INFLUENCE OF THE MAGNETIC FIELD AND IMPURITY ON THE COMMENSURATE–INCOMMENSURATE PHASE TRANSITION IN A QUASI-TWO-DIMENSIONAL MAGNETIC SYSTEM

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Abstract

A theory of thermodynamic properties of a spin density wave (SDW) in a quasi-two-dimensional system (with a preset impurity concentration x) is constructed. We choose an anisotropic dispersion relation for the electron energy and assume that external magnetic field $\boldsymbol{H}$ has an arbitrary direction relative to magnetic moment $\boldsymbol{M}_Q$. The system of equations defining order parameters M_Q^z, M_Q^σ, M_z, and M_σ is constructed and transformed with allowance for umklapp scattering (U-processes). Special cases when $\boldsymbol{H} \parallel \boldsymbol{M}_Q$ and $\boldsymbol{H} \perp \boldsymbol{M}_Q$ ($H_z H_\sigma = 0$) are considered in detail as well as cases of weak fields $\boldsymbol{H}$ of arbitrary direction. The condition for the transition of the system to the commensurate and incommensurate states of the SDW is analyzed. The concentration dependence of magnetic transition temperature T_M is calculated, and the components of the order parameter for the incommensurate phase are determined. The phase diagram (T, $\tilde{x}$) is constructed.

1. Introduction

There are a large number of publications focused on the discovery and study of the properties of new high-temperature superconducting materials based on FeAs. These studies have been initiated in [1], and subsequent studies resulted in compounds with a superconducting transition temperature of $Tc \approx 55$ K [2−6].

A distinguishing feature of these materials — ferropnictides and ferrochalcogenides — is their multiband structure [7-13].

Various approaches to describing superconductivity and magnetism (based on the band structure of each compound, the possibility of violation of the nesting conditions, deformation of the Fermi surface, and so on) are being used at present for a new class of FeAs-based compounds [14–21]. In our opinion, it is necessary to analyze the properties of FeAs-based materials to determine their magnetic properties and magnetic phase transitions disregarding their possible superconductivity.

An interesting feature of some new materials is the possibility of a phase transition to the commensurate or incommensurate state of the SDW. In the case of a transition to the incommensurate state, which is observed in many Fe-based compounds (see, e.g., [22–27]), interesting features appear in the behavior of physical quantities as a function of temperature and impurity concentration. In particular, a gapless state can be formed and metal properties can be exhibited [28−32].

Here, we analyze the properties of a quasi-two-dimensional system with an anisotropic energy spectrum and take into account the nesting condition on the Fermi surface, which facilitates the emergence of magnetism owing to the SDW, as well as U-processes.

2. Hamiltonian of the system and basic equations

Using the mean field approximation, we can write Hamiltonian of a quasi-two-dimensional system in the form:

$$\mathcal{H} = \sum_{k,\alpha} (\varepsilon_{\vec{k}} - \mu) a^{+}_{\vec{k}\vec{\alpha}} a_{\vec{k}\vec{\alpha}} - \sum_{\vec{k},\alpha,\beta} \vec{H}\vec{\sigma}_{\alpha,\beta}\, a^{+}_{\vec{k}\vec{\alpha}} a_{\vec{k}\vec{\beta}} + \frac{U}{N} \sum_{\vec{k},\vec{k}',\vec{q}} a^{+}_{\vec{k}\uparrow} a_{\vec{k}+\vec{q}\uparrow} a^{+}_{\vec{k}'\downarrow} a_{\vec{k}'-q\downarrow}, \quad (1)$$

where:

$$\sigma = \pm 1(\uparrow,\downarrow), \quad \varepsilon_{\vec{k}\sigma} = \varepsilon_{\vec{k}} - \mu - \sigma\widetilde{H}_z, \quad \widetilde{H}_z = H_z + M_z,$$
$$\widetilde{H}^{\sigma} = H^{\sigma} + M^{\sigma}, \quad M^{\sigma} = M_x + i\sigma M_y, \quad M^{\sigma}_Q = M^x_Q + i\sigma M^y_Q, \quad H^{\sigma} = H_x + i\sigma H_y, \quad (2)$$

μ is the chemical potential, and H_x, H_y, H_z are the external magnetic field components.
Here, we assume that the magnetic field direction is arbitrary relative to magnetization parameter $\vec{M}_Q$.

The components of order parameter $\vec{M}_Q$ and of spontaneous magnetization $\vec{M}$ are defined as

$$M^z_Q = \frac{1}{2}\, gT \sum\nolimits_{\vec{k},n,\sigma} \sigma G_{\sigma\sigma}(\vec{k}+\vec{Q},\vec{k},\omega_n), \quad (3)$$

$$M^{\sigma}_Q = gT \sum\nolimits_{\vec{k},n} G_{-\sigma\sigma}(\vec{k}+\vec{Q},\vec{k},\omega_n), \quad (4)$$

$$M_z = M^z_{Q=0} = \frac{1}{2}\, g\, T \sum\nolimits_{\vec{k},n,\sigma} \sigma G_{\sigma\sigma}(\vec{k},\vec{k},\omega_n),$$

$$M^{\sigma} = M^{\sigma}_{Q=0} = gT \sum_{\vec{k},n} (G_{-\sigma\sigma}\vec{k},\vec{k},\omega_n), \quad (5)$$

where $g=U/N$; N is the total number of lattice states, and $\mathrm{G}_{\sigma\sigma'}(\vec{\mathrm{k}}',\vec{\mathrm{k}},\omega_n)$ is the one-particle Green's function in the $(\vec{k},\omega)$ representation.

