SUPERCONDUCTING TRANSITION TEMPERATURE AND HEAT CAPACITY JUMP IN QUASI-TWO-DIMENSIONAL ANISOTROPIC SYSTEMS DOPED WITH CHARGE CARRIERS

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Abstract

Phase transitions in quasi-two-dimensional systems doped with atoms with different valences, at various temperatures are investigated. The transitions into the magnetic state of spin density wave which appear due to the nesting on the Fermi surface and the transition into incommensurable state of spin density wave are considered along with the appearnce of superconductivity. The main system of equation is presented, the difference of free energies in different phases, superconducting transition temperature and heat capacity jump are calculated. The behavior of mentioned quantities as a function of temperature and charge carrier density is researched.

1. Introduction

The description of the properties of FeAs based high-Tc superconducting systems (Fe – pnictids and Fe - chalcogenids) requires taking into account the following peculiarities of these systems: the overlapping on the Fermi surface of few energy bands (both electron- and hole-type bands); reduced dimensionality of the system and the anisotropy of dispersion law for the energy of electrons and holes of different bands; the existence of symmetry points where the following relation takes place:

$$\varepsilon_n(\vec{k}) = -\varepsilon_n(\vec{k} + \vec{Q}) \tag{1}$$

(ε_n is the energy of charge in *n-th* band, $\vec{Q}$ is the wave vector of spin density wave); phase transitions into magnetic (SDW) and superconducting (SC) when temperature and charge carrier density vary; the bands filling degree when doping.

An important number of articles, monographs and reviews are dedicated to the theory of many-band superconductors (see the references given in [1] – [4]). These researches have been started long before the discovery of HTSC and are based on the model independently developed by Moscalenco [5] and Suhl et al. [6]. Presently, along with the term “many-band” for modern HTSC compounds the term “many-orbital superconductivity” is used. In our opinion, this fact is determined by presence of several energy bands (both electron– and hole – type) on the Fermi surface. In this case, the two – or many – band model [5, 6] is developed and adjusted to the concrete HTSC compound, according to experimental data. For example, a review of modern researches on FeAs – based modern compounds is given in [7] (see also the references in [4]).

An important problem when the physical properties of above mentioned systems are researched is the identification of mechanisms leading to the appearance of magnetism (SDW state) and superconductivity (SC) and the coexistence of these states. One of such mechanisms is the transition of the system into gapless magnetic state (phase transition commensurability – incommensurability) when the wave vector of spin density wave is $Q \neq 2\ k_F$. Some partial researches in this direction are performed in [4, 8].

Here, in this paper these researches are developed further: free energy in the phase of coexistence of SDW and SC is calculated, the type of phase transition (first or second kind) is determined when superconductivity appears on the background of SDW, the temperature of superconducting transition T_c and heat capacity jump in the point $T = T_c$ are calculated. Also, the behavior of above mentioned thermodynamic quantities as functions of temperature and charge carrier density is analyzed.

2. The Hamiltonian of the system and basic equations

We think that a quality correlation between superconductivity and magnetism is possible to obtain using the following Hamiltonian:

$$H = \sum_{\vec{k},\sigma}\left(\varepsilon(\vec{k}) - \mu\right)a^{+}_{\vec{k}\sigma}\, a_{\vec{k}\sigma} - \sum_{\vec{k}\vec{k}'} V\left(\vec{k}\vec{k}'\right)a^{+}_{\vec{k}\uparrow}a^{+}_{-\vec{k}\downarrow}\;\; a_{-\vec{k}'\downarrow}a_{\vec{k}'\uparrow} + $$
$$+ \sum_{\vec{k}\vec{k}\vec{q}} I\left(\vec{k}\vec{k}'\right) a^{+}_{\vec{k}\uparrow}a_{\vec{k}+\vec{q}\uparrow}a^{+}_{\vec{k}'\downarrow}a_{\vec{k}'-\vec{q}\downarrow}. \quad (2)$$

Here V and I – effective constants of superconducting and magnetic interaction of electrons, $\vec{k}$ – quasi - momentum, $\varepsilon(\vec{k})$ – energy of electron, σ – spin of electron, which takes the values $\uparrow$ and $\downarrow$, $a^{+}_{\vec{k}\sigma}, a_{\vec{k}\sigma}$- operators of appearance or annihilation of electrons (with momentum $\vec{k}$ and spin σ), $\vec{q}$ corresponds to those values of electron momentum which lead to the nesting condition (1), μ is chemical potential.

