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The free energy functional for a spin singlet ferromagnetic superconductor

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The aim of this paper is to investigate the coexistence of ferromagnetic and superconducting phase for a system of itinerant fermions using a functional method from the field theory. In this way we present a microscopic derivation of Ginzburg-Landau free energy functional for the singlet Cooper pairing system, where the ferromagnetic order appears as a consequence of spontaneously broken spin-rotation symmetry and a contact interaction both for the Heisenberg and the singlet pairing terms was considered. The result is the expanded form of the free functional energy up to 4-th term. Finally we are focusing on the 4-th term of the free energy functional expansion which exhibits both ferromagnetic and superconducting order.

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1. Introduction

The possibility of such a coexistence was first pointed out by Ginzburg under the condition that magnetization is less than the thermodynamic critical field [1]. The earliest experimental investigations [2] started for superconductors with a ferromagnetic impurity. The theoretical description of such kind of systems was performed by Abrikosov [3] who used the RKKY interaction in which ferromagnetic impurities interact with conduction electrons and the magnetization was considered an external parameter, independent of the superconducting gap. In this case it was emphasized that the energy of the normal ferromagnetic state is lower than the energy for the superconducting state so that the coexistence is unfavorable. In [4] Fulde and Ferrell studied superconductivity in strong exchange field produced by aligned ferromagnetic impurities and predicted the occurrence of a new type of depaired superconducting state. The possibility of a p-wave superconducting state in itinerant ferromagnetism was predicted in [5]. In this case, the pairing mechanism is mediated by the exchange of longitudinal spin fluctuations. Finally it was shown that when approaching the transition point from either ferromagnetic or paramagnetic side, the transition temperature goes through a maximum value then falls to zero so that even the superconductivity is interpreted as arising from magnetic mediation, it appears in the paramagnetic phase. The first experimental observation of coexistence was made for ferromagnetic compound UGe2 [6]. The coexistence has also been shown to exist in ZrZn2 and URhGe [7, 8]. In all these materials the superconducting phase is completely covered within the ferromagnetic phase and disappears in paramagnetic region. This fact may confirm the hypothesis that the same electrons are responsible for both ferromagnetic and superconducting states. Based on these experiments, the theoretical investigation of the coexistence was performed by Blagoev el al. [9, 10]. An itinerant ferromagnetic model in a mean field approach in which the magnetic electrons are also responsible for Cooper pairing was developed by Karchev et al. in [11]. Following this model, the behavior of the specific heat is similar to that found in UGe2 experimentally [12]. The calculation of the density of states, nuclear relaxation rate, ultrasonic attenuation and electromagnetic absorption in the model given by [11] was presented in [13].

2. Theory

To analyze the problem of ferro-super phase coexistence, we consider the model Hamiltonian

$$\begin{aligned} H-\mu N = &\int d^3r \sum_\sigma \psi_\sigma^+(\vec{r})\left[-\frac{\nabla^2}{2m}-\mu\right]\psi_\sigma(\vec{r}) \\ &-\frac{J}{2}\int d^3r\,\vec{S}(\vec{r})\vec{S}(\vec{r}) \\ &-g\int d^3r\,\psi_\uparrow^+(\vec{r})\psi_\downarrow^+(\vec{r})\psi_\downarrow(\vec{r})\psi_\uparrow(\vec{r}), \end{aligned} \tag{1}$$

where $\psi_\sigma^+(\vec{r})$, $\psi_\sigma(\vec{r})$ are the fermionic field operators corresponding to spin value $\sigma:(\uparrow,\downarrow)$, $\vec{S}(\vec{r})$ - spin density operator on the site $\vec{r}$, $\frac{J}{2}$ - the Heisenberg coupling constant and g - Cooper pairing coupling constant.