If the Fermi level is shifted from the middle of the band due to the introduction of an impurity with concentration x into the system, we must take into account the charge conservation conditions:

$$x = T \sum\nolimits_{\vec{k}\sigma} \sum\nolimits_n \left[G_{\sigma\sigma}(\vec{k},\vec{k},\omega_n) - G^{(-)}_{\sigma\sigma}(\vec{k},\vec{k},\omega_n)\right]. \quad (6)$$

where $G_{\sigma\sigma}(\vec{k}\,\vec{k},\omega_n)$ temperature Green's function in representation $(\vec{k},\omega\;)$ and $G^{(-)}_{\sigma\sigma}(\vec{k},\vec{k},\omega_n)$ can be obtained from $G_{\sigma\sigma}(\vec{k}\,\vec{k},\omega_n)$ by the substitution $\varepsilon_1 = \varepsilon'_{\vec{k}} \to -\varepsilon_1$ and $\varepsilon_2 = \varepsilon'_{\vec{k}+\vec{Q}} \to -\varepsilon_2$.

On the basis of Hamiltonian (1) and relations (3)–(5), we obtain the following set of equations for the Green's functions:

$$\begin{aligned}(i\omega_n - \varepsilon_{\vec{k}\sigma}) G_{\sigma\sigma'}(\vec{k},\vec{k}',\omega_n) + \sigma M^z_Q G_{\sigma\sigma'}(\vec{k}+\vec{Q},\vec{k}',\omega_n) + \\ + \sigma M^z_Q G_{\sigma\sigma'}(\vec{k}-\vec{Q},\vec{k}',\omega_n) + M^{-\sigma}_Q G_{-\sigma\sigma'}(\vec{k}+\vec{Q},\vec{k}',\omega_n) + \\ + M^{-\sigma}_Q G_{-\sigma\sigma'}(\vec{k}-\vec{Q},\vec{k}',\omega_n) + \widetilde{H}^{-\sigma} G_{-\sigma\sigma'}(\vec{k},\vec{k}',\omega_n) = \delta_{kk'}\delta_{\sigma\sigma'}\end{aligned} \quad (7)$$

If vector $\vec{Q}(Q_x, Q_y)$ is incommensurate with the reciprocal lattice vectors, the resultant set of equations is of an infinitely large order. To avoid these difficulties, we here use the computational technique developed in [29‒32] for a spin density wave (SDW) transition in a quasi-two-dimensional system.

The method involves analysis of normal processes (without U-processes) at the first stage: paired electrons and holes in this case must be in a unit cell; that is, in the 2D case, the following conditions must be satisfied:

$$|k_x| < Q_x^0, \quad |k_x + Q_x| < Q_x^0, \quad |k_y| < Q_y^0, \quad |k_y + Q_y| < Q_y^0, \tag{8}$$

where

$Q_x^0 = \pi/a$, $Q_y^0 = \pi/b$; a and b are the lattice constants.

With allowance for relations (8) (normal processes), we obtain the following system of equations for the Green's functions $G_{\sigma\sigma}(\vec{k}, \mathrm{k}, \omega_n)$, $G_{-\sigma\sigma}(\vec{k}, \vec{\mathrm{k}}, \omega_n)$, $G_{\sigma\sigma}(\vec{k} + \vec{Q}, \vec{k}, \omega_n)$ and $G_{-\sigma\sigma}(\vec{k} + \vec{Q}, \vec{\mathrm{k}}, \omega_n)$:

$$\begin{pmatrix} i\omega_n - \varepsilon_{\vec{k},\sigma} & \sigma M_Q^z & \widetilde{H}^{-\sigma} & M_Q^{-\sigma} \\ \sigma M_Q^z & i\omega_n - \varepsilon_{\vec{k}+\vec{Q},\sigma} & M_Q^{-\sigma} & \widetilde{H}^{-\sigma} \\ \widetilde{H}^{\sigma} & M_Q^{\sigma} & i\omega_n - \varepsilon_{\vec{k},-\sigma} & -\sigma M_Q^z \\ M_Q^{\sigma} & \widetilde{H}^{\sigma} & -\sigma M_Q^z & i\omega_n - \varepsilon_{\vec{k}+\vec{Q},-\sigma} \end{pmatrix} \cdot \begin{pmatrix} G_{\sigma\sigma}(\vec{k}, \vec{k}, \omega_n) \\ G_{\sigma\sigma}(\vec{k} + \vec{Q}, \vec{k}, \omega_n) \\ G_{-\sigma\sigma}(\vec{k}, \vec{k}, \omega_n) \\ G_{-\sigma\sigma}(\vec{k} + \vec{Q}, \vec{k}, \omega_n) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}. \tag{9}$$

To avoid cumbersome calculations, we will give the solution to system (9) in Appendix A in [31].

System of equations for order parameter $\vec{M}_Q$ and spontaneous magnetization $\vec{M}$ see also in [31, 32].