Within such approach the ratio between parameters V and I or the superconducting transition temperature T_c and magnetic transition temperature T_M is important. The second term in this expression contains $V > 0$ and describes the formation of Cooper pairs, the third one describes the appearance of SDW at $I > 0$. We consider a non-phonon mechanism of superconductivity based on direct repulsion of electrons. The non-phonon mechanism which leads to the values $V > 0$ in Hamiltonian (2) isn't clearly determined. According to many researchers, superconductivity in FeAs-based compounds appears due to spin fluctuations, i.e. magnetic mechanism [7]. But strong magnetic fluctuations which are able to lead to the formation of Cooper pairs aren't discovered in all these compounds. In the same time, all of them are many-band systems. Therefore, the appearance of additional electron-electron inter- and intra-band interactions V_{nm} ($n; m = 1, 2$ in the case of two-band system), which contribute to the efficiency of system transition into superconducting state, is inherent for such systems. In particular, when inter-band constants of electron interaction are higher than intra-band ones ($V_{11}V_{22} - V_{21}V_{12} < 0$) within a non-phonon mechanism high values of Tc are possible when two-band system is doped with charge carriers [9, 4]. In our opinion, such an electronic mechanism of superconductivity could be named inter-band mechanism.

Using the Green functions method [10], in middle – field approximation, we obtain from (2) a self-consistent system of equations for determining the order parameter of SC (Δ), order parameter of SDW (M), and chemical potential μ (see, for details [8, 11]):

$$\frac{1}{V} = \frac{1}{4}\int_{-\widetilde{W}}^{\widetilde{W}} d\varepsilon N(\varepsilon)\sum_{\alpha,\beta}\Phi_1\left(\varepsilon, \mu_\beta^\alpha, M, \Delta\right),$$

$$\frac{1}{I} = \frac{1}{4}\int_{-\widetilde{W}}^{\widetilde{W}} d\varepsilon N(\varepsilon)\sum_{\alpha,\beta}\Phi_2\left(\varepsilon, \mu_{\alpha\beta}, M, \Delta\right),$$

$$x = \int_{-\widetilde{W}}^{\widetilde{W}} d\varepsilon N(\varepsilon)\sum_{\alpha\beta}\Phi_3(\varepsilon, \mu_{\alpha\beta}, M, \Delta), \tag{3}$$

here $N(\varepsilon)$ – electron state density for quasi-two-dimensional anisotropic system with cosines-type dispersion law:

$$\varepsilon(\vec{k}) = -W_1 cosk_x a - W_2 cosk_y b, \tag{4}$$

$$\Phi_1\left(\varepsilon, \mu_{\alpha\beta}, M, \Delta\right) = \frac{M^2 + Y}{Y}\cdot\frac{th\frac{\sqrt{X_1}}{2T}}{\sqrt{X_1}} - \frac{M^2 - Y}{Y}\cdot\frac{th\frac{\sqrt{X_2}}{2T}}{\sqrt{X_2}},$$

$$\Phi_2\left(\varepsilon, \mu_{\alpha\beta}, M, \Delta\right) = \frac{\Delta^2 + \left(\mu_{\alpha\beta}\right)^2 + Y}{Y}\cdot\frac{\mathrm{th}\frac{\sqrt{X_1}}{2T}}{\sqrt{X_1}} - \frac{\Delta^2 + \left(\mu_{\alpha\beta}\right)^2 - Y}{Y}\cdot\frac{th\frac{\sqrt{X_2}}{2T}}{\sqrt{X_2}},$$

$$\Phi_3\left(\varepsilon, \mu_{\alpha\beta}, M, \Delta\right) = \frac{\Delta^2 + \left(\mu_{\alpha\beta}\right)^2 + \varepsilon^2 + Y}{Y}\cdot\frac{th\frac{\sqrt{X_1}}{2T}}{\sqrt{X_1}} - \frac{\Delta^2 + \left(\mu_{\alpha\beta}\right)^2 + \varepsilon^2 - Y}{Y}\cdot\frac{th\frac{\sqrt{X_2}}{2T}}{\sqrt{X_2}}, \tag{5}$$

$$X_{1,2} = \varepsilon^2 + \left(\mu_{\alpha\beta}\right)^2 + M^2 + \Delta^2 \pm 2Y, \qquad Y = \sqrt{\left(\mu_{\alpha\beta}\right)^2\left(\varepsilon^2 + M^2\right) + M^2\Delta^2},$$

where

$$\mu_{\alpha\beta} = \mu + \alpha\eta_a + \beta\eta_b; \;\; \eta_a = \frac{W_1 a q_x}{2}; \; \eta_b = \frac{W_2 b q_y}{2}; \;\; \alpha, \beta = \pm 1 \tag{6}$$

η_a, η_b are the constants of the incommensurability parameter of SDW, q_x, q_y – components of the deviation of SDW vector from $2k_F$.

