\omega_n) \tag{2}$$

$$\Delta_P = g_P \langle \varphi_Q \rangle = \frac{g_P}{\omega_0(Q)} \langle b_Q + b^{+}_{-Q} \rangle \tag{3}$$

where $\langle \varphi_Q \rangle$ is the amplitude of the wave shifts; $\omega_0(Q)$ is the phonon frequency; $g_s$ and $g_P$ are the BCS and effective Peierls interaction constants respectively.

Excluding the amplitude $\langle \varphi_Q \rangle$ of the wave shifts from (3) and using the equation of motion for the phonon averages (see [26]) one obtains the self-consistent system of equations for the order parameters $\Delta_s$ (equation (2)) and $\Delta_P$:

$$\Delta_P = \tfrac{1}{2} g_P T \sum_{K,\sigma} \sum_{\omega_n} G^{\sigma\sigma}_{K-Q,K}(\omega_n). \tag{4}$$

$F^{\downarrow\uparrow}_{-K,K}$ and $G^{\sigma\sigma}_{K-Q,K}$ are the Fourier components of the thermal Green function defined by

$$\begin{aligned} F^{\downarrow\uparrow}_{-K,K}(\tau - \tau') &= -\langle T a^{+}_{-K\downarrow}(\tau) a^{+}_{K\uparrow}(\tau') \rangle \\ G^{\sigma\sigma'}_{K,K'}(\tau - \tau') &= -\langle T a_{K\sigma}(\tau) a^{+}_{K'\sigma'}(\tau') \rangle. \end{aligned} \tag{5}$$

On the grounds of the Hamiltonian (1) for the Green functions $G^{\sigma\sigma}_{K-Q,K}$, $G^{\sigma\sigma}_{K,K}$, $F^{\downarrow\uparrow}_{-K,K}$, we obtain

$$\begin{aligned} G^{\sigma\sigma}_{K-Q,K}(\Omega_{n\sigma}) &= -\Delta_P[(\Omega_{n\sigma}+\varepsilon_1)(\Omega_{n\sigma}+\varepsilon_2) - \Delta_P^2 - \Delta_s^2]/D('_{n\sigma}) \\ G^{\sigma\sigma}_{K,K}(\Omega_{n\sigma}) &= [(\Omega_{n\sigma}+\varepsilon_1)(\Omega_{n\sigma}^2 - \varepsilon_2^2 - \Delta_s^2) - \Delta_P^2(\Omega_{n\sigma} - \varepsilon_2)]/D(\Omega_{n\sigma}) \\ F^{\downarrow\uparrow}_{-K,K}(\Omega_{n\sigma}) &= -\Delta_s(\Omega_{n\sigma}^2 - \varepsilon_2^2 - \Delta_s^2 - \Delta_P^2)/D(\Omega_{n\sigma}) \end{aligned} \tag{6}$$

where

$$\Omega_{n\sigma} = \mathrm{i}\omega_n + \sigma H_0 \qquad \sigma = \pm 1 \qquad \varepsilon_1 = \varepsilon_K - \mu \qquad \varepsilon_2 = \varepsilon_{K-Q} - \mu$$

$$\begin{aligned} D(\Omega_{n\sigma}) = {}& \Omega_{n\sigma}^4 - \Omega_{n\sigma}^2(\varepsilon_1^2 + \varepsilon_2^2 + 2\Delta_P^2 + 2\Delta_s^2) + \Delta_s^2(\varepsilon_1^2 + \varepsilon_2^2) \\ & + \varepsilon_1^2\varepsilon_2^2 - 2\varepsilon_1\varepsilon_2\Delta_P^2 + (\Delta_P^2 + \Delta_s^2)^2. \end{aligned} \tag{7}$$

Assume that the band energies are given by

$$\varepsilon_K = -W\cos(Kd). \tag{8}$$

Inserting equations (6) into the system of equations (2), (4) and integrating over energy as was done in [27], we obtain the system of equations for determination of the order parameters $\Delta_s$ and $\Delta_P$:

$$\ln\left(\frac{T}{T_{s0}}\right) = 2\pi T \sum_{n>0} \left\{ -\tfrac{1}{4} \sum_{\alpha,j} \mathrm{Im}\left[\left(1 + j\frac{\mu_\alpha}{E}\right)\frac{1}{\varepsilon_j^\alpha}\right] - \frac{1}{\omega_n} \right\} \tag{9}$$

$$\ln\left(\frac{T}{T_{P0}}\right) = 2\pi T \sum_{n>0} \left[ -\tfrac{1}{4} \sum_{\alpha,j} \mathrm{Im}\left(\frac{1}{\varepsilon_j^\alpha}\right) - \frac{1}{\omega_n} \right] \tag{10}$$