3. Normal and U-processes

Let us choose the anisotropic dispersion relation for the electron energy

$$\varepsilon(\vec{k}) = -W_1 \cos(k_x a) - W_2 \cos(k_y b), \tag{10}$$

which takes into account the interaction between the nearest neighbors. It can easily be seen that for $\mu = 0$ and $x = 0$, $q_x = q_y = 0$, $Q_x^0 = \frac{\pi}{a}$, $Q_y^0 = \frac{\pi}{b}$, the nesting condition $\varepsilon(k) = -\varepsilon(k - Q^0)$ holds. In this case, the commensurate SDW state is formed and a dielectric gap appears on the entire Fermi surface. For$x \neq 0$ and q_x, $q_y \neq 0$ condition (8) leads to the relations $q_x < k_x < Q_x^0$, $q_y < k_y < Q_y^0$. As noted above, in the case of normal processes, 2D summation over $\vec{k}$ in [3] and (6) takes into account a part of the Brillouin zone.

In this case, U-processes are taken into account by summation in [3] and (6) over $\vec{k}$ in the intervals $-Q_x^0 < k_x < Q_x^0$ and $-Q_y^0 < k_y < Q_y^0$. Consequently, the entire Brillouin zone participates in electron–hole pairing. Let us pass from summation over $\vec{k}$ to integration with respect to energy in each term of Eqs. (3)‒(6) in accordance with the formula

$$\sum_k F\left(\vec{k},\dots\right) = \frac{1}{(2\pi)^2}\int_{-Q_0^x}^{Q_0^x} dk_x \int_{-Q_0^y}^{Q_0^y} dk_y\, F\left(\varepsilon_1,\varepsilon_{2,}\dots\right), \quad (11)$$

where

$\varepsilon_1 = \varepsilon'\left(\vec{k}\right) = \varepsilon_{1x} + \varepsilon_{1y} - \mu$ и $\varepsilon_2 = \varepsilon'(k+Q) = \varepsilon_{2x} + \varepsilon_{2y} - \mu$, $\varepsilon_{1x} = -W_1 cos\,(a\,k_x)$, $\varepsilon_{1y} = -W_2 cos\left(b\,k_y\right)$, $\varepsilon_{2x} = +W_1\cos\,[a\,(k_x+q_x)]$, $\varepsilon_{2y} = W_2\cos\,[b\left(k_y+q_y\right)$.

Following the technique developed in [29‒32], we can reduce expression (15) to the form

$$\sum_k F\left(\vec{k},\dots\right) = \frac{1}{4}\int_{-\widetilde{W}}^{\widetilde{W}} N(\varepsilon)\,d\varepsilon \sum_{\alpha,\beta} F\left(\varepsilon_1 = \varepsilon - \mu_\beta^\alpha;\ \varepsilon_2 = -\left(\varepsilon+\mu_\beta^\alpha\right),\dots\right). \quad (11a)$$

Here

$$\widetilde{W} = W_1 + W_2,\ \ \mu_\beta^\alpha = \mu + \alpha\eta_a + \beta\eta_b,\ \ \eta_a = \frac{W_1 a q_x}{2},\ \ \eta_b = \frac{W_2 b q_y}{2},\ \ \alpha;\beta = \pm 1. \quad (12)$$

Thus, double integration of $F\left(\vec{k},\dots\right)$ with respect to k_x and k_y can be reduced to integration of expression $\frac{1}{4}\,N(\varepsilon)\,F\,(\varepsilon,\dots)$ with respect to energy ε in the interval $-\widetilde{W} < \varepsilon \ll \widetilde{W}$, where N(ε) is the density of electron states of the 2D system [33], which is determined from dispersion relation (10).

Further, all researches are executed taking into account U-processes. We will consider some cases of the chosen direction of a magnetic field.

Case a. The transverse magnetic field is $\widetilde{H}_z = M_z = M_Q^\sigma = 0$; $\psi = \pi/2$. In this limit, formulas for order parameter M_Q^z and spontaneous magnetization M^σ lead to the following equations:

$$1 = -\frac{1}{4}g\sum_{\beta,\alpha,\sigma\prime,\sigma\prime\prime}\sigma'\int_{-\widetilde{W}}^{\widetilde{W}} N(\varepsilon)\,\frac{d\varepsilon}{4\xi_{\sigma\prime\prime}(\varepsilon)}\ th\,\frac{E^\beta_{\alpha\sigma\prime\sigma\prime\prime}}{2T},$$

$$M^\sigma = \frac{1}{4}\,g\sum_{\beta,\alpha,\sigma\prime,\sigma\prime\prime}\sigma'\,\sigma''\int_{-\widetilde{W}}^{\widetilde{W}} N(\varepsilon)\,\frac{(\varepsilon-\sigma''H^\sigma)}{\xi_{\sigma\prime\prime(\varepsilon)}}\,th\,\frac{E^\beta_{\alpha\sigma\prime\sigma\prime\prime}}{2T}\,d\varepsilon,$$

$$x = 2N_0\sum_{\alpha\beta\sigma'\sigma''}\int_0^{\widetilde{w}}\frac{N(\varepsilon)}{N_0}\left\{\frac{th\frac{\beta\left(\tilde{\varphi}_{\sigma'\sigma''}-\mu_{\alpha\beta}\right)}{2}}{4\tilde{\varphi}_{\sigma'\sigma''}\varepsilon\widetilde{H}}\left[(\varepsilon+\tilde{\varphi}_{\sigma'\sigma''})\left(\widetilde{H}^2+2\sigma''\widetilde{H}\varepsilon\right)+\right.\right. \quad (13)$$