The expressions (4) – (5) are given in final form after series of transformation of main equations. In particular, summation over Matsubara frequency is performed and transition to the integration over energy taking into account the umklapp - processes leading to the relation $Q \neq 2k_F$ is made (for details, see [8, 11, 12]).

The properties of the system in SDW state ($\Delta = 0, M \neq 0$) are researched in details in our series of works [4, 11, 12]. Here, we will consider the possibility of coexistence of magnetism and superconductivity ($\Delta \neq 0$, $M \neq 0$) in quasi-two-dimensional doped anisotropic system. In order to reveal the efficiency of such coexistence, the difference of free energies $F(\Delta, M) - F(0, M)$ has to be researched as a function of temperature and charge carrier density along with self-consistent solution of system of equations (3).

3. Calculation of free energy and heat capacity jump at $T = T_c$

In order to determine the free energy we use the identity:

$$F\,(\Delta, M) - F\,(0{,}0) = \int_0^{\Delta} \Delta'^2\, d\Delta' \frac{d}{d\Delta'}\left(\frac{1}{V}\right) + \int_0^{M} M'^2 dM' \frac{d}{dM'}\left(\frac{1}{I}\right)\Big|_{V=0}. \tag{7}$$

Integrating by parts, we will bring it to the form:

$$F\,(\Delta, M) - F(0{,}0) = \frac{\Delta^2}{V} + \frac{M^2}{I} - 2\int_0^{\Delta} \Delta' d\Delta' \frac{1}{V} - 2\int_0^{M} M' dM' \left(\frac{1}{I}\right)_{V=0} \tag{8}$$

Using expressions (3) and integrating over order parameters Δ' and M', we bring the difference of free energies to the form:

$$F(\Delta, M) - F\,(0{,}0) = \frac{\Delta^2}{V} + \frac{M^2}{I} - T \int_{-\widetilde{W}}^{\widetilde{W}} N\,(\varepsilon)\, d\varepsilon \sum_{\alpha\beta} \left\{ \ln ch\, \frac{\sqrt{X_1}}{2T} + \ln ch \frac{\sqrt{X_2}}{2T} - \ln ch \frac{\sqrt{X_1^{00}}}{2T} - \ln ch\, \frac{\sqrt{X_2^{00}}}{2T} \right\}, \tag{9}$$

where X_1 and X_2 are determined by formulas (4), and $X_{1,2}^{00} = X_{1,2}\,|_{M=\Delta=0}$. As it follows from the results obtained earlier [8], in this examined system superconducting state appears on the background of magnetic ordering. Thus, it makes sense to consider the difference of free energies in the form:

$$\delta\, F = F\,(\Delta, M) - F\,(0, M) = \frac{\Delta^2}{V} - T \sum_{\alpha\beta} \int_{-\widetilde{W}}^{\widetilde{W}} N\,(\varepsilon) d\varepsilon\; \cdot \sum_{\alpha\beta} \left\{ \frac{\ln ch\, \sqrt{X_1}}{2T} + \ln ch \frac{\sqrt{X_2}}{2T} - \ln ch \frac{\sqrt{X_1^o}}{2T} - \ln ch \frac{\sqrt{X_2^o}}{2T} \right\},$$

$$X_1^o = X_1|_{\Delta=0}\;, \quad X_2^o = X_2|_{\Delta=0}. \tag{10}$$

Further we examine the temperature range close to superconducting transition temperature $(T \sim T_c)$. We expand the difference of free energies (10) over small parameter Δ^2

$$\delta\, F = F\,(\Delta, M) - F\,(0, M) = \frac{\Delta^4}{4}\,[-f_1 + \Delta^2 f_2 + \ldots], \tag{11}$$

and represent the equation for superconducting transition temperature (3) in the form:

$$\frac{1}{V} = f_o - \frac{1}{2} f_1\, \Delta^2 + \frac{3}{8}\, \Delta^4\, f_2 + \ldots, \tag{12}$$

where

$$f_0 = \frac{1}{2} \int_0^{\widetilde{W}} d\varepsilon\, N\,(\varepsilon) \sum_{\alpha\beta} \Phi_1\left(\varepsilon, \mu_\beta^\alpha, M\,\Delta\right)\Big|_{\Delta=0}$$

$$= \frac{1}{2} \int_0^{\widetilde{W}} d\varepsilon\, N\,(\varepsilon) \sum_{\alpha\beta} \left[\frac{M^2 + Y}{Y} \cdot \frac{th \frac{\sqrt{X_1}}{2T}}{\sqrt{X_1}} - \frac{M^2 - Y}{Y} \cdot \frac{th \frac{\sqrt{X_2}}{2T}}{\sqrt{X_2}} \right],$$