**Table 1.** The results obtained by solution of the system of equations (12).

| $H_0/T_{P0}$ | $\mu/T_{P0}$ | $\eta_q/T_{P0}$ | $T_P/T_{P0}$ | $H_0/T_{P0}$ | $\mu/T_{P0}$ | $\eta_q/T_{P0}$ | $T_P/T_{P0}$ |
|---|---|---|---|---|---|---|---|
| 0.0 | 0.0 | 0.0 | 1.0 | 0.2 | 1.08 | 0.134 | 0.54 |
| 0.0 | 0.5 | 0.0 | 0.94 | 0.2 | 1.09 | 0.359 | 0.51 |
| 0.0 | 1.0 | 0.0 | 0.68 | 0.2 | 1.1 | 0.553 | 0.49 |
| 0.0 | 1.073 | 0.059 | 0.56 | 0.2 | 1.2 | 0.966 | 0.39 |
| 0.0 | 1.08 | 0.354 | 0.54 | 0.3 | 1.08 | 0.0 | 0.54 |
| 0.0 | 1.09 | 0.520 | 0.52 | 0.3 | 1.09 | 0.196 | 0.51 |
| 0.0 | 1.1 | 0.601 | 0.50 | 0.3 | 1.1 | 0.452 | 0.48 |
| 0.0 | 1.2 | 0.977 | 0.41 | 0.3 | 1.2 | 0.943 | 0.36 |

$$\alpha, j = \pm 1 \qquad \mu_\alpha = \mu + \alpha\eta_q \qquad \eta_q = Wdq/2 \qquad q = Q - 2K_F \tag{11}$$
$$\varepsilon_j^\alpha = \sqrt{(E + j\mu_\alpha)^2 - \Delta_P^2} \qquad E = \sqrt{(i\omega_n + H_0)^2 - \Delta_s^2}.$$

$T_{s0}$ and $T_{P0}$ are the temperatures of the superconducting transition (in the absence of dielectric order) and the dielectric transition (in the absence of superconductivity and when $\mu = 0$).

At $Q \neq 2K_F(\eta_q \neq 0)$, renormalisation of the parameter occurs, namely the parameters $\mu_+ = \mu + \eta_q$ and $\mu_- = \mu - \eta_q$ appear. The difference between $\mu_+$ and $\mu_-$ arises because the Umklapp processes in the quasi-one-dimensional system are taken into account.

Following [19, 22], the wavevector $Q$ of the CDW (or $\eta_q$) is determined from the condition of maximality of the Peierls transition temperature $T_P$. From equation (10) at $\Delta_s = 0, \Delta_P \rightarrow 0$, one obtains, in order to determine the maximal $T_P$ and the corresponding $\eta_q$, the system of equations

$$\begin{aligned} \ln(T_P/T_{P0}) &= -F(\mu, \eta_q, T_P, H_0) \\ \partial F(\mu, \eta_q, T_P, H_0)/\partial\eta_q &= 0 \end{aligned} \tag{12}$$

where

$$F(\mu, \eta_q, T_P, H_0) = \mathrm{Re}\left[\tfrac{1}{4}\sum_{\alpha,\sigma}\psi\left(\tfrac{1}{2} - \frac{i(\mu_\alpha + \sigma H_0)}{2\pi T_P}\right)\right] - \psi(\tfrac{1}{2}) \tag{13}$$
$$\sigma = \pm 1 \qquad \alpha = \pm 1.$$

It should be noted that such an approach to determine $Q$ at the point $T = T_P$ is equivalent to the approach considered in [28], where $Q$ is determined from the condition of the free-energy minimum near the transition temperature $T_P$. The results of the numerical solutions of the system of equations (12) are given in table 1. It is easy to see from this table that, when the magnetic field increases, $\mu_c$ also increases and the system goes into a phase with $Q \neq 2K_F$ ($\eta_q \neq 0$). Therefore at $\mu \neq 0$ the magnetic field contributes to the stabilisation of the CDW state with $Q = 2K_F$. One can understand this result by comparing equation (12) at $\eta_q = 0$ with the same equation at $H_0 = 0$. One obtains mathematically equivalent equations. Therefore, $H_0$ plays the same role as $\eta_q$, i.e. it stabilises the CDW state. That is why at $H_0 \neq 0$, for the transition into the state with $Q \neq 2K_F$ to occur, it is required that $\mu_c'(H_0) > \mu_c'(0) = \mu_c$ (here $\mu_c'(H_0)$ is the value of $\mu$ at which the solution of the system of equation (12) with $\eta_q \neq 0$ appears). Thus the statement in [19] that in the magnetic field a transition into the state with $q \neq 0$ is possible at $\mu_c'(H_0) < \mu_c$ has no grounds.

To understand the role of $H_0$, let us consider the electronic density of states $N(\mu)$ at the Fermi surface obtained from the imaginary part of the function $G^{\sigma\sigma}_{K,K}(\Omega_{n\sigma})$ (equation (6)):

$$N(\mu) = \tfrac{1}{4}N_0 \,\mathrm{Re}\left(\sum_{\sigma,\alpha} \frac{|\mu_\alpha + \sigma H_0|}{\sqrt{(\mu_\alpha + \sigma H_0)^2 - \Delta^2}}\right) \qquad \sigma, \alpha = \pm 1. \tag{14}$$

At $\eta_q = 0$, one has the condition $|\mu - H_0| \leqslant |\mu + H_0| < \Delta$ which corresponds to the fact that the dielectric gap on the Fermi surface appears, and the conditions $|\mu - \mathrm{H}_0| < \Delta < |\mu + \mathrm{H}_0|$ and $\Delta < |\mu - H_0| \leqslant |\mu + H_0|$ correspond to the appearance of a gapless CDW state. These results are reminiscent of the situation in the quasi-one-dimensional antiferromagnetic superconductor [29] when in a certain range of values of the magnetic field a gapless state appears and as a result the magnetic field gives rise to SC.