$$\left.+(\varepsilon-\tilde{\varphi}_{\sigma'\sigma''})\widetilde{H}^2\right] - \frac{th\dfrac{\beta\left(\tilde{\varphi}'_{\sigma'\sigma''}+\mu_{\alpha\beta}\right)}{2}}{4\tilde{\varphi}'_{\sigma'\sigma''}\varepsilon\widetilde{H}}\left[\left(-\varepsilon+\tilde{\varphi}'_{\sigma'\sigma''}\right)\left(\widetilde{H}^2+2\sigma''\widetilde{H}\varepsilon\right)+\right.$$

$$\left.\left.+\left(-\varepsilon+\tilde{\varphi}'_{\sigma'\sigma''}\right)\widetilde{H}^2\right\}d\varepsilon,$$

where

$$\tilde{\varphi}_{\sigma'\sigma''} = \sqrt{M_Q^2+\left(\widetilde{H}+\varepsilon\right)^2},\quad \tilde{\varphi}'_{\sigma'\sigma''} = \sqrt{M_Q^2+\left(\widetilde{H}-\varepsilon\right)^2}.$$

Case b. The longitudinal magnetic field is $H^\sigma = M^\sigma = M_Q^\sigma = 0$; $\psi = 0$. This gives

$$A\,(\varepsilon) = 2[\varepsilon^2 + \left(M_Q^z\right)^2]^{\frac{1}{2}},\qquad \xi_{\sigma''}(\varepsilon) = \left|A(\varepsilon) - 2\sigma''^{\widetilde{H}_z}\right|,$$

$$E^\beta_{\alpha\sigma\prime\sigma\prime\prime} = -\mu_\alpha^\beta - \frac{1}{2}\,\sigma'\xi_{\sigma\prime\prime}(\varepsilon). \quad (14)$$

System of equations can be transformed to

$$M_Z = \frac{1}{2} g \sum_{\beta,\alpha,\sigma\prime,\sigma\prime\prime} \sigma' \sigma'' \int_{-\widetilde{W}}^{\widetilde{W}} \frac{N(\varepsilon)}{4}\, th \frac{E_\alpha^\beta\, \sigma'\sigma''}{2T} d\varepsilon,$$

$$1 = -\frac{1}{4} g \sum_{\beta,\alpha,\sigma\prime,\sigma\prime\prime} \sigma' \int_{-\widetilde{W}}^{\widetilde{W}} \frac{N(\varepsilon)}{4\, A\,(\varepsilon)}\, th \frac{E_\alpha^\beta\, \sigma'\sigma''}{2T}\, d\varepsilon,$$

$$x = 2N_0 \sum_{\alpha\beta\sigma'\sigma''} \int_0^{\widetilde{w}} \frac{N(\varepsilon)}{N_0} \Bigg\{ \frac{th \frac{\beta\left(\tilde{\varphi}_{\sigma'\sigma''} - \mu_{\alpha\beta}\right)}{2}}{2\tilde{\varphi}_{\sigma'\sigma''}\widetilde{H}A_k} \Big[(\varepsilon + \tilde{\varphi}_{\sigma'\sigma''}) \left(\widetilde{H}^2 + \sigma''\widetilde{H}A_k - \sigma\widetilde{H}_Z(\varepsilon + \tilde{\varphi}_{\sigma'\sigma''}) \right) + (\varepsilon - \tilde{\varphi}_{\sigma'\sigma''})\widetilde{H}^2 + \tilde{\psi} \Big]$$

$$- \frac{th \frac{\beta\left(\tilde{\varphi}'_{\sigma'\sigma''} + \mu_{\alpha\beta}\right)}{2}}{2\tilde{\varphi}'_{\sigma'\sigma''}\widetilde{H}A_k} \Big[\left(-\varepsilon + \tilde{\varphi}'_{\sigma'\sigma''}\right) \left(\widetilde{H}^2 + \sigma''\widetilde{H}A_k - \sigma\widetilde{H}_Z\left(-\varepsilon + \tilde{\varphi}'_{\sigma'\sigma''}\right) \right) + \left(-\varepsilon + \tilde{\varphi}'_{\sigma'\sigma''}\right)\widetilde{H}^2 + \tilde{\psi} \Big\} d\varepsilon, \tag{15}$$

where

$$\tilde{\varphi}_{\sigma'\sigma''} = 2\sqrt{\widetilde{H}^2 + M_Q^2 + \widetilde{H}A_k + \varepsilon^2}, \quad \tilde{\varphi}'_{\sigma'\sigma''} = 2\sqrt{\widetilde{H}^2 + M_Q^2 - \widetilde{H}A_k + \varepsilon^2}, \tag{16}$$

$$\tilde{\psi} = \sigma\widetilde{H}_z\left(\widetilde{H}_z^2 - M_Q^{z^2}\right), \qquad A_k = \left[\varepsilon^2 + M_Q^2\right]^{1/2}.$$

