ELECTRONIC DENSITY OF STATES IN STRONGLY ANISOTROPIC SYSTEMS IN THE PHASE OF COEXISTENCE OF MAGNETISM AND SUPERCONDUCTIVITY IN AN EXTERNAL MAGNETIC FIELD

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Abstract

A method for calculating the electronic density of states in the "mixed phase"—superconductivity (SC) and the magnetic state of the spin-density wave (SDW)—is proposed. The main mechanism for the appearance of this phase is considered to be the doping of the system and allowance for the lattice structure (umklapp processes). The effect of an external magnetic field and the possibility of increasing the superconducting transition temperature T_c are analyzed.

1. Introduction

Numerous experimental studies of the properties of modern high-temperature materials demonstrate a surprising property: magnetism accompanies superconductivity; superconductivity (SC) arises either against the background of a state of a spin density wave (SDW) or after the suppression of magnetism because of doping. Modern high-temperature materials contain a number of features in the electronic energy spectrum, namely: it is a multiband system (several energy bands are present on the Fermi surface). Herewith, each compound is characterized by a certain number of these bands, which can only be electronic, only of the hole-type, or alternate between the two in different ratios. This situation requires a separate approach, when considering compounds from the class of ferropnictides and ferrochalcogenides; different ideas about the mechanism of the appearance of SC in these systems are emerging (reviews of the works in [1–3]). At present, an agreement has been reached that, in systems with electron bands on the Fermi surface (FeAs plane is responsible for SC), the main mechanism of interaction in the appearance of superconductivity is the spin fluctuations. In other compounds with a basic superconducting plane FeSe, this mechanism cannot be implemented because of the lack of "nesting" in the electronic energy spectrum and the absence of a magnetic exchange interaction. In this case [3], the cause of high-temperature superconductivity is the numerous interband electron–electron interactions in a rarefied BCS type system [4]. It is of interest that, in modern high-temperature superconductors, phase transitions are observed, for example, the commensurate–incommensurate state of a spin density wave. As a result, a displacement of the dielectric gap relative to the Fermi level and the transition to a gapless magnetic system occur in these materials.

Another approach related to the role of the Fermi surface is given in [5, 6], which is based on the accounting of the changes of parameters (when doping) such as the change in the difference in the areas of the cavities of the Fermi surface of the bands under consideration and of the deviations from ellipticity.

As in our above-mentioned works and in [5, 6], the appearance of superconductivity near the temperature of the magnetic transition is essential for the appearance of a "mixed" phase (SC+ SDW). As noted above, the thermodynamic properties of this state are studied in both quasi-1D and -2D cases. Of undoubted interest are the kinetic properties of these systems. In the study of kinetic characteristics, an important step is to determine the electronic density of states in the mixed phase of two long-range orderings: superconductivity and the spin-density wave state. This paper is focused on this problem.

2. Hamiltonian of the System and Main Definitions

In the mean-field approximation, the Hamiltonian of the system under consideration has the form

$$\mathrm{H} = \mathrm{H}_0 + \mathrm{H}_{BCS} + \mathrm{H}_{SDW} + \mathrm{H}_{H_0}, \tag{1}$$

where

$$\begin{aligned}
\mathrm{H}_0 &= \sum_{k\alpha}\left[\left(\varepsilon(\vec{k}) - \mu\right) a^{\dagger}_{\vec{k}\alpha} a_{\vec{k}\alpha}\right],\\
\mathrm{H}_{BCS} &= \Delta \sum_{\vec{k}}\left(a^{\dagger}_{\vec{k}\uparrow} a^{\dagger}_{-\vec{k}\downarrow} + h.c.\right),\\
\mathrm{H}_{SDW} &= -M \sum_{\vec{k},\alpha,\beta}\left(\sigma^i\right)_{\alpha\beta}\left(a^{\dagger}_{\vec{k}\alpha} a_{\vec{k}+\vec{Q},\beta} + h.c.\right),\\
\mathrm{H}_{H_0} &= -\sum_{\vec{k},\alpha,\beta} H_0\left(\sigma^z\right)_{\alpha\beta} a^{\dagger}_{\vec{k}\alpha} a_{\vec{k}\beta}.
\end{aligned} \tag{2}$$