## 3. Free energy and magnetic susceptibility of the system

To calculate the difference between the free energies of the superconducting and dielectric phases we use the formula

$$\delta F = F(\Delta_s, \Delta_P, H_0) - F(0, \Delta_P, H_0) = \int_0^{\Delta_s} \Delta_s'^2 \frac{\mathrm{d}}{\mathrm{d}\Delta_s'}\left(\frac{1}{g_s}\right) \mathrm{d}\Delta_s'. \tag{15}$$

One can represent equation (9) as

$$\frac{1}{g_s} = 2\pi T N_0 \sum_{n>0} \left[-\tfrac{1}{4}\sum_{\alpha,j} \mathrm{Im}\left(1 + j\frac{\mu_\alpha}{E}\right)\frac{1}{\varepsilon_j^\alpha}\right]. \tag{16}$$

Inserting equation (16) into equation (15) and integrating over $\Delta_s'$, we obtain

$$\frac{\delta F}{N_0} = \Delta_s^2 \ln\left(\frac{T}{T_{s0}}\right) - \pi T \sum_{n>0}\sum_{\alpha,j}\left(\mathrm{Im}(\varepsilon_j^\alpha - \varepsilon_j^\alpha|_{\Delta_s=0}) - \frac{\Delta_s^2}{\omega_n}\right) \qquad \alpha, j = \pm 1. \tag{17}$$

Let us now determine the magnetic susceptibility. With this aim we represent the spin magnetic momentum of the system in the region of small magnetic fields in the form

$$M = 2H_0 N_0 + T\sum_n \sum_{K,\sigma} \sigma G^{\sigma\sigma}_{K,K}(\mathrm{i}\omega_n) \qquad \sigma = \pm 1. \tag{18}$$

Inserting into equation (18) the corresponding Green function (6) and carrying out the integration over the energy for magnetic susceptibility $\chi = M/H_0$, we obtain

$$\frac{\chi}{\chi_0} = 1 + \tfrac{1}{2}\pi T \sum_{n>0}\sum_{\alpha,j} \mathrm{Im}\left[\frac{-j\,\mathrm{i}\mu_\alpha \Delta_s^2}{(\omega_n^2 + \Delta_s^2)\varepsilon_{j0}^\alpha} + \frac{1}{(\varepsilon_{j0}^\alpha)^3}\left(\frac{\Delta_s^2(\mathrm{i}\sqrt{\omega_n^2 + \Delta_s^2} + j\mu_\alpha)}{\omega_n^2 + \Delta_s^2} - \Delta_P^2\right)\right]$$

$$\varepsilon_{j0}^\alpha = \varepsilon_j^\alpha|_{H_0=0} \qquad \chi_0 = 2N_0. \tag{19}$$

## 4. Penetration depth of the magnetic field

To determine the penetration depth of the magnetic field, we shall suppose that the vector potential $A$ is parallel to the nesting vector $Q$ and define the electromagnetic kernel by the relation $j = -Q_{\|}A$, where $j$ is the induced current. The calculation of $Q_{\|}$ is reduced to the determination of the thermodynamic causal Green function of the current operator $\hat{j}$ in the mixed SC + CDW phase. To calculate it, one uses the procedure developed in [29, 30]. After integrating over energy for the penetration depth $\lambda = Q_{\|}^{-1/2}$ of the magnetic field, we obtain

$$\left(\frac{\lambda}{\lambda_0}\right)^{-2} = \tfrac{1}{16}\pi T \sum_n \sum_{\alpha,\sigma=\pm 1} \mathrm{Im}\left(\frac{1}{(f_\alpha \sqrt{z_{\alpha\sigma}})^3}[f_\alpha(5z_{\alpha\sigma}^3 + 3\gamma_1 z_{\alpha\sigma}^2 - \gamma_2 z_{\alpha\sigma} - \gamma_3) - 2\sigma z_{\alpha\sigma}(z_{\alpha\sigma}^3 + \gamma_1 z_{\alpha\sigma}^2 + \gamma_2 z_{\alpha\sigma} + \gamma_3)]\right) \tag{20}$$

$$z_{\alpha\sigma} = \omega_n^2 + \Delta_P^2 + \Delta_s^2 - \mu_\alpha^2 + \sigma f_\alpha \qquad f_\alpha = 2\,\mathrm{i}\mu_\alpha\sqrt{\omega_n^2 + \Delta_s^2}$$

$$\gamma_1 = \omega_n^2 - \mu_\alpha^2 + \Delta_P^2 + 3\Delta_s^2$$

$$\gamma_2 = -\omega_n^4 + 2\omega_n^2(\Delta_s^2 - \Delta_P^2 - 5\mu_\alpha^2) + (\Delta_s^2 + \Delta_P^2 + \mu_\alpha^2) + 2(\Delta_s^4 - \Delta_P^4 - \mu_\alpha^4)$$

$$\gamma_3 = -\omega_n^6 - \omega_n^4(\Delta_s^2 + \mu_\alpha^2 + 3\Delta_P^2) + \omega_n^2(2\mu_\alpha^2\Delta_P^2 + 2\Delta_s^2\mu_\alpha^2 - 2\Delta_s^2\Delta_P^2 + \Delta_s^4 + \mu_\alpha^4 - 3\Delta_P^4) + 3\mu_\alpha^2(\Delta_s^4 + \Delta_P^4 - \mu_\alpha^2\Delta_P^2 + \mu_\alpha^2\Delta_s^2) - \Delta_s^2\Delta_P^4 + \Delta_s^4\Delta_P^2.$$

$\lambda_0$ is the penetration depth of the magnetic field in the usual superconductors when $T = 0$.

