Journal of Low Temperature Physics, Vol. 105, Nos. 3/4, 1996

Thermodynamics of D-Wave Pairing in Cuprate Superconductors

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The mechanism of d-pairing with account of antiferromagnetic spin fluctuations was considered. The thermodynamics of d-wave pairing in cuprate supercoductors was calculated. For the calculation the method of functional integrals was used. It has been shown that the temperature dependence of specific heat corresponds to d-pairing. The value of the jump of specific heat $\Delta/\gamma T_c$ for the compounds $YBa_2Cu_3O_{6.63}$ was given.

PACS numbers: 05.70 Ln, 05.70 Jk, 64.

1. INTRODUCTION

Some recent papers consider the mechanism of antiferromagnetic spin fluctuations [1,2]. Electron scattering on these fluctuations may cause the electron pairing with d-symmetry. Spin fluctuations play an important role in superconductors with heavy fermions [3]. In Pines papers [1,2] the calculation of superconducting gap, critical temperature, temperature dependence of resistance and many other values are discussed, but thernodynamics is not considered. The aim of our work is to calculate the thermodynamics of d-wave-pairing in cuprate superconductors, namely, the electronic specific heat and the jump of the specific heat.

Note that the energy gap of the $d_{x^2-y^2}$ state has the functional form in k space

$$\Delta(\mathbf{k}) = \mathbf{\Delta_o}[\cos(\mathbf{k_x a}) - \cos(\mathbf{k_y a})], \tag{1}$$

where Δ_o is the maximum gap value and a is the in-plane lattice constant. The gap is real with a strongly anosotropic magnitude featuring nodes along the (110) directions in k space and a sign change in the order parameter between the lobes in the k_x and k_y directions.

The thermodynamics of a superconductor at low temperatures is determined by excitations involving two quasiparticles. In conventional superconductors with the pairing of BCS type (s wave) the temperature dependence of the heat capacity is exponentional, namely, $\sim \exp^{-\Delta/k_B T}$. In superconductors with anisotropic pairing

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the temperature dependence of the heat capacity follows the power law T^n. The appearance of such temperature dependence is stipulated by the anisotropy pairing when the energy gap becomes zero at seperate curves of the Fermi surface.

2. SPECIFIC HEAT OF D-WAVE PAIRING

In order to calculate the thermodynamic potential it is necessary to calculate a big statistical sum

$$\exp[-\beta\Omega(\mu,\beta,g)] \equiv Tr\exp[-\beta(H-\mu N)], \quad \beta = 1/kT, \tag{2}$$

where μ is a chemical potential and $\Omega(\mu,\beta,g)$ is a thermodynamical potential, g is the interaction constant.

The antiferromagnetic spin fluctuations which result in d-pairing in cuprate superconduction are described by the Lagrangian in lattice representation [4]:

$$L = \sum_{\vec{n}} \psi_\alpha^+(\vec{n})(\frac{\partial}{\partial\tau} - \mu)\psi_\alpha(\vec{n}) - t\sum_{\vec{n},\vec{p}} \psi_\alpha^+(\vec{n})\psi_\alpha(\vec{n}+\vec{p})$$

$$+g\sum_{\vec{n}} \psi_\alpha^+(\vec{n})\left(\frac{\sigma^i}{2}\right)_{\alpha,\beta}\psi_\beta(\vec{n})S_i(\vec{n}) + \frac{1}{2}\sum_{\vec{n}\vec{m}} S_i(\vec{n})\chi_{ij}^{-1}(\vec{n},\vec{m})S_j(\vec{m}), \tag{3}$$

where the summation is over all knots of infinite lattice, $\vec{p}$ ia a unit vecor, which connects the neighboring knots, μ is a chemical potential, $\sigma_{\alpha,\beta}$ is the Pauli matrix, $S_i(\vec{n})$ is the operator of spin fluctuations in lattice representation, $\psi_\alpha^+(\vec{n})$ is the operator of an electron creation on n-th site, and $\psi_\alpha(n)$ is the operator of a hole creation on n-th site, α is a spin projection, t is a band halfwidth, $\chi_{ij}(\vec{n},\vec{m})$ is the spin correlation function, which is modulated by

$$\chi(q,\omega) = \frac{\chi_Q}{1+\xi^2(q-Q)^2 - i\omega/\omega_{SF}}, \quad q_x > 0, \quad q_y > 0, \tag{4}$$

where χ_Q is the static spin susceptibility at wave vector $Q = (\pi/a, \pi/a)$, ξ is the temperature-dependent antiferromagnetic correlation length, ω_{SF} is the paramagnon energy. All these parameters are taken from NMR experiments [1].