In order to write the partition function, we start from the functional integral formula for the action, which in our case is:

$$\begin{aligned} S &= \int_0^\beta d\tau \int d^3r \sum_\sigma \psi_\sigma^+(\vec r,\tau)\partial_\tau \psi_\sigma(\vec r,\tau) \\ &- \int_0^\beta d\tau \int d^3r \sum_\sigma \psi_\sigma^+(\vec r,\tau)\left[-\frac{\nabla^2}{2m}-\mu\right]\psi_\sigma(\vec r,\tau) \\ &+ \frac{J}{2}\int_0^\beta d\tau \int d^3r \vec S(\vec r)\vec S(\vec r) \\ &+ g\int_0^\beta d\tau \int d^3r \psi_\uparrow^+(\vec r)\psi_\downarrow^+(\vec r)\psi_\downarrow(\vec r)\psi_\uparrow(\vec r). \end{aligned} \tag{2}$$

Now we have to express the action (2) in terms of order parameters responsible for ferromagnetic and superconducting ordering. To do this we will introduce in (2) a spin related real vector field $\vec\chi(\vec r,\tau)$ and a complex field $\varphi^*(\vec r,\tau), \varphi(\vec r,\tau)$ related with the BCS term. Performing a Hubbard-Stratonovich transformation we obtain the action in terms of fluctuating fields:

$$\begin{aligned} S' &= \int_0^\beta d\tau \int d^3r \sum_\sigma \psi_\sigma^+(\vec r,\tau)\left[\partial_\tau+\frac{\nabla^2}{2m}+\mu\right]\psi_\sigma(\vec r,\tau) \\ &+ 2\int_0^\beta d\tau \int d^3r \vec\chi(\vec r,\tau)\vec S(\vec r,\tau) - \frac{2}{J}\int_0^\beta d\tau \int d^3r \vec\chi^2(\vec r,\tau) \\ &+ \int_0^\beta d\tau \int d^3r \left[\varphi(\vec r,\tau)\psi_\uparrow^+(\vec r,\tau)\psi_\downarrow^+(\vec r,\tau)\right] \\ &+ \int_0^\beta d\tau \int d^3r \varphi^*(\vec r,\tau)\psi_\downarrow(\vec r,\tau)\psi_\uparrow(\vec r,\tau) \\ &- \frac{1}{g}\int_0^\beta d\tau \int d^3r \varphi^*(\vec r,\tau)\varphi(\vec r,\tau). \end{aligned} \tag{3}$$

To get the free energy functional we will use the functional identity

$$\frac{Z}{Z_0} = \int d\psi^* d\psi d\chi d\varphi^* d\varphi e^{S'}, \tag{4}$$

where Z is the partition function. From this expression of the partition function, we can identify the effective Hamiltonian H_{ef} in terms of the fluctuating fields χ and φ .

Without any loss of generality we can set the magnetic vector field along *z*-axis: $\vec\chi = (0,0,\chi)$ and, after a few tricks, the fermionic terms in (3) can be righted down in the matrix form

$$\int_0^\beta d\tau \int d^3r \left(\psi_\uparrow^+(\vec r,\tau),\psi_\downarrow(\vec r,\tau)\right)\times\left(\hat M\right)\times\begin{pmatrix}\psi_\uparrow(\vec r,\tau)\\ \psi_\downarrow^+(\vec r,\tau)\end{pmatrix}, \tag{5}$$

where the matrix $\hat M$ is identified in the form:

$$\hat M = \begin{pmatrix} \partial_\tau+\frac{\nabla^2}{2m}+\mu+\chi(\vec r,\tau) & \varphi(\vec r,\tau) \\ \varphi^*(\vec r,\tau) & \partial_\tau-\frac{\nabla^2}{2m}-\mu+\chi(\vec r,\tau)\end{pmatrix}. \tag{6}$$