$$f_1 = -\int_0^{\widetilde{W}} d\varepsilon\, N\,(\varepsilon) \sum_{\alpha\beta} \frac{\partial}{\partial \Delta^2} \Phi_1\;\left(\varepsilon, \mu_\beta^\alpha, M, \Delta\right)\Big|_{\Delta=0} =$$

$$= -\int_0^{\widetilde{W}} d\varepsilon N(\varepsilon) \sum_{\alpha,\beta,j} \left\{ \frac{1}{4T_c ch^2\left(\frac{1}{2T}\sqrt{z_2 + 2jz_1}\right)} \times \right.$$

$$\times\left(\frac{1}{\sqrt{z_2+2jz_1}}+\frac{jM^2}{\sqrt{z_1{}^2z_2+2jz_1{}^3}}\right)\left(\frac{M^2}{\sqrt{z_1{}^2z_2+2jz_1{}^3}}+\frac{j}{\sqrt{z_2+2jz_1}}\right)-$$

$$-\frac{M^2th\left(\frac{1}{2T}\sqrt{z_2+2jz_1}\right)}{2}\cdot\left[\frac{1}{(z_1{}^2b+2jz_1{}^3)^{3/2}}\cdot(3jz_1M^2+z_1{}^2+z_2M^2)+\frac{j}{z_2+2jz_1}\times\right.$$

$$\left.\times\left(\frac{1}{M^2\sqrt{z_2+2jz_1}}+\frac{j}{\sqrt{z_1{}^2z_2+2jz_1{}^3}}\right)\right\},$$

Where

$$z_1=\mu_{\alpha\beta}\sqrt{\varepsilon^2+M^2},$$

$$z_2=\varepsilon^2+\left(\mu_{\alpha\beta}\right)^2+M^2,\qquad j=\pm 1.$$

$$f_2=\frac{2}{3}\int_0^{\widetilde{W}}d\varepsilon\, N(\varepsilon)\sum_{\alpha\beta}\frac{\partial^2}{\partial\Delta^4}\Phi_1\left(\varepsilon,\mu_\beta^\alpha,M,\Delta\right)\Big|_{\Delta=0}. \qquad (13)$$

From expression (11) follows that there are two possibilities of transition of magnetic system into superconducting state: 1) $\Delta = 0$ and 2) $\Delta^2 = f_1/f_2$. The first case corresponds to second-kind phase transition (at $f_1 > 0, f_2 < 0$), and the second case – to first-kind phase transition (at $f_1 < 0$, $f_2 < 0$). Here is crucial the sign of the coefficient f_1, depending on x and M. The point $f_1 = 0$ corresponds to the value $x = x_c$, when the type of phase transition is changing. The critical temperature is not a monotonic decreasing function of x. There is a range of ambiguous compliance between x and T_c. It an area of instability of normal state relative to the formation of Cooper pairs. Obviously, at $x > x_c$ the equation (12) has to be examined at $\Delta \neq 0$, which corresponds to first-kind phase transition. In particular, unambiguous dependence of T_c on x can be represented graphically, after calculating based on (10) the difference in free energy at low temperatures and determining x from the condition $\delta F = 0$ at $T=T_c = 0$.
Further, expanding over the quantity $(1 - T/T_c)$ in eq. (13) and considering only quadratic terms over the quantity Δ^2, it is easy to find the expression for order parameter:

$$\Delta^2=\frac{2}{f_1}\left(1-\frac{T}{T_c}\right)T_c\frac{\delta f_0}{\delta T}\Big|_{T=Tc}. \qquad (14)$$

Replacing (14) in (11), for free energy we obtain:

$$\delta F=-\frac{1}{f_1}\left(1-\frac{T}{T_c}\right)^2\left(\frac{\delta f_0}{\delta T}\Big|_{T=Tc}\right)^2. \qquad (15)$$

Therefore, based on (15), for specific heat jump in the point $T=T_c$ we obtain the expression:

$$\delta C=C(\Delta,M)-C(0,M)=-T\frac{\delta^2}{\delta T}\delta F=\frac{2}{f_1}T_c\left(\frac{\delta f_0}{\delta T}\Big|_{T=Tc}\right)^2. \qquad (16)$$

4. Phase transitions

The system of equations (3) – (5) contains the possibility for describing various phase transitions in examined system when temperature T and charge carrier density x change. This system contains parameter of magnetic ordering M, superconducting order parameter Δ, chemical potential μ, and also the components of incommensurability of magnetic state η_a and η_b.