4. Critical temperature of transition to a magnetic state: Phase transitions

Given above the equations as a result of a number of mathematical transformations and transition to an integration on energy in compliance with formula (11a), it is possible to simplify significantly [31, 32]. We use, in particular, ratios $H_z H^\sigma = 0$ and $M_Q^\sigma = 0$. In a limit of zero value of a magnetic field ($H \to 0$) we obtain systems of the equations for determination of parameter of magnetic phase M, and at $M \to 0$ we obtain temperature of magnetic streamlining T_M. This system of the equations has the form

$$1 = \frac{1}{4} g \sum_{\beta,\alpha,\sigma',\sigma\prime\prime} \sigma'\sigma'' \int_0^{\widetilde{w}} \frac{N(\varepsilon)\left(2\widetilde{H}cos^2\psi - \sigma''A\,(\varepsilon)\right)}{2\xi_{\sigma\prime\prime}(\varepsilon)A(\varepsilon)}\, th\, \frac{E_{\alpha\sigma\prime\sigma\prime\prime}^\beta}{2T}\, d\varepsilon, \tag{17}$$

$$M = \frac{1}{8} g \sum_{\beta,\alpha,\sigma',\sigma\prime\prime} \sigma'\sigma'' \int_0^{\widetilde{w}} \frac{N(\varepsilon)\left(A(\varepsilon) - 2\sigma''\widetilde{H}\right)}{2\xi_{\sigma\prime\prime}(\varepsilon)}\, th\, \frac{E_{\alpha\sigma\prime\sigma\prime\prime}^\beta}{2T}\, d\varepsilon. \tag{18}$$

which is supplemented with the equations, the incommensurability of a condition of SDW allowing determining the parameter of an order defined from conditions of a minimum of free energy at $M \to 0$

$$\frac{\delta}{\delta\eta_{a,b}}[F(M) - F(0)] = 0. \tag{19}$$

Considering quasi-two-dimensionality and anisotropy of the considered system, we use determination of the density of electronic states for this system:

$$\frac{N(\varepsilon)}{N_0} = \frac{\theta\left((1+\eta)^2-\lambda^2\right)}{\sqrt{\eta}} \left\{\theta(\lambda^2 - (\eta-1)^2)K(k) + \frac{\theta\left((\eta-1)^2-\lambda^2\right)}{k} K\left(\frac{1}{k}\right)\right\}, \qquad (20)$$

where

$$k = \frac{\sqrt{(1+\eta)^2-\lambda^2}}{\left(2\sqrt{\eta}\right)}, \quad \lambda = \frac{\varepsilon}{w_1}, \qquad \eta = \frac{w_2}{w_1}. \qquad (21)$$

$K(k) = F\left(\frac{\pi}{2}, k\right)$ is full elliptic integral of the first sort.

The system of the equations derived above decides by numerical methods

To determine magnetic transition temperature T_M for $\widetilde{H} = 0$, we solve system of equations (17)–(19) using electron density of states (20). It is convenient to begin analyzing this system of equations assuming that $\eta_a = \eta_b = 0$. In this simplified case, we find that the T_M/T_{M0} ratio decreases with increasing $\tilde{x}$ up to a critical point (T_M, x_c) denoted by the cross in Fig. 1. In the vicinity of this point, a solution corresponding to instability of the SDW state exists.

The solution to system of equations (24)–(26) without the above simplifications at point gives values of parameters η_a and $\eta_b \neq 0$ associated with violation of nesting and displacement of the Fermi surface (q_x, $q_y \neq 0$). It should be noted that the free energy of the system under investigation as a function of temperature has two minima. One of these minima disappears for $\eta_a = \frac{W_1 a q_x}{2}$ and $\eta_b = \frac{W_2 b q_y}{2} = 0$. Deviation of these parameters from zero lowers the energy of the system and stabilizes the magnetic state via a transition from the commensurate SDW state to the incommensurate SDW state (dashed curve in Fig. 1). Thus, the solid curve in Fig. 1 shows the dependence of T_M/T_{M0} on $\tilde{x}$ for the phase transition to the commensurate SDW state, while the dashed curve demonstrates the transition to the incommensurate SDW state.

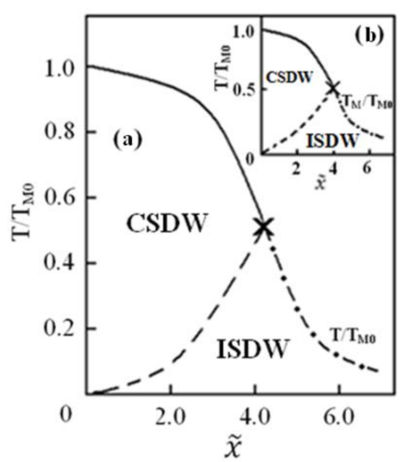

Fig. 1. Phase diagram (T, $\tilde{x}$); CSDW and ISDW are the commensurate and incommensurate states of the spin density wave, respectively; (a) isotropic energy spectrum ($W_2/W_1 = 1$); (b) anisotropic energy spectrum ($W_2/W_1 = 1.3$). At the branching point (×), $T_M/T_{M0} = 0.49$ (a) and 0.52 (b).

To construct the $(T, \tilde{x})$, phase diagram, we must analyze the behavior of the SDW state for $T < T_M$ [31,32].

On the basis of these theory graphic dependences, the corresponding quantities are given below.

Figure 1 shows the $(T, \tilde{x})$ phase diagram as the result of analysis of the solutions to these main equations at $T < T_M$ and determination of the dependence of parameter η_a on temperature (Fig. 2) and on impurity concentration (Fig. 3).