## 5. Numerical solutions and discussion of results

The coexistence of the SC and of the CDW state is determined by the condition $\Delta_s \neq 0$ and $\Delta_P \neq 0$, which corresponds to the non-zero solution of the system of equations (9), (10). Together with this, it is necessary that the free-energy difference $\delta F = F(\Delta_P, \Delta_s) - F(\Delta_P, 0)$ determined by equation (17) be a negative quantity. This corresponds to the fact that the appearance of SC on the background of the CDW state is energetically convenient.

In the considered model there are two independent parameters: $p = T_{s0}/T_{P0}$ and $\bar{\mu} = \mu/T_{P0}$. The value of $\eta_q$ is determined from equations (12). A quasi-one-dimensional system is considered in the magnetic field $H_0$ at the temperature $T$. The numerical solutions of the above-mentioned system of equations carried out for various values of $\bar{\mu}$ and $p$ throughout the temperature range from 0 to $T_P$ are given in figures 1 and 2.

In figure 1($a$) the dependence of the order parameters $\Delta_s/\Delta_{s0}$ and $\Delta_P/\Delta_{P0}$ on temperature at $\bar{\mu} = 1.073$ and $p = 0.6$ is given. Curves labelled A–C are related to $\Delta_s/\Delta_{s0}$ and curves labelled A′–C′ to $\Delta_P/\Delta_{P0}$. In this figure, curves A and A′ correspond to $\rho = H_0/T_{P0} = 0$, $\bar{\eta}_q = \eta_q/T_{P0} = 0.059$, curves B and B′ to $\rho = 0.2$, $\bar{\eta}_q = 0$, and curves C and C′ $\rho = 0.3$, $\bar{\eta}_q = 0$.

In figure 1($b$) the dependences of the order parameters $\Delta_s/\Delta_{s0}$ and $\Delta_P/\Delta_{P0}$ as functions of temperature at $p = 0.57$ and $\bar{\mu} = 1.075$ for the values $\rho = 0$ ($\bar{\eta}_q = 0.205$) and $\rho = 0.2$ ($\bar{\eta}_q = 0$) are presented (curves A and A′ and curves B and B′, respectively). Here at $\rho = 0$ the SC appears on the background of a dielectric state at the point $T_{s1} =$