As it was shown earlier [8, 4], superconductivity in examined system appears at $T_M > T_c$ on the background of incommensurable state of SDW. This fact corresponds to the necessity of examining the system (3) in two cases: 1) $M \neq 0$, $\Delta = 0$ and 2) $M \neq 0$, $\Delta \neq 0$. When the temperature of superconducting transition T_c is calculated is sufficient to examine the limiting cases $M \neq 0$, $\Delta \to 0$.

In the case 1) we have a system of equations, describing SDW state in the absence of superconductivity, and in the case 2) this system contains the definition of quantities T_c, $M(T_c)$, μ, and also the values of η_a and η_b.

The obtained above main equations are a complex system and its solving may be performed numerically.

For the case 1), which corresponds to SDW state, we examine the system of equations:

$$\frac{1}{V} = \frac{1}{2}\int_0^{\widetilde{W}} \frac{N(\varepsilon)d\varepsilon}{\sqrt{\varepsilon^2 + M^2}} \sum_{\alpha\beta j} \frac{\left[M^2 + j\mu_{\alpha\beta}\sqrt{\varepsilon^2 + M^2}\right] th\frac{1}{2T}\left(\sqrt{\varepsilon^2 + M^2} + j\mu_{\alpha\beta}\right)}{j\mu_{\alpha\beta}\left[\sqrt{\varepsilon^2 + M^2} + j\mu_{\alpha\beta}\right]},$$

$$\frac{1}{I} = \frac{1}{2}\int_0^{\widetilde{W}} \sum_{\alpha\beta j} \frac{N(\varepsilon)d\varepsilon}{\sqrt{\varepsilon^2 + M^2}} th\frac{1}{2T}\left(\sqrt{\varepsilon^2 + M^2} + j\mu_{\alpha\beta}\right), \qquad (17)$$

$$x = \int_0^{\widetilde{W}} \sum_{\alpha\beta j} \frac{N(\varepsilon)d\varepsilon}{\sqrt{\varepsilon^2 + M^2}} \frac{\left[\varepsilon^2 + \mu_{\alpha\beta}^2 + j\mu_{\alpha\beta}\sqrt{\varepsilon^2 + M^2}\right] th\frac{1}{2T}\left(\sqrt{\varepsilon^2 + M^2} + j\mu_{\alpha\beta}\right)}{j\mu_{\alpha\beta}\left[\sqrt{\varepsilon^2 + M^2} + j\mu_{\alpha\beta}\right]},$$

together with two additional equations that allow to determine the dependence of quantities η_a and η_b from T and x:

$$\frac{\delta}{\delta\eta_a}[F(M) - F(0)] = \sum_{\alpha\beta j} j\alpha \int_0^{\widetilde{W}} N(\varepsilon)d\varepsilon \left[th\frac{1}{2T}\left(\sqrt{\varepsilon^2 + M^2} + j\mu_{\alpha\beta}\right) - th\frac{1}{2T}\left(\varepsilon + j\mu_{\alpha\beta}\right)\right] = 0$$

$$\frac{\delta}{\delta\eta_b}[F(M) - F(0)] = \sum_{\alpha\beta j} j\beta \int_0^{\widetilde{W}} N(\varepsilon) \times$$

$$\times\, d\varepsilon \left[th\frac{1}{2T}\left(\sqrt{\varepsilon^2 + M^2} + j\mu_{\alpha\beta}\right) - th\frac{1}{2T}\left(\varepsilon + j\mu_{\alpha\beta}\right)\right] = 0, \qquad (18)$$

where $F(M) - F(0)$ is the difference of free energies.

In Fig. 1 the phase diagram (T, $\tilde{x}$) is shown as a result of the analysis of the solutions of these equations and determination of dependence of parameters η_a, η_b on temperature and impurity concentration [8, 11].

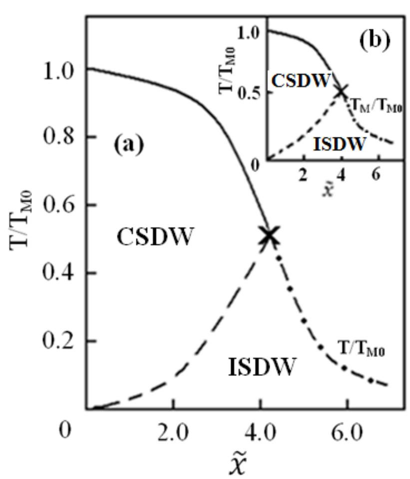

Fig. 1. Phase diagram (T, x̃). *CSDW* – commensurable, and *ISDW* – incommensurable spin density wave (a) case of isotropic energy spectrum (W_2 / W_1=1), (b) – case of anisotropic energy spectrum (W_2 / W_1=1.3). In the branching point marked with a cross, we have: case (a) $T_M/T_{M0} = 0.49$, case (b) $T_M/T_{M0} = 0.52$.