With the above formulas the partition function (4) is

$$\begin{aligned} \frac{Z}{Z_0} &= \int d\chi d\varphi^* d\varphi \exp\left\{-\frac{1}{g}\int_0^\beta d\tau \int d^3r \varphi^*(\vec r,\tau)\varphi(\vec r,\tau)\right\} \\ &\times \exp\left\{-\frac{2}{J}\int_0^\beta d\tau \int d^3r \chi^2(\vec r,\tau) + \ln\left(\det\frac{\hat M}{\hat M_0}\right)\right\}. \end{aligned} \tag{7}$$

where $\hat M_0 = \hat M_{(\varphi^*=\varphi=\chi=0)}$. Let us now put $\hat M$ in the form

$$\hat M = \hat M_0 + \chi\hat I + \hat\Phi = \hat M_0\left(\hat I + \hat M_0^{-1}\chi + \hat M_0^{-1}\hat\Phi\right) \tag{8}$$

where $\hat I$ is the identity operator,

$$\hat\Phi = \begin{pmatrix} 0 & \varphi(\vec r,\tau) \\ \varphi^*(\vec r,\tau) & 0\end{pmatrix}, \tag{9}$$

and

$$\hat M_0^{-1} = \hat G(\vec r,\tau) \tag{10}$$

is the matrix form for the Green function

$$\hat G = \begin{pmatrix} G_+ & 0 \\ 0 & G_-\end{pmatrix}, \tag{11}$$

whose elements satisfy the equations of motion:

$$\left[\partial_\tau \pm\left(\frac{\nabla^2}{2m}+\mu\right)\right]G_\pm(\vec r,\tau;\vec r\,',\tau') = \delta(\vec r-\vec r\,')\delta(\tau-\tau'). \tag{12}$$

In order to get the effective Hamiltonian in terms of a power series of χ and φ we will make use of the identity

$$\ln\left(\det\frac{\hat M}{\hat M_0}\right) = tr\ln\left(\frac{\hat M}{\hat M_0}\right), \tag{13}$$

expand the logarithm function and compute the trace operator.

With respect to (8, 9, 10) and (11), eq. (13) can be written in the form:

$$tr\ln\left(\frac{\hat M}{\hat M_0}\right) = tr\ln\left[\hat I + G\left(\chi I + \hat\Phi\right)\right]. \tag{14}$$

Let us put

$$\hat{A} = \chi \hat{I} + \hat{\Phi} = \begin{pmatrix} \chi(\vec{r},\tau) & \varphi(\vec{r},\tau) \\ \varphi^*(\vec{r},\tau) & \chi(\vec{r},\tau) \end{pmatrix} \quad (15)$$

and now expand the logarithm in (13) in terms of matrix $\hat{A}$:

$$tr \ln\left(\frac{\hat{M}}{\hat{M}_0}\right) = tr\left\{\hat{G}\hat{A} - \frac{1}{2}\left(\hat{G}\hat{A}\right)\left(\hat{G}\hat{A}\right) + \frac{1}{3}\left(\hat{G}\hat{A}\right)\left(\hat{G}\hat{A}\right)\left(\hat{G}\hat{A}\right) - \frac{1}{4}\left(\hat{G}\hat{A}\right)\left(\hat{G}\hat{A}\right)\left(\hat{G}\hat{A}\right)\left(\hat{G}\hat{A}\right) + \ldots\right. \quad (16)$$

As it can be observed, the above formula plays the leading role in determining the free energy functional using (4) identity. The procedure to follow in order to compute (16) is to introduce the Fourier transform for $\hat{G}$ and $\hat{A}$, then to explicitly write down the summations over matrix indices, then integrate over impulses $\vec{k}$ and to perform the summation over fermionic Matsubara frequencies $\omega_n = (2n+1)\pi T$. Note than the order of the last two computing steps must be changed if the convergence problems appear.

3. Results and discussion

Following the above model we will discuss the 2-nd and the 4-th order terms of (16) making use of the Fourier transformations of the Green functions given by (12):

$$G_{\pm}\left(\vec{k},\omega\right) = \frac{1}{i\omega \mp \bar{\varepsilon}_{\vec{k}}}\,, \quad (17)$$

where $\bar{\varepsilon}_{\vec{k}} = \varepsilon_{\vec{k}} - \mu$.