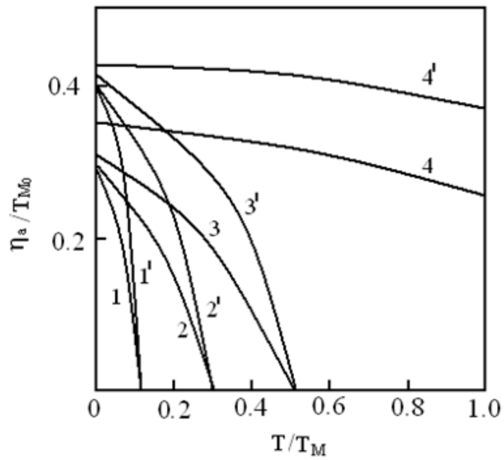

Fig. 2. Temperature dependences of parameter η_a (curves *1–4* correspond to the isotropic case; *1'–4'*, to the anisotropic case) for $\tilde{x}$ = 1, 2, 4, 5, respectively.

Plotting these solutions for η_a and analogous solutions for η_b in the diagram in Fig. 1, we can separate the domains of commensurate ($\eta_a = \eta_b \neq 0$) and incommensurate states of the spin density wave. The dashed curve on the phase diagram (see Fig. 1) separates the incommensurate SDW state (in the low-temperature region) from the commensurate state (in the high-temperature region). Comparison of the two diagrams in Fig. 1 demonstrates the effect of anisotropy of the energy spectrum on the $(T, \tilde{x})$ phase diagram. It can be seen that anisotropy of the energy spectrum increases the ISDW domain (it shifts the dashed curve to the region of higher temperatures). Figures 1a and 1b illustrate the isotropic case ($W_1 = W_2$) and anisotropic case ($W_2/W_1 = 1.3$), respectively.

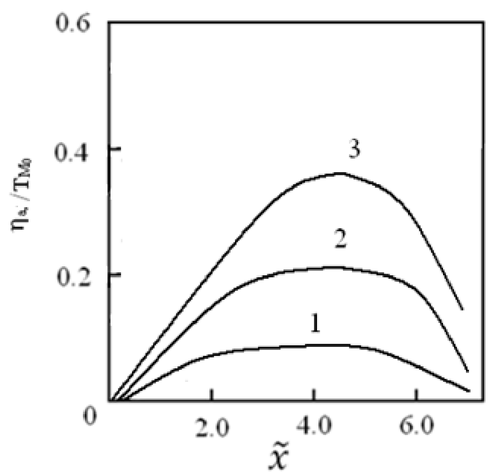

Fig. 3. Dependences of η_a/T_M on $\tilde{x}$ for T/T_{M0} = 0.1 (curve *1*), 0.2 (*2*), and 0.4 (*3*).

Figure 4 shows the M_Q/M_0 ratio as a function of T/T_{M0} with increasing $\tilde{x}$.

It can be seen that the value of M_Q decreases with increasing $\tilde{x}$ as well as with increasing T.

Figure 5 shows the increase in parameters η_a , η_b with increasing impurity concentration and the dependence of these parameters on the anisotropy of the energy spectrum: $\eta_a = \eta_b$ in the isotropic case and $\eta_a \neq \eta_b$ in the anisotropic case.

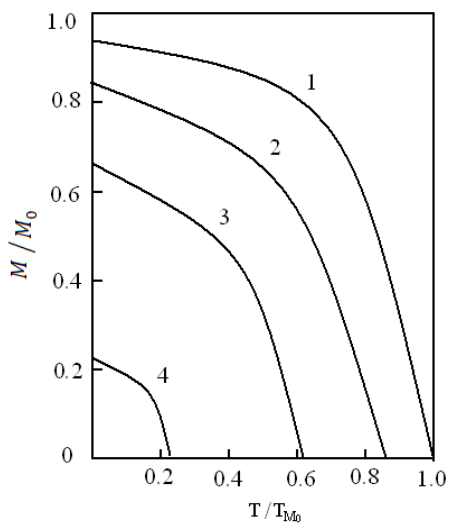

Fig. 4. Temperature dependences of order parameter M/M_0 for small magnetic fields $\widetilde{H}$≈0.15· T_{M0} for $\widetilde{x}$ = 0.5 (curve 1), 2 (*2*), 3 (*3*), and 4 (*4*).

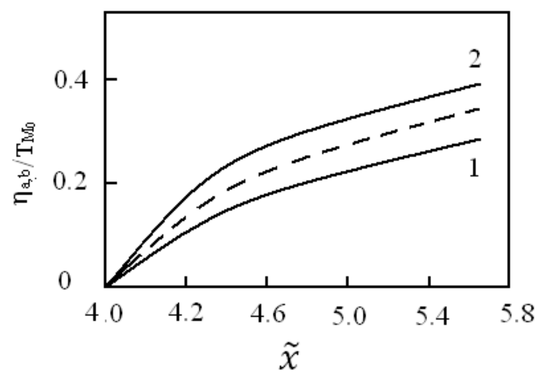

Fig. 5. Dependence of parameters η_a and η_b (curves 1 and *2*, respectively) on $\tilde{x}$ for $T = T_M$ for the anisotropic case (W_2/W_1 = 1.3); dashed curve corresponds to the isotropic case $\eta_a = \eta_b$.