The dashed curve in the phase diagram of Fig. 1 separates incommensurable SDW (ISDW) state (low temperatures range) from commensurable one (high temperatures range). The comparison of two diagrams in Fig.1 (a and b) demonstrates the influence of the anisotropy of energy spectrum on phase diagram (T, $\tilde{x}$). It follows that the anisotropy of energy spectrum increases the area of ISDW (shifts the dashed curve to the area of higher temperatures). It is chosen: (1a) – isotropic case ($W_1 = W_2$); (1b) – anisotropic case $W_2/W_1=1.3$. Thus, both in isotropic and anisotropic case, the magnetic state of spin density wave splits into commensurable and incommensurable one.

As a result the dielectric gap shifts relative to the Fermi surface (q_x,; $q_y \neq 0$) and, therefore, free carriers appear on the Fermi surface. In such a way, the examined here mechanism (violation of nesting and shifting of dielectric gap) may lead to the transition of the system to gapless magnetic state and to the possibility of appearance of superconductivity.

The limiting case $M \neq 0$, $\Delta \to 0$, $T = T_c$ leads to the system of eq. (17), where we have to consider $T = T_c$. The obtained in this way system demonstrates the appearance of superconductivity in the magnetic phase, i.e. determines the coexistence of magnetism and superconductivity.

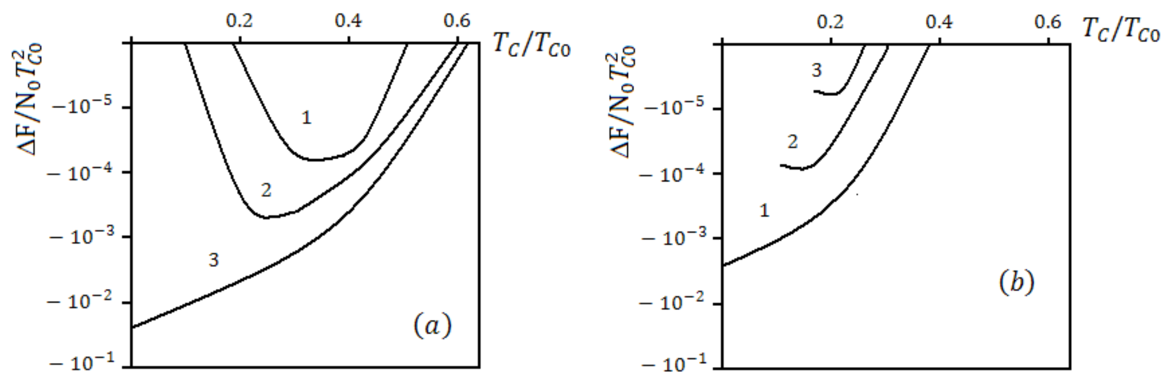

Fig. 2. Temperature dependence of free energy difference at various values of parameters $\tilde{x}$ *and t.* Case (a) curve 1 corresponds to $\tilde{x} = 3.6$ and $t=0.8$, curve 2 – to $\tilde{x} = 4.2$ and $t=0.6$, curve 3 – to $\tilde{x} = 4.6$ and $t=0.4$. Case (b) curve 1 corresponds to $\tilde{x} = 6$ and $t=0.3$, curve 2 – to $\tilde{x} = 4$ and $t=0.2$, curve 3 - $\tilde{x} = 2$ and $t=0.1$.

The quantities $t = T_{c0}/T_{M0}$, $\tilde{x} = x/2N_0$ and T are important theory parameters. Here T_{c0} and T_{M0} are renormalized temperatures of superconducting and magnetic transitions.