Expression (1) contains terms responsible for superconductivity, magnetism, and the interaction of electrons with an external magnetic field. We chose representation in which we have a parallel magnetic field ($\vec{H}_0 \parallel \vec{M}$) for $i = z$ and a perpendicular magnetic field ($\vec{H}_0 \perp \vec{M}$) for $i = x$, Q is the wave vector of SDW; σ is the Pauli matrix:

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}; \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{3}$$

In expression (2), $a^{\dagger}_{\vec{k}\alpha}$ and $a_{\vec{k}\alpha}$ are the creation and annihilation operators of electrons with momentum $\vec{k}$ and projection of spin $\alpha = \uparrow, \downarrow$, μ is the deviation from the middle filling of the energy band and $\varepsilon(\vec{k})$ is the energy of electron. The Δ and M quantities are the superconducting and magnetic order parameters:

$$\begin{aligned}
\Delta &= VT \sum_{\vec{k},\omega_n} F^{\downarrow\uparrow}_{-\vec{k}\vec{k}}(\omega_n),\\
M &= \frac{1}{2} IT \sum_{\vec{k},\omega_n,\alpha}\left(\sigma^z\right)_{\alpha\alpha} G^{\alpha\alpha}_{\vec{k}-\vec{Q},\vec{k}}(\omega_n),\\
\omega_n &= \left(2n+1\right)\pi T, \quad n = \pm 1, \pm 2, \ldots
\end{aligned} \tag{4}$$

Here, *V* and *I* are the BCS and exchange interaction constants, respectively; $F^{\downarrow\uparrow}_{-\vec{k}\vec{k}}$ and $G^{\alpha\alpha}_{\vec{k}-\vec{Q},\vec{k}}$ are the Fourier representations of the temperature Green's functions (anomalous and normal, respectively), ω_n – the Matsubara frequency, and *T* is the temperature.

We consider a quasi-1D system with the dispersion law:

$$\varepsilon(\mathrm{k}) = -W\cos kd, \tag{5}$$

where *W* is the half-width of the energy band and *d* is the lattice constant. With the middle filling of the energy band $\mu = 0$ and the external magnetic field $H_0 = 0$, the nesting condition is satisfied:

$$\varepsilon(k) = -\varepsilon(k + Q_0) \tag{6}$$

Herewith, the quasi-1D system is in the magnetic state of the SDW with the wave vector $Q_0 = \pi/d$. The deviation from the middle filling of the energy band $\mu \neq 0$, as well as the inclusion of an external magnetic field $\vec{H}_0$, violate the nesting condition; as a result, there are phase transitions of the commensurable–incommensurable state of the SDW; an order parameter that determines this incommensurability arises. Herewith, the dielectric gap shifts with respect to the Fermi surface, and the magnetic system transits into a gapless state: free carriers appear on the Fermi surface; as a result, the coexistence of superconductivity and magnetism is possible.

This mechanism for the appearance of superconductivity against the background of magnetism has been studied, for example, in our works [3, 7, 8]. In these papers, the thermodynamic properties of doped systems of reduced dimensionality are mostly analyzed. A further stage of the research consists in a more detailed study of the effect of an external magnetic field on the thermodynamic properties of the systems under consideration and the study of the effect of the lattice structure (umklapp process) on the kinetic characteristics of the mixed state (SC + SDW). The first step to solve this problem is to calculate the density of electronic states. We start from the mean-field approximation. This approach is possible, if we consider a three-dimensional system in which the motion of electrons is one-dimensional. The three-dimensionality of the system cancels the existing fluctuations, which makes it possible to apply the mean-field theory (justification see in our above works). In Hamiltonian (1), the parameters of the magnetic M and superconducting Δ long-range orders are determined by equations (4). Applying the method of temperature Green's functions [9] based on Hamiltonian (1), we obtain for the introduced Green's functions in the case of a parallel magnetic field $\vec{H}_0 \parallel \vec{M}$ the following expressions:

$$G^{\uparrow\uparrow}_{kk}(\omega_n) = -\frac{\left\{(i\omega_n + H_0 + \varepsilon_1)\left[-(i\omega_n + H_0)^2 + \varepsilon_2^2 + \Delta^2\right] + M^2\,(i\omega_n + H_0 - \varepsilon_2)\right\}}{D_{H_0}\omega_n},$$

$$F^{\downarrow\uparrow}_{-kk} = \frac{\Delta\left\{-(i\omega_n + H_0)^2 + \varepsilon_2^2 + \Delta^2 - M^2\right\}}{D_{H_0}(\omega_n)}, \tag{7}$$

$$\mathrm{G}^{\sigma\sigma}_{\vec{\mathrm{k}}-\vec{\mathrm{Q}},\vec{\mathrm{k}}}(\omega_n) = \sigma\,\frac{\mathrm{M}[\mathrm{M}^2 - \Delta^2 - (i\omega_n + H_0 + \varepsilon_1)(i\omega_n + H_0 + \varepsilon_2)}{D_{H_0}(\omega_n)}.$$

Here

$$D_{(H_0)}(\omega_n) = (i\omega_n + H_0)^4 - (i\omega_n + H_0)^2(\varepsilon_1^2 + \varepsilon_2^2 + 2M^2 + 2\Delta^2) + \\ +\varepsilon_1^2\varepsilon_2^2 - 2M^2\varepsilon_1\varepsilon_2 + \Delta^2\left(\varepsilon_1^2 + \varepsilon_2^2\right) + \left(M^2 - \Delta^2\right)^2. \tag{8}$$

Substituting necessary Green's functions (7) into expressions (4), we obtain a system of equations for order parameters Δ and M. One can solve this system numerically for given values of parameters μ and H_0. First, we should choose 1D or 2D cosine law of dispersion and convert from summation over $\vec{k}$ to integration with respect to energy, taking into account the transition of the system to the incommensurate state of the SDW (see, e.g., [3, 7, 8]). Below, we present a method for taking into account the umklapp processes associated with a change in the wave vector of a spin density wave $Q \neq 2k_F$ of a quasi-1D system.

3. Calculation of the Density of Electronic States

The relation determines the density of electronic states with allowance for umklapp processes and in the presence of an external magnetic field ($\vec{H}_0 \parallel \vec{M}$):

$$N^{\uparrow}(\omega) = N_N^{\uparrow}(\omega) + N_u^{\uparrow}(\omega), \tag{9}$$

where $N_N^{\uparrow}(\omega)$ is determined by the normal processes and $N_u^{\uparrow}(\omega)$ by the umklapp processes in the magnetic field H_0 chosen in the direction $\vec{M}$.

We first consider normal processes:

$$N_N^{\uparrow}(\omega) = \frac{1}{\pi} \sum_{q<k<Q_0} \mathrm{Im} G_{kk}^{\uparrow\uparrow}(\mathrm{z})\Big|_{z=\omega-i\delta}. \tag{10}$$

The domain of sum in formula (10) is determined by the conditions $|\mathrm{k}| < \mathrm{Q}_0$ and $|\mathrm{k} - \mathrm{Q}| < \mathrm{Q}_0$, where $Q = Q_0 + q$ ($q = k_F$).

In accordance with (7), we have

$$G_{kk}^{\uparrow\uparrow}(\mathrm{z}) = -\frac{D_1\left(H_0, z\right)}{D\left(H_0, z\right)}, \tag{11}$$

where

$$D_1\left(H_0, z\right) = \left[z + H_0 + \varepsilon_1\right]\left[-\left(z + H_0\right)^2 + \varepsilon_2^2 + \Delta^2\right] + M^2\left(z + H_0 - \varepsilon_2\right),$$

$$D\left(H_0, z\right) = \left(z + H_0\right)^4 - \left(z + H_0\right)^2 [\left(\varepsilon_1^2 + \varepsilon_2^2 + 2M^2 + 2\Delta^2\right) + \\ +\varepsilon_1^2\varepsilon_2^2 - 2M^2\varepsilon_1\varepsilon_2 + \Delta^2\left(\varepsilon_1^2 + \varepsilon_2^2\right) + \left(\mathrm{M}^2 - \Delta^2\right)^2,$$

$$\varepsilon_1 = \varepsilon_{\vec{k}} - \mu, \quad \varepsilon_2 = \varepsilon_{\vec{k}-\vec{Q}} - \mu,$$