It is convinient to use the formalism of continual integration for Fermi systems. The big statistical sum can be written in the form of functional integral [4,5]:

$$e^{-\beta\Omega} = N\int\prod_{\vec{m}} dS_i(\vec{n})d\psi_\alpha^+(\vec{n},\tau)d\psi_\alpha(\vec{n},\tau)\exp\left\{-\int_0^\beta d\tau L(\tau)\right\}, \tag{5}$$

where $\beta = 1/kT$, N ia a normalization multiplier.

Detailed calculations of the big statistical sum are givem in [4]. In the weak coupling approximation (lowest order in g^2) we have calculated the thermodynamic potential:

$$\Omega(\Delta) = V\int\frac{d^2k}{(2\pi)^2}\left\{-\frac{2}{\beta}\ln\frac{\mathrm{ch}\frac{\beta}{2}(\sqrt{(\varepsilon(\vec{k})-\mu)^2+\Delta(\vec{k})^2})}{\mathrm{ch}\frac{\beta\varepsilon}{2}}+\right.$$

$$+\frac{\Delta(\vec{k})^2}{2\sqrt{(\varepsilon(\vec{k})-\mu)^2+\Delta(\vec{k})^2}}\mathrm{th}\frac{\sqrt{(\varepsilon(\vec{k})-\mu)^2+\Delta(\vec{k})^2}}{2}\Bigg\}. \tag{6}$$

Here V is a two dimensional volume (the area of the cuprate layered), $\Delta(\vec{k})$ is a superconductivity gap, $\vec{k}$ is a momentum of an electron, $\varepsilon(\vec{k}) = -2t[\cos(k_x a) + \cos(k_y a)]$ describes the spectrum of two-dimensional electron. The heat capacity was calculated using the formula:

$$C = -T\frac{\partial^2\Omega}{\partial T^2}. \tag{7}$$

We have done the computer calculations for $YBa_2Cu_3O_{6.63}$. The equation for the gap Δ was obtained in Refs. [2,4]. The gap value depends on the spin correlation function. Data needed for the definition of the correlator were taken from [2]. For the calculation we take the following parameters: $\omega_{SF}(T_C) \approx 7.7\ mev$, $\chi_S(Q) = 44\ ev$, $\xi/a \approx 2.5$, $t = 2\ ev$, $\mu = 0.25$, $T_c = 95$ K . We chose the value of constant g which satisfy the relation $2\Delta/kT_c = 3.4$, as was derived in [2]. The results of the numerical calculation are shown in Fig. 1. (curve 1). The calculations show the linear behaviour of the ratio of the specific heat to temperature, C/T, in the range from zero to critical temperature. The curve 2 in Fig. 1. shows the temperature dependence which corresponds to the BCS model (s pairing).