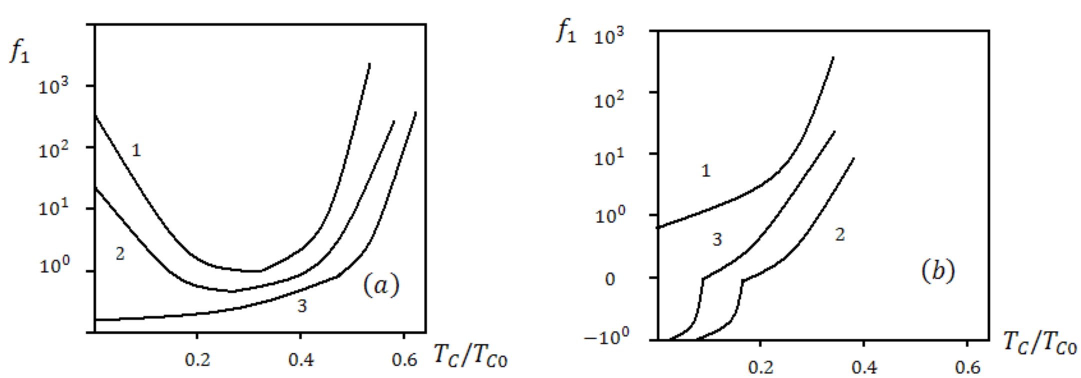

Fig. 3. The dependence of coefficient f_1 on critical temperature of superconducting transition. The curves are marked similarly to Fig. 2. The values of parameters $\tilde{x}$ and t is similar to Fig. 2.

In Fig. 2 the temperature dependence of free energy difference at various values of t and $\tilde{x}$ parameters is shown. From these results follows that in a wide range of temperatures the difference of free energies has a negative value, which speaks that the appearance of superconductivity on the background of incommensurable SDW state is profitable. Wherein second – order phase transitions are possible in low temperatures range (Fig. 2a, curves 1-3) and first – order ones in low temperatures range (Fig. 2b, curves 2 and 3). The same result we obtain when the function $f_1(T)$ from (13) is studied (Fig. 3). The type of phase transition is determined by the ratio between quantities T_{C0} and T_{M0}. We have a second – order phase transition to superconducting state (Fig. 3a) where $f_1 > 0$ in the whole range of examined values of T_c and first – order one $f_1 < 0$ (Fig 3b, curves 2 and 3).

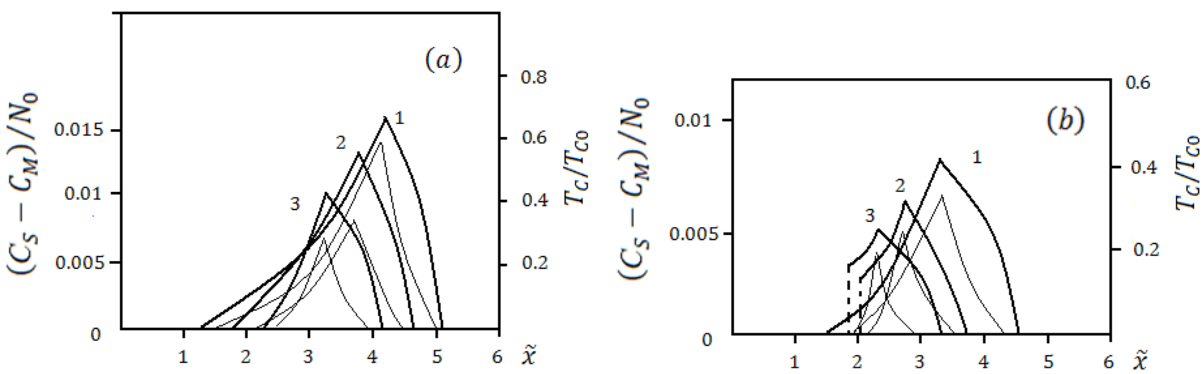

Fig. 4. The dependence of temperature of superconducting transition (bold curves) and $\frac{C_S - C_M}{N_0}$ on charge carrier density. Case (a) curve 1 corresponds to *t=0.8*, curve 2 – to *t=0.6*, curve 3 – to *t=0.4*. Case (b) curve 1 corresponds to *t=0.3*, curve 2 - *t=0.2*, curve 3 - *t=0.1*.

The dependence on charge carrier density of two quantities T_c/T_{c0} (bold curves 1-3) and $\delta C/N_0 = \left(C(\Delta, M) - C(0, M)\right)/N_0$ (thin curves 1-3) is presented in Fig. 4 a, b. As it follows from this figure the quantities T_c/T_{c0} and $\delta C/N_0$ reach the maximum at nearly the same values of carrier density $\tilde{x}_{max}$. Superconducting state occurs at doping in the point $\tilde{x} = \tilde{x}_{c1}$, reaches the maximum value in the point $\tilde{x} = \tilde{x}_{max}$ and vanish at the point $\tilde{x} = \tilde{x}_{c2}$. The behavior of T_c/T_{c0} is presented in the form of deformed bell-shaped curve. The absence of symmetry in this dependence on carrier density is explained by the influence of magnetic state on superconductivity. Indeed, the definition of T_c contains the magnetic order parameter $M(T_c)$, which suppresses superconductivity. The value of this quantity in the area $\tilde{x} < \tilde{x}_{max}$ is bigger than in the area $\tilde{x} > \tilde{x}_{max}$, that is manifested in the form of dependence T_c/T_{c0} on $\tilde{x}$.