To perform the integration in (10), we use the cosine law (5), representing ε_1 and ε_2 as follows:

$$\begin{aligned}
&\varepsilon_1 = \varepsilon_{k-q/2}\cos\frac{qd}{2} - \mu_\pm = \varepsilon - \mu_\pm, \\
&\varepsilon_2 = -\left[\varepsilon_{k-q/2}\,cos\frac{qd}{2} + \mu_\pm\right] = -\left(\varepsilon + \mu_\pm\right), \\
&\mu_\pm = \mu \pm \eta, \quad \eta = W\sin\frac{qd}{2}.
\end{aligned} \tag{12}$$

We will consider small deviations of the wave vector of the spin density wave from 2k$_f$ ($q/2k_F << 1$); therefore, we will assume $\sin(\frac{qd}{2}) \approx \frac{qd}{2}$; $\cos(\frac{qd}{2}) \approx 1$.

We substitute (11) into (10) and reduce $N_N^{\uparrow}(\omega)$ to the form:

$$N_N^{\uparrow}(\omega) = \frac{1}{2\pi^2}\,\mathrm{Im}\int_{-W_1}^{W_1} N(\varepsilon_{k-q/2})\,d\,\varepsilon_{k-q/2}\,\left.\frac{D_1\left(\varepsilon_{k-q/2},\ H_0,\ \mu_-\right)}{D_{H_0}\left(\varepsilon_{k-q/2},\ H_0,\ \mu_-\right)}\right|_{z=\omega-i\delta} \tag{13}$$

where

$$W_1 = W\cos\frac{qd}{2}\,, \quad N(\varepsilon_{k-q/2}) = \frac{1}{d\sqrt{W^2 - \varepsilon_{k-q/2}^2}} \tag{14}$$

The account of umklapp processes reduces to additional summation over the domain $-Q_0 < k < q$, that is

$$N_u^{\uparrow}\left(\omega\right) = \frac{1}{2\pi^2}\int_{-Q_0}^{q} dk\ \mathrm{Im}G_{kk}^{\uparrow\uparrow}(\mathrm{z})\big|_{z=\omega-i\delta} \tag{15}$$

The domain of integration in this expression is conveniently divided into three sections: $-Q_0 < k < -Q_0 + \frac{q}{2}$, $-Q_0 + \frac{q}{2} < k < \frac{q}{2}$ and $\frac{q}{2} < k < q$.

In the first and last terms, we proceed to integration with respect to $\varepsilon_{k-q/2}$; in the second term of this expression, we replace k by $-k$ and then proceed to integration over $\varepsilon_{k+q/2}$. As a result, expression (15) has the form:

$$\begin{aligned}
N_u^{\uparrow}\ (\omega) = {} & \frac{1}{2\pi^2}\ \mathrm{Im}\int_{-W_1}^{W} d\varepsilon_{k-q/2}\,N\left(\varepsilon_{k-q/2}\right)\left.\frac{D_1\left(\varepsilon_{k-q/2},\ H_0,\mu_-\right)}{D_{H_0}\left(\varepsilon_{k-q/2},\ H_0,\mu_-\right)}\right|_{z=\omega-i\delta} + \\
& + \frac{1}{2\pi^2}\,\mathrm{Im}\int_{-W}^{W} N\left(\varepsilon_{k+q/2}\right)d\,\varepsilon_{k+q/2}\left.\frac{D_1\left(\varepsilon_{k+q/2},\ H_0,\ \mu_+\right)}{D_{H_0}\left(\varepsilon_{k+q/2},\ H_0,\mu_+\right)}\right|_{z=\omega-i\delta} + \\
& + \frac{1}{2\pi^2}\ \mathrm{Im}\int_{-W}^{-W_1} N\left(\varepsilon_{k-q/2}\right)d\varepsilon_{k-1/2}\ \left.\frac{D_1\left(\varepsilon_{k-q/2},\ H_0,\ \mu_-\right)}{D_{H_0}\left(\varepsilon_{k-q/2},\ H_0,\ \mu_-\right)}\right|_{z=\omega-i\delta}
\end{aligned} \tag{16}$$