Note that the incommensurable condition of SDW arises at a defined value of parameter $\eta = \eta_a + \eta_b$ at the corresponding impurity concentration value. Thus, each of components η_a and η_b can accept different values. In our opinion, this suggests the possibility of spin polarization of electrons in both one-dimensional ($q_x = 0$, $q_y \neq 0$ or $q_x \neq 0$, $q_y = 0$) and two-dimensional directions ($q_x \neq 0$, $q_y \neq 0$). In the channelized model, it is defined by the direction of a vector $\boldsymbol{Q}$. As appropriate there is a shift of the Fermi level in relation to a dielectric crack.

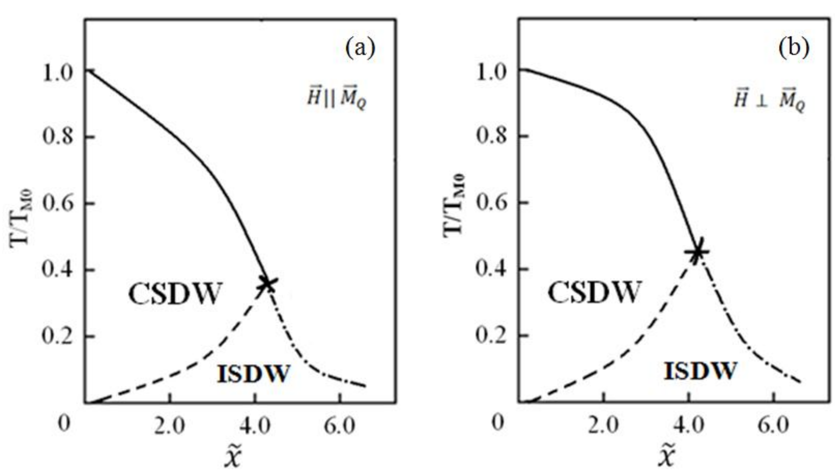

Fig. 6. Phase diagram (T, $\tilde{x}$) in magnetic fields $\boldsymbol{H} \parallel \boldsymbol{M}_Q$ (a) and $\boldsymbol{H} \perp \boldsymbol{M}_Q$ (b). (a) (b)

Let us return the phase diagram (Figs. 1a, 1b) and try to determine the effect of magnetic field on this diagram. It was found that for a longitudinal magnetic field $\vec{H} \,||\, \vec{M}_Q$ ($\psi = 0$), the T_M value is noticeably suppressed by the magnetic field, while a transverse field ($\psi = \pi/2$) weakly affects magnetic transition temperature T_M. This result changes the (T_M, x) phase diagram for $\boldsymbol{H} \parallel \boldsymbol{M}_Q$: the cross on the curve describing the dependence of T_M on $\tilde{x}$ in the longitudinal field is displaced to the region of lower temperatures (i.e., the region of solutions η_a and $\eta_b \neq 0$ in the phase diagram is shifted downwards). As a result, the dashed curve separating the CSDW state from ISDW state is shifted towards lower temperatures. Therefore, the ISDW domain decreases in a longitudinal magnetic field. Conversely, for $\vec{H} \perp \vec{M}_Q$, the phase diagram changes insignificantly. These results are shown in Figs. 6a and 6b.

5. Conclusions

This aim of this study was a theoretical description of the properties of new FeAs-based high-temperature superconducting materials at temperatures $T \leq T_M$, where T_M is the magnetic transition temperature. Our analysis was based on the Hubbard Hamiltonian in the mean field approximation, nesting on the Fermi surface, and rearrangement of the energy spectrum. We proceeded from a quasi-two-dimensional system approximating layered structures inherent in these materials, assuming that magnetism is associated with the spin density wave. The commensurability–incommensurability phase transition appearing, among other things, due to allowance for U-processes in SDW-induced magnetism is a very interesting phenomenon.

Using Green's functions and determining the order parameters corresponding to M_Q^z, M_Q^σ, M_z and M^σ, we succeeded in describing the dependence of magnetic transition temperature T_M on concentration and also analyzed the behavior of M_Q at $T < T_M$. In this way, we could construct the $(T, \tilde{x})$ phase diagram containing the commensurate and incommensurate states of the SDW. The latter stabilizes the state of the spin density wave. We have analyzed the effect of anisotropy of the energy spectrum and external field on the $(T, \tilde{x})$ phase diagram. It is shown that the ISDW region is considerably reduced for $\tilde{H} || \vec{M}_Q$, while its decrease for $\tilde{H} \perp \vec{M}_Q$ is insignificant. A magnetic field (especially longitudinal) lowers the probability of formation of a semimetallic state and, hence, emergence of superconductivity. In fact, a metal state facilitating the emergence of superconductivity appears against the background of the spin density wave. It should be noted that magnetic transition temperature T_M is strongly suppressed in a longitudinal magnetic field ($\tilde{H} || \vec{M}_Q$) and is weakly suppressed in a transverse field ($\tilde{H} \perp \vec{M}_Q$).

Note that anisotropy of the energy spectrum affects the general pattern of the SDW state.