The 2-nd order term. Writing down the explicit form of the 2-nd term from (16)

$$\begin{aligned} H_{ef}^{(2)} &= -\frac{1}{2}\sum_{i,k}\int_0^{\beta} d\tau_1 d\tau_2 \int d^3r_1 d^3r_2 \times \\ &\times\left[G_{ii}\left(\vec{r}_1,\tau_1,\vec{r}_2,\tau_2\right)A_{ik}\left(\vec{r}_2,\tau_2\right)\right]\times \\ &\times\left[G_{kk}\left(\vec{r}_1,\tau_1,\vec{r}_2,\tau_2\right)A_{ki}\left(\vec{r}_2,\tau_2\right)\right] \\ &+\frac{1}{g}\int_0^{\beta} d\tau \int d^3r\left|\varphi(\vec{r},\tau)\right|^2 + \frac{2}{J}\int_0^{\beta} d\tau\int d^3r\chi^2(\vec{r},\tau) \end{aligned} \quad (18)$$

and using the identity

$$\frac{1}{\sqrt{\beta V}}\int_0^{\beta} d\tau\int d^3r A_{ik}(\vec{r},\tau)e^{i\left(\vec{k}\vec{r}-\omega\tau\right)} \equiv A_{ik}\left(\vec{k},\omega\right) \quad (19)$$

it can be expressed in terms of fluctuating fields order parameters χ, φ:

$$\begin{aligned} H_{ef}^{(2)} &= -\frac{1}{2\beta V}\sum_{\vec{k},\vec{q}}\ \sum_{\omega,\omega'} \times \\ &[G_+\left(\vec{k},\omega\right)G_+\left(\vec{k}-\vec{q},\omega-\omega'\right)\chi\left(\vec{q},\omega'\right)\chi\left(-\vec{q},-\omega'\right) + \\ &G_+\left(\vec{k},\omega\right)G_-\left(\vec{k}-\vec{q},\omega-\omega'\right)\varphi\left(\vec{q},\omega'\right)\varphi^*\left(-\vec{q},-\omega'\right) + \\ &G_-\left(\vec{k},\omega\right)G_+\left(\vec{k}-\vec{q},\omega-\omega'\right)\varphi^*\left(\vec{q},\omega'\right)\varphi\left(-\vec{q},-\omega'\right) + \\ &G_-\left(\vec{k},\omega\right)G_-\left(\vec{k}-\vec{q},\omega-\omega'\right)\chi\left(\vec{q},\omega'\right)\chi\left(-\vec{q},-\omega'\right)] \\ &+\frac{1}{g}\int_0^{\beta} d\tau\int d^3r\left|\varphi(\vec{r},\tau)\right|^2 + \frac{2}{J}\int_0^{\beta} d\tau\int d^3r\chi^2(\vec{r},\tau) \end{aligned} \quad (20)$$

As it can be expected, eq. (20) exhibits no-vanishing terms of 2-nd power of the fluctuating fields with temperature dependent coefficients which can be determined in a usual G-L theory manner.

The 4-th order term. The most interesting component of the free energy is the fourth order power term. In order to compute it we make use of the approximation in [3] by considering equal arguments in performing the summation over the matrix indices in the 4-th term in (16):

$$\begin{aligned} H_{ef}^{(4)} &= -\frac{1}{4\beta V}\sum_{\vec{k},\omega}\ \sum_{i,j,k,l}\int_0^{\beta} d\tau\int d^3r G_{ii}\left(\vec{k},\omega\right)\times \\ &A_{ij}\left(\vec{r},\tau\right)G_{jj}\left(\vec{k},\omega\right)A_{jk}\left(\vec{r},\tau\right)G_{kk}\left(\vec{k},\omega\right)\times \\ &\times A_{kl}\left(\vec{r},\tau\right)G_{ll}\left(\vec{k},\omega\right)A_{li}\left(\vec{r},\tau\right) \end{aligned} \quad (21)$$