Based on (13) and (16) for total electronic density of states taking into accounts both normal and umklapp processes, we obtain the following expression:

$$N^{\uparrow}(\omega)=\frac{1}{2\pi^2 dW\cos\frac{dq}{2}}\,\mathrm{Im}\left(\int_{-W}^{W}d\varepsilon\frac{D_1(\varepsilon,H_0,\mu_-)}{D_{H_0}(\varepsilon,H_0,\mu_-)}+\right.$$
$$\left.\left.+\int_{-W}^{W}d\varepsilon\frac{D_1(\varepsilon,\ H_0,\ \mu_+)}{D_{H_0}(\varepsilon,\ H_0,\ \mu_+)}\right)\right|_{z=\omega-i\delta} \tag{17}$$

In expression (17), we perform integration in the complex domain closing the integration contour in the upper half-flatness. As a result, we obtain:

$$N^{\uparrow}(\omega)=\frac{1}{4\pi dWcos\frac{qd}{2}}\ \mathrm{Re}\ \left\{I(z,H_0,\mu_-)+I(z,H_0,\mu_+)\right\}\Big|_{z=\omega-i\delta} \tag{18}$$

where

$$I(z,H_0,\mu_\pm)=\frac{C(z,H_0,\mu_\pm)}{B(z,H_0,\mu_\pm)}\cdot$$
$$\cdot\left[\frac{1}{\sqrt{A(z,H_0,\mu_\pm)+B(z,H,\mu_\pm)}}-\frac{1}{\sqrt{A(z,H_0,\mu_\pm)-B(z,H_0,\mu_\pm)}}\right]-$$
$$-(z+H_0+\mu_\pm)\left[\frac{1}{A(z,H_0,\mu_\pm)+B(z,H_0,\mu_\pm)}+\frac{1}{\sqrt{A(z,H_0,\mu_\pm)-B(z,H_0,\mu_\pm)}}\right], \tag{19}$$
$$A(z,H_0,\mu_\pm)=(z+H_0)^2+\mu_\pm^{\,2}-M^2-\Delta^2,$$

Let us write the square roots in the above expressions in accordance with their definition:

$$\sqrt{a+ib}=\frac{sign b}{\sqrt{2}}\left[a+\sqrt{a^2+b^2}\right]^{1/2}+\frac{i}{\sqrt{2}}\left[\sqrt{a^2+b^2}-a\right]^{1/2} \tag{20}$$

We proceed to the representation $z=\omega-i\delta$, using the definition of the square roots (20). As a result, we reduce the total electronic density of states to the form:

$$\frac{N(\omega)}{N_0}=Re\left\{I(\omega,H_0,\mu_-)+I(\omega,H_0,\mu_+)\right\} \tag{21}$$

where

$$I(\omega,H_0,\mu_\pm)=\frac{C}{B}\left[F_1-F_2\right]-\left[\omega+H_0+\mu_\pm\right]\cdot\left[F_1+F_2\right],$$
$$C=C\left(\omega,H_0,\mu_\pm\right)=-2\mu_\pm\left(\omega+H_0\right)\left(\omega+H_0+\mu_\pm\right)+2\mu_\pm{}^2, \qquad (22)$$
$$B=B\left(\omega,H_0,\mu_\pm\right)=-2\,sign\left(\omega+H_0\right)^2\left[\mu_\pm{}^2\left(\omega+H_0\right)+M^2\Delta^2-\mu_\pm{}^2\Delta^2\right]^{1/2},$$