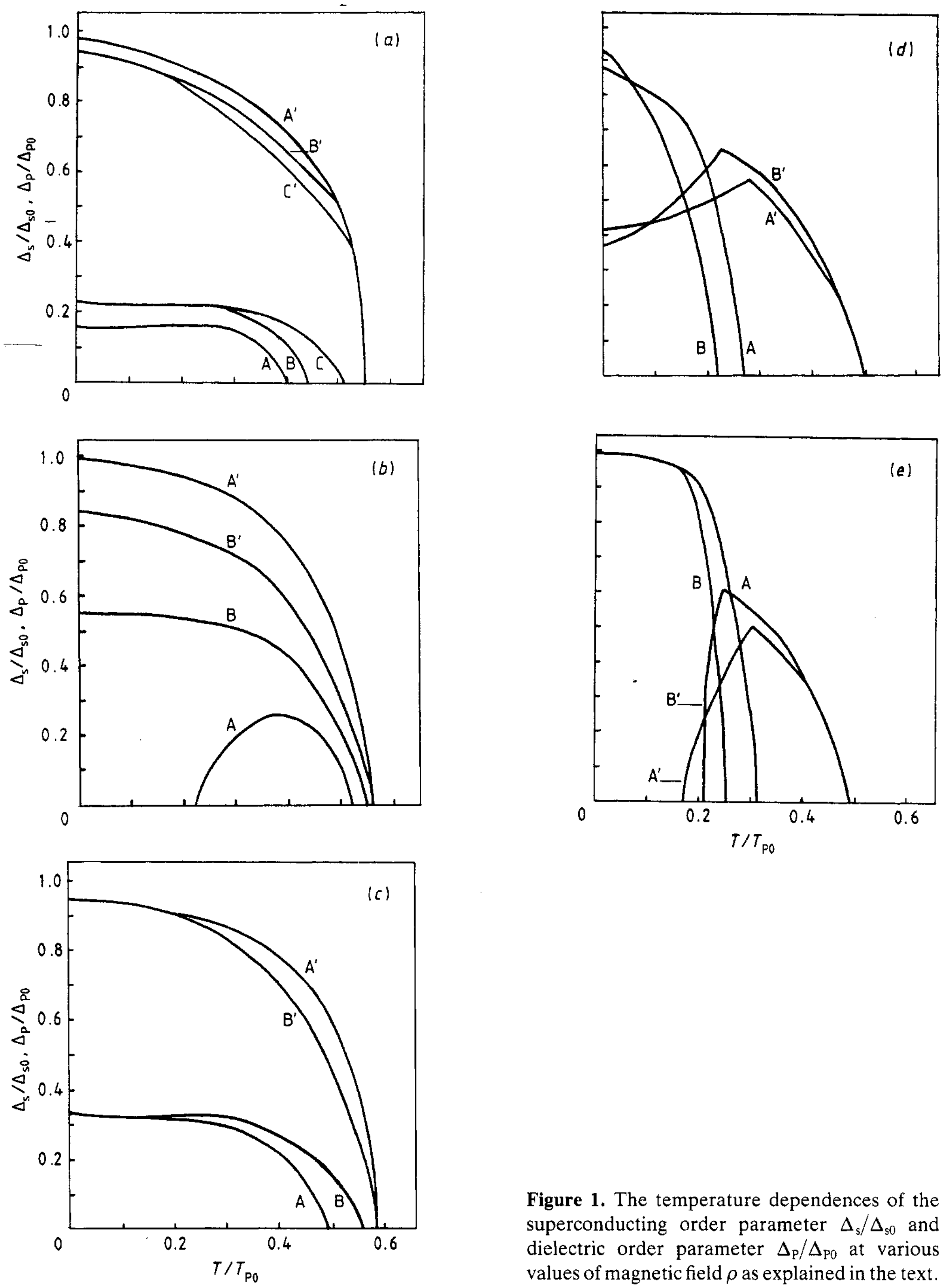


**Figure 1.** The temperature dependences of the superconducting order parameter $\Delta_s/\Delta_{s0}$ and dielectric order parameter $\Delta_P/\Delta_{P0}$ at various values of magnetic field $\rho$ as explained in the text.

$0.23T_{P0}$ and is suppressed by 'dielectrisation' at the point $T_{s2} = 0.53T_{P0}$. A return to the dielectric state occurs. As $\rho$ increases, this effect disappears and SC exists throughout the temperature interval from $T_{s3} = 0.56T_{P0}$ to 0, i.e. the magnetic field restores the superconducting phase within this temperature interval.

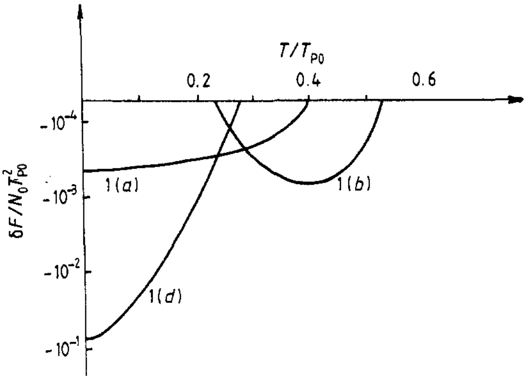


**Figure 2.** The temperature dependences of the free-energy difference at $\rho = 0$ for cases presented in figures 1($a$), 1($b$) and 1($d$).

In figure 1($c$) the temperature dependences of the order parameters $\Delta_s/\Delta_{s0}$ and $\Delta_P/\Delta_{P0}$ at $p = 0.6$, $\bar{\mu} = 1.068$ for $\rho = 0$ and $0.27$ ($\bar{\eta}_q = 0$) are shown (curves A and A′ and curves B and B′, respectively).

In figure 1($d$) the same dependences are shown at $p = 0.35$, $\bar{\mu} = 1.1$ for values of $\rho = 0$ ($\bar{\eta}_q = 0.601$) and $\rho = 0.2$ ($\bar{\eta}_q = 0.553$) (curves A and A′ and curves B and B′, respectively). At the point $T = T_s$ the superconducting parameter sharply increases and thereby suppresses the parameter $\Delta_P$.

Figure 1($e$) gives the dependences of the parameters $\Delta_s/\Delta_{s0}$ and $\Delta_P/\Delta_{P0}$ on temperature at $p = 0.38$ and $\bar{\mu} = 1.1$ for values $\rho = 0$ ($\bar{\eta}_q = 0.601$) in curves A and A′ and for $\rho = 0.2$ ($\bar{\eta}_q = 0.553$) in curves B and B′. From this figure, in the region of low temperatures the 'dielectrisation' is completely suppressed and the system is in the superconducting phase.

The corresponding temperature dependences of the difference $\delta F$ in free energies at $\rho = 0$ is calculated from (17) and the system of equations for the cases in figures 1($a$), ($b$) and ($d$) are presented in figure 2. These results are in agreement with conclusions about the possibility of coexistence of SC and CDW in a certain temperature range.

As follows from the results obtained above, the behaviour of the system varies greatly and depends essentially on the values of $p$ and $\mu$. There are two different regions in the ranges of $p$ and $\bar{\mu}$ in which the non-zero solutions $\Delta_s$ and $\Delta_P$ of the system of equations (9), (10) exist. In the first region the values of $p$ and $\bar{\mu}$ are in the intervals $0.56 \leqslant p \leqslant 0.63$ and $1.048 \leqslant \bar{\mu} \leqslant 1.076$. The characteristic features of this region are as follows.