and, with respect to (11) and (15) we put it in the following form:

$$\begin{aligned} H_{ef}^{(4)} &= -\frac{1}{4\beta V}\sum_{\vec{k},\omega}\int_0^{\beta} d\tau\int d^3r \times \\ &\{\ \left(G_+^4\left(\vec{k},\omega\right) + G_-^4\left(\vec{k},\omega\right)\right)\chi^4\left(\vec{r},\tau\right) + \\ &4[\ G_+^3\left(\vec{k},\omega\right)G_-\left(\vec{k},\omega\right) + G_+^2\left(\vec{k},\omega\right)G_-^2\left(\vec{k},\omega\right) + \\ &G_+\left(\vec{k},\omega\right)G_-^3\left(\vec{k},\omega\right)\ ]\chi^2\left(\vec{r},\tau\right)\left|\varphi\left(\vec{r},\tau\right)\right|^2 + \\ &2G_+^2\left(\vec{k},\omega\right)G_-^2\left(\vec{k},\omega\right)\left|\varphi\left(\vec{r},\tau\right)\right|^4\ \} \end{aligned} \quad (21)$$

Now, using (18) we can perform the summation over fermionic frequencies and, up to integrate over $\vec{k}$, we get:

$$H_{ef}^{(4)} = -\frac{1}{4\beta V}\int d^3 r d\tau \times \sum_{\vec{k}} \left\{ -\frac{2\pi}{24T^4} \frac{ch\left(\frac{\bar{\varepsilon}_{\vec{k}}}{T}\right) - 2}{ch^4\left(\frac{\bar{\varepsilon}_{\vec{k}}}{2T}\right)} \chi^4(\vec{r},\tau) + \frac{1}{4T\bar{\varepsilon}_{\vec{k}}^{\,3}} \frac{sh\left(\frac{\bar{\varepsilon}_{\vec{k}}}{T}\right) - \frac{\bar{\varepsilon}_{\vec{k}}}{T}}{ch^2\left(\frac{\bar{\varepsilon}_{\vec{k}}}{T}\right)} |\varphi(\vec{r},\tau)|^4 + \frac{1}{2T^3\bar{\varepsilon}_{\vec{k}}} \frac{th\left(\frac{\bar{\varepsilon}_{\vec{k}}}{2T}\right)}{ch^2\left(\frac{\bar{\varepsilon}_{\vec{k}}}{2T}\right)} |\varphi(\vec{r},\tau)|^2 \chi^2(\vec{r},\tau) \right\}. \quad (22)$$

Numerical computing of integral over $\vec{k}$ leads to no vanishing terms so that the free energy of the system contains both ferromagnetic and superconducting order. Once we get the free energy functional form, the critical temperature can be determined along with the other physical quantities (specific heat, critical exponents) and this will be the object of a further work.

4. Conclusions

As is seen from the above calculations, this theory gives a generalized Ginzburg-Landau free energy for a system where two order parameters exist: in this case the the magnetic order parameter (magnetization) and superconducting order parameter. The coupling between the two fields comes from the quadric term $|\varphi(\vec{r},\tau)|^2 \chi^2(\vec{r},\tau)$. This term is the one which make it possible a phase coexistence between the two fields. The second order term is also very important because from it we can calculate the transition temperature for the two order parameters using the specific values for relevant systems.

Also, it is possible to calculate the specific heat and its discontinuity in the transition point. The theory can also be extended to the case when an external magnetic field is present in the system and we can calculate the magnetic susceptibility.

However, the most important problem is related to the phase coexistence. This implies a common critical temperature and the existence of simultaneously non-vanishing order parameters. All these problems needs a numerical calculation which will be done in a future publication.

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