$$F_1=F_1\left(\omega,H_0,\mu_\pm\right)=-sign\left[\omega+H_0-\frac{\mu_\pm\left(\omega+H_0\right)}{\sqrt{\mu_\pm{}^2\left(\omega+H_0\right)^2+M^2\Delta^2-\ \mu_\pm{}^2\Delta^2}}\right]\cdot$$
$$\cdot\left[\left(\omega+H_0\right)^2+\mu_\pm{}^2-M^2-\Delta^2+\ B\right]^{-1/2},$$
$$F_2=F_2\left(\omega,H_0,\mu_\pm\right)=-sign\left[\omega+H_0+\frac{\mu_\pm\left(\omega+H_0\right)}{\sqrt{\mu_\pm{}^2\left(\omega+H_0\right)^2+M^2\Delta^2-\mu_\pm{}^2\Delta^2}}\right]\cdot$$
$$\cdot[\left(\omega+H_0\right)+\mu_\pm{}^2-M^2-\Delta^2\left]-B\right]^{-1/2},$$
$$N_0=4\pi dWcos\frac{\pi d}{2}$$

Expressions (18)–(22) determine the electronic density of states in the mixed phase (SC + SDW) for a given value of the external magnetic field H_0 and the deviation from the middle filling of the energy band μ in the phase of coexistence of superconductivity and the incommensurate state of SDW due to an external magnetic field H_0 and the deviation of vector of a spin density wave from $2k_F$. In detail, one can obtain further calculations in general only by numerical methods. The problem becomes simpler, if we consider the nucleation of weak superconductivity against the background of the SDW. In this case, we pass to the limiting transition Δ << M.

As a result, we obtain

$$\frac{N\left(\omega\right)}{N_0}=\mathrm{Re}\left\{\frac{\left|\omega+H_0+\mu_-\right|}{\sqrt{\left(\omega+H_0+\mu_-\right)^2-M^2}}+\frac{\left|\omega+H_0+\mu_+\right|}{\sqrt{\left(\omega+H_0+\mu_+\right)^2-M^2}}\right\} \qquad (23)$$

It follows that N (ω) ≠ 0, if $\left|\omega+H_0+\mu_-\right|<|\mathrm{M}|$ and $\left|\omega+H_0+\mu_+\right|<|M|$. For temperature higher then critical temperature of SC transition T_c , we have the state of the SDW.

Let us consider some limiting cases:

1. H_0=0, $\mu_\pm=\mu\pm\eta,\ \eta=0$. The system is in a dielectric state (in the commensurate state of the SDW), the nesting condition (6) is satisfied.
2. H_0 =0, $\mu_\pm=\mu\pm\eta,\ \eta\neq 0$

For $\mu = \mu_c$ the system goes to the phase of the incommensurate state of the spin density wave with incommensurability parameter η. In the domain $\mu > \mu_c$, an ambiguous correspondence arises between the temperature of the magnetic transition T_M and μ; that is, the state of the SDW becomes unstable. The phase transition to the incommensurate state of the SDW, taking into account the umklapp processes, contributes to the stabilization of the state by transition to a semi metallic state ($Q \neq 2k_F$, $\eta \neq 0$). There is a possibility of the appearance of superconductivity.

The inclusion of an external magnetic field makes a definite contribution to the η value; consequently, in a definite range of magnetic field values, it accelerates the transition to the above-mentioned metallic state and, accordingly, leads to an increase in the superconducting transition temperature. The same situation occurs when the charge density wave and superconductivity arise in the system (see, e.g., [10]). Consequently, in strongly anisotropic systems in the phase of coexistence of superconductivity and spin density wave, as well as superconductivity and charge density wave, the temperature of the superconducting transition can increase with increasing external magnetic field.

4. Conclusions

Using the Green's function method, we have determined the electronic density of states of a quasi-1D system in the mixed phase of the coexistence of superconductivity and the incommensurable state of the spin density wave in the presence of an external magnetic field. Herewith, we have taken into account the effect of the umklapp processes (lattice structure). Under the assumption of the generation of weak superconductivity against the background of the SDW, we have analyzed various limiting cases. As a result, we have discussed the possibility of implementing the mixed phase of the incommensurate state of SDW with superconductivity. We have shown that the inclusion of an external magnetic field of a certain range contributes to an increase in the temperature of the superconducting transition. This is an unusual and surprising picture illustrating the favorable effect of an external magnetic field on superconductivity.

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