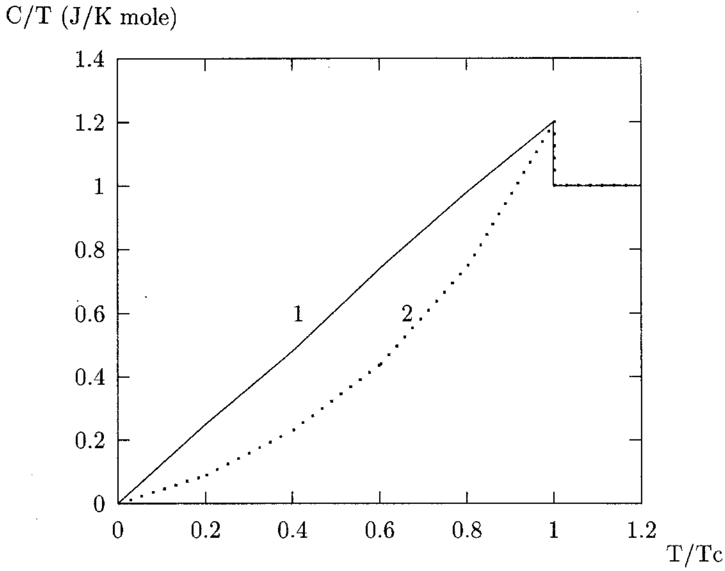

Fig. 1. Temperature dependence of the specific heat which corresponds to: 1 - d-wave pairing, 2 - s-wave pairing.

3. THE JUMP OF THE SPECIFIC HEAT OF D-WAVE PAIRING

Basing on Eq. (6) it was obtained the jump for the thermodynamical potential near T_c :

$$\Omega(\Delta) - \Omega(0) = \frac{V}{8} \int \frac{d^2k}{(2\pi)^2} \frac{\Delta_i^4(\vec{k})}{[\varepsilon(\vec{k}) - \mu]^2}$$

$$\left\{ \frac{\beta}{2} \left(1 - \mathrm{th}^2 \frac{\beta(\varepsilon(\vec{k}) - \mu)}{2} \right) - \frac{1}{(\varepsilon(\vec{k}) - \mu)} \mathrm{th} \frac{(\varepsilon(\vec{k}) - \mu)}{2} \right\}, \tag{8}$$

where $\Omega(\Delta)$ and $\Omega(0)$ – are the thermadynamical potentials at $T < T_c$ and $T > T_c$, respectively.

In spite of the presence of the factors $(\varepsilon(\vec{k}) - \mu)$ in the denominator of formula , it is not difficult to test that the singularity on the Fermi surface $\varepsilon(\vec{k}) - \mu$ is absent. Eqs. (6-8) (at $T \sim T_c$) can be a basis for calculation of different thermodynamic quantities.

The jump of specific heat was calculated by

$$\Delta C = -T \frac{\partial^2 \Delta \Omega}{\partial T^2}. \tag{9}$$

We provided computer calculations of the value of $R = \Delta C / \gamma T_c$. For the compounds $YBa_2Cu_3O_{6.63}$ the parameter R was equal to 1.5 ($\gamma = 16$ mJ/mol K^2).

4. CONCLUSION

It follows from the calculations that the temperature dependence of the specific heat corresponds to T^2. In the paper [6] the specific heat in the superconducting state of the heavy Fermion considering all symmetry allowed gap functions was modelled. It was shown that the d-symmetry resulted in the linear dependence of C/T on temperature. s-symmetry is connected with nonlinear dependence of this value on temperature. The similiar rezult was obtained in this paper for antiferromagnetic spin fluctuations in cuprate superconductors. The linear dependence of C/T on temperature has been observed in experintantal work [7] for YBaCuO systems.

The problem of the definition of the gap symmetry in cuprate superconductors in the main one. There are many experiments devoted to the investigation of d-wave symmetry of the superconducting gap [8-12]. In particular, note the new experiments. The authors of Ref. 10 investigated the quantization of magnetic flux. in the ring containing three Josephson junctions on the grain-boundaries. It was established that the sign of the order parameter in $YBa_2Cu_3O_{7-\delta}$ depends on the direction. This behaviour corresponds to the $d_{x^2-y^2}$ symmetry. The experiments on the Josephson junction (DC SQUID) [11] also confirm the d-wave pairing. The temperature dependence of the antiferromagnetic spin fluctuations achieved in our work corresponds to d-wave pairing. The present thermodynamical calculations may be the additional test in the definition of the symmetry of the gap in the cuprate superconductors.

ACKNOWLEDGMENTS

Tha authors thank Prof. J.Kirtley and Prof. V.Gusynin for the discussion of this results.

This work was supported by the program of NATO Research Felloships.

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