(i) $\Delta_s < \Delta_P$ throughout the temperature region $0 < T < T_s$.
(ii) There is an increase in the value $T_s$ when the magnetic field increases.
(iii) With increase in $\rho$, $\Delta_s$ increases including when $T = 0$ only for $\bar{\mu} > \bar{\mu}_c = 1.073$.

As is known, the magnetic field destroys the Cooper pairs in the usual superconductors. However, in the present case, when dielectric-type ordering takes place and the magnetic field is sufficiently weak, it influences the quasi-particle energy spectrum rather than destroys the Cooper pairs. Such unusual behaviour of the system's low-temperature phase in a magnetic field in our view is conditioned by the fact that in going from the initial metal state to the CDW state a shift in the dielectric gap with reference to the Fermi level (since $Q \neq 2K_F$) occurs in the energy spectrum of the system. Therefore, along with the electrons penetrating to the conductive band owing to their thermal excitation through the gap, the additional electrons that turn out to be above the gap owing to such restructuring of the energy spectrum also take part in the superconducting ordering. The position of the dielectric gap in the energy spectrum is defined by the parameter $\eta_q$. When $\eta_q = 0$ (commensurable phase), the gap forms in the middle of the energy band and, when $\eta_q \neq 0$ (incommensurable phase), it is shifted towards the Fermi level of the initial metal system. The magnetic field affecting the system suppresses the incommensurable phase, namely with increasing $\rho$ the parameter $\eta_q \to 0$. As a result the number of electrons above the gap increases and therefore the order parameter $\Delta_s$ increases even at $T = 0$ as $\rho$ increases until $\eta_q = 0$ while $\Delta_P$ decreases (see figures 1(*a*) and 1(*b*)). Also the magnetic field promotes the penetration of the electrons which appear owing to the thermal destruction of the electron–hole pairs through the dielectric gap which arises in the conductive band. When the values of the parameter $p$, characterising the strength of the interaction of Cooper pairs, are large enough, these electrons can contribute to the superconducting ordering. As a result, $T_s$ increases.

The appearance of a gapless state in a definite region of values of $\mu$ or external magnetic field $H_0$ as in the case of the quasi-one-dimensional antiferromagnet [29] is essential for superconductivity to appear. To explain the appearance of superconductivity in a ferromagnet in the region of strong external magnetic fields [31] the idea in [32] about the compensation of the internal field by the external field has been used.

The situation in antiferromagnetic and ferromagnetic systems differs from that considered in our paper. In the case of the magnetic system, as a rule, there are two groups of electrons: one is responsible for the SC and the other for magnetism. In our case there is a group of electrons which is responsible for SC and for CDW. In consequence the order parameters $\Delta_s$ and $\Delta_P$ are determined by the system of equations (9), (10) and the competition of coexistence of these two orderings is strict. A system state of semiconducting type but without an energy gap in the excitation spectrum occurs only in the second region ($0.1 \leqslant p \leqslant 0.45$ and $1.09 \leqslant \bar{\mu} \leqslant 1.4$) and therein the mechanism of destruction of Cooper pairs in a magnetic field is more essential. Thus, $T_s$ decreases as the magnetic field increases. As $\Delta_s$ and $\Delta_P$ are mutually dependent quantities, the decrease in $\Delta_s$ gives rise to the increase in $\Delta_P$ with increase in the magnetic field (figures 1(*d*) and (*e*)).

In figure 3(*a*) the temperature dependence of the spin magnetic susceptibility $\chi/\chi_0$ in the CDW state (the chain curve corresponds to $\bar{\mu} = 0$ and the broken curve to $\bar{\mu} = 1.075$) and in the mixed SC + CDW phase (the full curves correspond to the same parameters as in figures 1(*b*) and 1(*c*)). A comparison of the chain curve with the broken curve shows that on increase in $\bar{\mu}$ the slope of the curve in the above dependence changes. In addition to this, the whole curve is shifted to the left which corresponds to the appearance of $\chi \neq 0$ at a lower temperature than in the case $\mu = 0$. Thus, in the first region of parameters $p$ and $\bar{\mu}$ (both in the CDW state and in the mixed phase) at $T = 0$, $\chi = 0$ and increases rapidly with rise in temperature.

In figure 3(*b*) the dependence of magnetic susceptibility corresponding to the second region of the parameters $p$ and $\bar{\mu}$ on temperature is presented. The broken curve refers to the case of the CDW state at $\bar{\mu} = 1.1$ and the full curves refer to the mixed phase at the parameter values corresponding to figures 1(*d*) and 1(*e*). One has that in the absence of SC at point $T = 0, \chi \neq 0$. The gapless CDW state occurs here. In the mixed SC + CDW phase at point $T = 0$, $\chi = 0$ and rapidly increases with rise in temperature.

Thus, one obtains that the behaviour of the quantity $\chi$ as a function of temperature strongly depends on the parameter $\mu$ both in the CDW state and in the mixed phase. In the CDW state the rise in $\mu$ is analogous to the influences of the impurity through the effect of destruction of the electron–hole pairs [20].