In these figures the curves for the specific heat are lesser deformed than the curves for T_c, due to the presence of additional factors in the definition of δC in (16).

The concrete values of theory parameters t and $\tilde{x}$ are given in figures captions. An example of experimental results related to FeAs – based HTSC compounds is given in Fig. 5. The comparison of our curves given in Fig. 4 with experimental ones from Fig. 5 suggests that qualitative dependence of T_c on $\tilde{x}$ is in agreement with experimental data [13].

In the case of heat capacity jump qualitative agreement may be obtained if it assumed that there is a peak in the dependence of electron state density N_0 on $\tilde{x}$ similar to the dependence $T_c(\tilde{x})$. The presented theory doesn't contain other possibilities. It is natural that the examined description of coexistence of magnetism and superconductivity based on a simple model (1) isn't enough for obtaining complete agreement with experimental data related to complex FeAs-based compounds.

Perhaps, it may be necessary to take into account the overlapping of energy bands on the Fermi surface, additional electron – electron interactions, associated with consideration of charge and spin fluctuations etc. Reasoning on this subject can be found in experimental studies (see, for instance [13]).

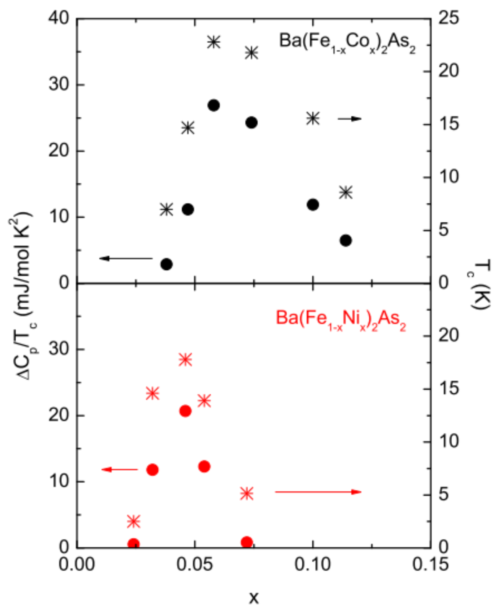

Fig. 5. $\Delta C_p/T_c$ (little circles, left axis) and T_c (asterisks, right axis) as functions on impurity concentration x, $Ba(Fe_{1-x}Co_x)_2As_2$ (the upper part) and $Ba(Fe_{1-x}Ni_x)_2As_2$ (the bottom part). The graph corresponds to Fig. 2 in [13] here $\Delta C_p = C_S - C_M$.

5. Conclusions

This paper is focused on the identification of various phase transitions in quasi-two-dimensional lattice with a cosine – type electron energy dispersion law and the presence in the system of interactions responsible for magnetic phase (SDW) and superconductivity.

Chemical doping with impurity leads to the violation of nesting on Fermi surface and instability of SDW state. In this case, the taking into account of umklapp - processes changes the value of wave vector of spin density wave. At $Q \neq 2k_F$ the dielectric gap shifts relative to Fermi surface. As a result, the system passes into stable gapless magnetic state (incommensurable SDW state). Free carriers appear on Fermi surface and possibility for superconductivity is opened. Thus, we may conclude:

1. When quasi-two-dimensional system is doped with impurity with increasing of charge carrier concentration $\tilde{x}$ successive phase transitions commensurable state of spin density wave (CSDW) - incommensurable state of spin density wave (ISDW).
2. On the background of ISDW formation of Cooper pairs and coexistence of magnetic and superconducting states are possible when $T_c < T_M$. If $T_c > T_M$ superconductivity doesn't appear.
3. The area where superconductivity and magnetism coexist is determined mainly by the value of the parameter $t = T_{C0}/T_{M0}$.

4. The dependence of T_c/T_{c0} on impurity concentration $\tilde{x}$ is presented in the form of deformed bell-shaped curve. Superconductivity appears in the point $\tilde{x}_{c1}$, reaches the maximum in the point $\tilde{x}_{max}$, and vanishes at $\tilde{x}_{c2}$. The type of phase transition determines the value of parameter t. In the area of low temperatures and small $\tilde{x}$ the phase transition is first-order one. Qualitative agreement with experimental data for a number of $FeAs$-based compounds.

5. Heat capacity jump $\delta C = C(\Delta, M) - C(0, M)$ as a function of $\tilde{x}$ has the same bell-shape but is less deformed then in the case of T_c/T_{c0} due to an additional factor in the definition of this value.

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