References

[1] Y. Kamihara, T. Watanabe, M. Hirano, et al. Chem. Soc. 130, 3296 (2008).
[2] Xiyu Zhu, Huong Vang, Lu Fang, et al., Supercond. Sci. Technol. 21, 105001 (2008).
[3] M. V. Sadovskii, Phys.—Usp. 51 (12), 1201 (2008).
[4] A. L. Ivanovskii, Phys.—Usp. 51 (12), 1229 (2008).
[5] YU. A. Izyumov and E. Z. Kurmaev, Phys.—Usp. 51 (12), 1261 (2008).
[6] Kenji Ishida, Yusuke Nakai, and Hideo Hasono, J. Phys. Soc. Jpn. 78, 062001 (2009).
[7] V. A. Moskalenko, M. E. Palistrant, and V. M. Vakalyuk, Sov. Phys.—Usp. 34 (8), 717 (1991).

[8] V. A. Moskalenko, L. Z. Kon, and M. E. Palistrant, Low_Temperature Properties of Metals with Specific Features of the Band Spectrum (Shtiintsa, Chernigov, 1989) [in Rus.].
[9] V. A. Moskalenko, L. Z. Kon, and M. E. Palistrant, Teoria Supraconductibilităţ ii Multiband (Tehnica, Bucharest, Romania, 2008) [in Rom.]; http:www.theory/V.Barsan/eboks//Mosc.-2008.
[10] M. E. Palistrant, Condens. Matter Phys. 12, 677 (2009).
[11] M. E. Palistrant and L. Z. Kon, Ukr. J. Phys. 55, 44 (2010).
[12] M. E. Palistrant, and V. A. Ursu, JETP 104 (1), 51 (2007); M. E. Palistrant, and V. A. Ursu, J. Supercond. Novel Magn. 21 (3), 171 (2008).
[13] M. E. Palistrant, J. Supercond. Novel Magn. 23, 1427 (2010).
[14] V. Raghu, Hiao_Liang Oi, Chao_Xing Liu, D. J. Scalapino, and Shou_Cheng Zhang, Phys. Rev. B: Condens. Matter 77, 220503(R) (2008); arXiv:0804.1113.
[15] C. Cao, P. J. Hirschfeld, and H. P. Cheng, Phys. Rev. B: Condens. Matter 77, 2205060(R) (2008).
[16] M. M. Korshunov and I. Eremin, arXiv:0804.1793.
[17] V. Barzykin and L. P. Gor'kov, JETP Lett. 88 (2), 131 (2008).
[18] M. G. Vavilov, A. V. Chubukov, and A. B. Vorontsov, Supercond. Sci. Technol. 23, 054011 (2010); M. G. Vavilov, A. V. Chubukov, and A. B. Vorontsov, arXiv:0912.3556.
[19] A. B. Vorontsov, A. V. Vavilov, and A. V. Chubukov, Phys. Rev. B: Condens. Matter 81, 174538 (2010); arXiv:1003.2389v1.
[20] E. Z. Kuchinskii, I. A. Nekrasov, and M. V. Sadovskii, JETP Lett. 91 (10), 518 (2010); E. Z. Kuchinskii, I. A. Nekrasov, and M. V. Sadovskii,arXiv:1004.0801v1.
[21] M. K. Forthaus, K. Sengupta, O. Heyer, et al., Phys. Rev. Lett. 105, 157001 (2010); M. K. Forthaus, K. Sengupta, O. Heyer, et al., arXiv:1009.3787v1.
[22] E. E. Rodriguez, C. Stock, K. Krycka, et al., Phys. Rev. B: Condens. Matter 83, 134438 (2011); E. E. Rodriguez, C. Stock, K. Krycka, et al., arXiv:1012.5311.
[23] Jiangping Hu, Bao Xu, Wuming Liu, et al., Phys. Rev. B: Condens. Matter 85, 144403 (2012); Jiangping Hu, Bao Xu, Wuming Liu, et al., arXiv:1106.5169.
[24] M. Klansjek, M. Horvatic, C. Berthier, et al., arXiv:1202.6374.
[25] Shuai Jiang, Hui Xing, Guofang Xuanet al., Phys. Rev. B: Condens. Matter 80, 184514 (2009); Shuai Jiang, Hui Xing, Guofang Xuan, et al., arXiv:0911.0273.
[26] J. J. Ying, J. C. Liang, X. G. Luo, et al., Phys. Rev. B: Condens. Matter 85, 144514 (2012); J. J. Ying, J. C. Liang, X. G. Luo, et al., arXiv:1202.3589.
[27] Huiqian Luo, Rui Zhang, M. Laver, et al., arXiv:1203.2759v1.
[28] M. E. Palistrant and I. V. Pădure, Phys. Lett. A 111, 445 (1985); M. E. Palistrant and I. V. Pădure, Theor. Math. Phys. 62 (1), 78 (1985).
[29] M. E. Palistrant and V. M. Vakalyuk, Sov. J. Low Temp. Phys. 18 (8), 597 (1992).
[30] M. E. Palistrant, Theor. Math. Phys. 168 (3), 1290 (2011).
[31] M. E. Palistrant and V. A. Ursu, Zh. Exp. Teor. Fiz. 143 (4), 1 (2013).
[32] M. E. Palistrant, V. A. Ursu, M. Calalb, J. Supercond. Novel Magn. 27 (5), 1299 (2014).
[33] D. F. Digor and M. E. Palistrant, Mold. J. Phys. Sci. 9 (3–4), 311 (2010).
[34] I. S. Gradshteyn and I. M. Ryzhik, Table of Integrals, Series and Products (Fizmatgiz, Moscow, 1962; Academic, New York, 1980).