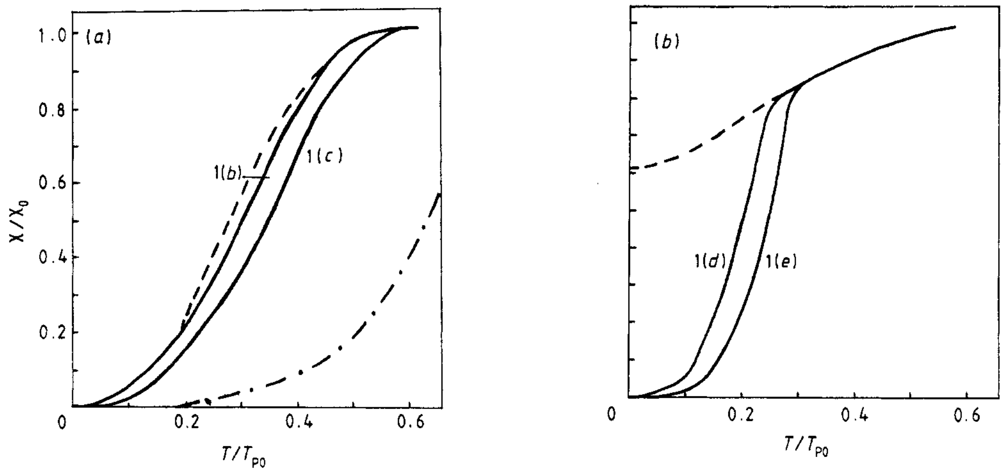


**Figure 3.** Spin magnetic susceptibility $\chi/\chi_0$ as a function of temperature $T/T_{P0}$ for different cases as explained in the text.

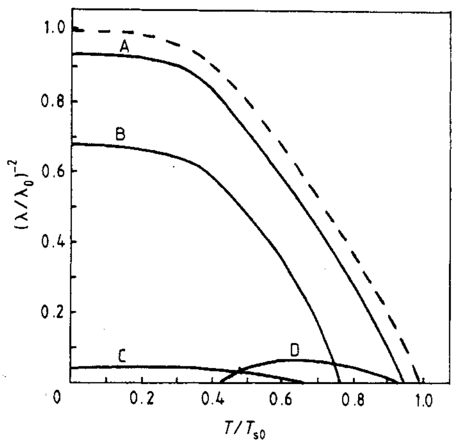


**Figure 4.** The temperature dependences of the quantity $(\lambda/\lambda_0)^{-2}$ for different theory parameters as explained in the text.

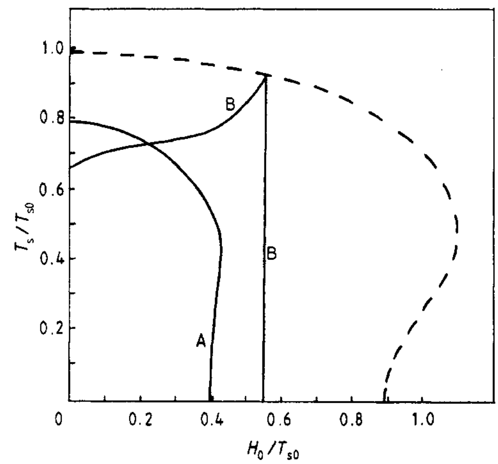


**Figure 5.** The dependences of the superconducting transition temperature $T_s$ as a function of magnetic field for different cases as explained in the text.

In figure 4 the dependence of the quantity $(\lambda/\lambda_0)^{-2}$ on temperature, obtained from the system of equations (9) and (10), and from equation (20), is shown. Curve A in this figure corresponds to the case $p = 0.38$, $\bar{\mu} = 1.2$, curve B to $p = 0.35$, $\bar{\mu} = 1.1$, curve C to $p = 0.6$, $\bar{\mu} = 1.073$, and curve D to $p = 0.57$, $\bar{\mu} = 1.075$. The broken line corresponds to the case of the usual superconductor. The comparison of the dependences in curves A–D with the broken curve shows that the behaviour of $(\lambda/\lambda_0)^{-2}$ as a function of temperature can differ from the BCS case both qualitatively and quantitatively. In particular, curves C and D show the high values of the penetration depth and its slight dependence on temperature.

In conclusion, in figure 5 the dependence of the superconducting transition temperature $T_s$ on the magnetic field in the mixed phase is presented. Curve A corresponds to $\bar{\mu} = 1.1, p = 0.35$ and curve B to $\bar{\mu} = 1.073, p = 0.6$. The broken curve corresponds to the case of the usual superconductor. As was mentioned above, along with the usual behaviour of the value $T_s$ as a function of the magnetic field (curve A) we have its increase with increase in magnetic field up to the value $T_s = T_P$ at the point $H_0 = H_{cr} \simeq 0.53\ T_{s0}$ (curve B). At $H_0 > H_{cr}$, we assume that $T_s = 0$ in accordance with the condition about the possibility of formation of superconducting ordering on the background of the CDW state ($T_s \leqslant T_P$) [27]. As follows from this figure the paramagnetic critical field of the mixed SC + CDW phase is less than its value for the superconducting phase $H_P \simeq 0.84T_{S0} = \Delta_s(0)/\sqrt{2}$. The increase in the critical temperature with increase in the magnetic field is observed in the region of values $0 < H_0 < H_P$.

## 6. Conclusions

The problem that we attempted to tackle was the investigation of the thermodynamic and magnetic properties of strongly anisotropic systems in the region of low temperatures. The investigations were carried out using the one-dimensional model and the slight deviation from the half-filling of the conductive band ($\mu \ll W$), Umklapp processes being taken into account. This deviation is rather real in systems with overlapping energetic bands on the Fermi surface, when one of the bands undergoes restructuring through the transition to the CDW state and the second remains unchanged and acts like a reservoir. This situation may happen, for example, in the chain A15 compounds. In addition to this, $\mu$ may change when an impurity is introduced into a strongly anisotropic system. In this case, to equations (9), (10) must be added one further equation, following from the law of charge conservation.

It should be noted that the model in [33] with partial 'dielectrisation' of the Fermi surface is rather successful in describing the properties of the anisotropic systems. In fact this model may be regarded as a simplified two-band model, where one band is responsible for SC and the other for CDW when all constants of the effective electron–electron interaction (both intra-band and inter-band) are considered to be equal. In real systems it seems that one should take into account both the partial 'dielectrisation' and the effects connected with $\mu \neq 0$. For the case of SC and SDW, such investigations have in part been carried out in [34].

It should be noted also that in some cases the behaviour of the quasi-one-dimensional system considered above, for which in the mixed SC + CDW phase the parameters of the theory are $p$ and $\mu$, is analogous to the behaviour of that in the model in [33] in which in the same phase the main parameters are $p$ and $N_1/N_2$ (where $N_1/N_2$ is the ratio of the densities of the electronic states in the corresponding parts of the Fermi surface). In connection to this the model considered above with $\mu \neq 0$ could be seen either as an alternative to the model in [33] or as an addition to it.

## References

[1] Schegolev I F 1972 *Phys. Status Solidi* a **12** 9
[2] Bechgaard K, Jacobsen C S, Mortensen K, Pedersen H J and Thorup N 1980 *Solid State Commun.* **33** 1119

[3] Scott J C, Pederser H J and Bechgaard K 1980 *Phys. Rev. Lett.* **45** 2125
[4] Zeller H R 1973 *Festkörperprobleme* (*Advances in Solid State Physics*) vol 131, ed. H J Queisser (Oxford: Pergamon) p 31
[5] Ichikava M and Fischer O 1977 *Solid State Commun.* **24** 747
[6] Chan S K and Hein V 1973 *J. Phys. F: Met. Phys.* **3** 795
[7] Budzin A I and Bulaevsky L N 1984 *Usp. Fiz. Nauk* **144** 415
[8] Johnston D C, Stokes J P, Hsich P L and Gruner G 1983 *J. Physique Coll.* **44** C3 1749
[9] Richard J and Monceau P 1980 *Solid State Commun.* **33** 635
[10] Johnston D C 1984 *Phys. Rev. Lett.* **52** 2049
[11] Bulaevsky L N 1975 *Usp. Fiz. Nauk* **115** 263
[12] Peierls R E 1955 *Quantum Theory of Solids* (Oxford: OUP) p 108 ff
[13] Frölich H 1954 *Proc. R. Soc.* A **223** 296
[14] Kuper C G 1955 *Proc. R. Soc.* A **227** 214
[15] Mattis D C 1970 *Phys. Rev. Lett.* **25** 376
[16] Rice M J and Strössler S 1973 *Solid State Commun.* **13** 125
[17] Allender D, Bray J W and Bardun J 1974 *Phys. Rev.* B **9** 119
[18] Lee P A, Rice T M and Anderson P W 1973 *Phys. Rev. Lett.* **31** 462
[19] Leung M C 1974 *Solid State Commun.* **15** 879; 1975 *Phys. Rev.* B **11** 4272
[20] Landau L D and Lifshitz E M 1964 *Statistical Physics* (Moscow: Nauka)
[21] Roshen W A 1985 *Phys. Rev.* B **31** 7296
[22] Timerov R H 1977 *Zh. Eksp. Teor. Fiz.* **72** 2309
[23] Palistrant M E and Chernei M D 1987 *Fiz. Nizk. Temp.* **13** 1054
[24] Levin K, Mills D L and Cunningham S L 1974 *Phys. Rev.* B **10** 3821
[25] Levin K, Cunningham S L and Mills D L 1974 *Phys. Rev.* B **10** 3832
[26] Kopayev Y V and Timerov R H 1972 *Zh. Eksp. Teor. Fiz.* **63** 290
[27] Palistrant M E and Padure I V 1985 *Teor. Mater. Fiz.* **62** 117
[28] Ashkenazi J, Kuper C G, Revzen M, Ron A and Schmeltzer D 1984 *Solid State Commun.* **51** 135
[29] Suzumura Y and Nagi A D 1981 *Solid State Commun.* **40** 651
[30] Machida K 1984 *J. Phys. Soc. Japan.* **53** 712
[31] Meul H W, Rossel C, Deeroux M and Fischer O 1984 *Phys. Rev. Lett.* **53** 497
[32] Jaccarino V and Peter M 1962 *Phys. Rev. Lett.* **9** 290
[33] Bilbro G and McMillan W L 1976 *Phys. Rev.* B **14** 1887
[34] Palistrant M E and Padure I V 1985 *Phys. Lett.* **111**A 445; 1987 *Teor. Mater. Fiz.* **70** 443