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FUNCTIONAL INTEGRAL OF ANTIFERROMAGNETIC SPIN FLUCTUATIONS IN HIGH-TEMPERATURE SUPERCONDUCTORS

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The Schwinger–Dyson equations and equation for free energy are derived in the approximation of weak coupling interaction for antiferromagnetic spin fluctuations in high temperature superconductors. For the calculations the method of functional integrals was used. The thermodynamic of the system is calculated near T_c and the evaluations of the parameter $\Delta C/\gamma T_c$ are given.

1. Introduction

The main question in the theory of superconductivity is what mechanism provides the electron pairing. In BCS theory it is the electron–phonon interaction. Some recent models postulate the mechanism of antiferromagnetic spin fluctuations.[1–3] Electron scattering on these fluctuations may cause the electron pairing.[4] Spin fluctuations play an important role in superconductors with heavy fermions.[5] In Pines' papers[2,6] the calculations of superconducting gap, critical temperature, temperature dependence of resistance, and many other values are discussed, but thermodynamics is not considered. It is interesting to calculate a jump of thermal capacity near T_c and the parameter $\Delta C/\gamma T_c$, which equals 1.42 in BCS theory. The aim of this work is to calculate the thermodynamics of antiferromagnetic spin fluctuations using the method of functional integral.

Following Pines[1] we used Hamiltonian, taking into account spin fluctuations, in the form

$$H = H_o + H_{\text{int}}\,, \tag{1}$$

where H_o is the Hamiltonian of free electrons. The interaction is described by

$$H_{\text{int}} = \frac{1}{\Omega}\sum_{\eta} g(q)s(q)S(-q)\,, \tag{2}$$

where Ω is the volume of a cell and $g(q)$ is the interaction constant.

$$s(q) = \frac{1}{2}\sum_{\alpha,\beta,k} \Psi^{+}_{k+q,\alpha}\sigma_{\alpha\beta}\Psi_{k\beta} \tag{3}$$

is the operator of spin density, where $\sigma_{\alpha\beta}$ is the Pauli matrix, $\Psi^+_{k+q,\alpha}$ is the operator of electron creation with momentum $k+q$ and projection α, and $\Psi_{k\beta}$ is the operator of hole creation with momentum k and projection β; $S(-q)$ is the operator of spin fluctuations with correlation function $\chi(q, \omega)$.[2]

It should be noted that experiments on NMR show that a symmetry of pairing states is $d_{x^2-y^2}$.

2. Big Statistic Sum

Let us write the Hamiltonian in lattice representation:

$$\begin{aligned} H &= -t\sum_{\mathbf{n},\mathbf{p}} \psi^+_\alpha(\mathbf{n})\psi_\alpha(\mathbf{n}+\mathbf{p}) + \frac{1}{2}\sum_{\mathbf{n},\mathbf{m}} S_i(\mathbf{n})\chi^{-1}_{ij}(\mathbf{n},\mathbf{m})S_j(\mathbf{m}) \\ &\quad + g\sum_{\mathbf{n}} \psi^+_\alpha(\mathbf{n})\left(\frac{\sigma^i}{2}\right)_{\alpha\beta}\psi_\beta(\mathbf{n})S^i(\mathbf{n})\,, \\ H &= H_\circ + H_{\text{int}}\,, \\ H_\circ &= -t\sum_{\mathbf{n},\mathbf{p}} \psi^+_\alpha(\mathbf{n})\psi_\alpha(\mathbf{n}+\mathbf{p}) + \frac{1}{2}\sum_{\mathbf{n},\mathbf{m}} S_i(\mathbf{n})\chi^{-1}_{ij}(\mathbf{n},\,\mathbf{m})S_j(\mathbf{m})\,, \end{aligned} \tag{4}$$

where the summation is over all knots of infinite lattice (a lattice length is equal to a), ρ is a unit vector, which connects the neighboring knots, and S^i is a spin operator. $N = \sum_{\mathbf{n}} \psi^+_\alpha(\mathbf{n})\psi_\alpha(\mathbf{n})$ is an operator of particles number, t is a band halfwidth, and $\chi_{ij}(\mathbf{n},\,\mathbf{m})$ is a spin correlation function.

It is necessary to calculate a big statistical sum

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

where μ is a chemical potential and $\Omega(\mu,\,\beta,\,q)$ is a thermodynamical potential. It is convenient to use the formalism of continual integration for Fermi systems. The big statistical sum can be written in the form of functional integral[7]

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

where

$$\begin{aligned} L(\tau) &= \sum_{\mathbf{n}} \psi^+_\alpha(\mathbf{n},\,\tau)\left(\frac{\partial}{\partial\tau}-\mu\right)\psi_\alpha(\mathbf{n},\,\tau) - t\sum_{\mathbf{n},\mathbf{p}}\psi^+_\alpha(\mathbf{n},\,\tau)\psi_\alpha(\mathbf{n}+\mathbf{p},\,\tau) \\ &\quad + g\sum_{\mathbf{n}}\psi^+_\alpha(\mathbf{n},\,\tau)\left(\frac{\sigma^i}{2}\right)_{\alpha,\beta}\psi_\beta(\mathbf{n},\,\tau)S^i(\mathbf{n},\,\tau) \\ &\quad + \frac{1}{2}\sum_{\mathbf{n},\mathbf{m}} S_i(\mathbf{n},\,\tau)\chi^{-1}_{ij}(\mathbf{n},\,\mathbf{m},\,\tau)S_j(\mathbf{m},\,\tau)\,, \end{aligned} \tag{6}$$

where $L(\tau)$ is the Lagrangian system. N is a normalization multiplier:

$$N^{-1} = \int \prod_{\mathbf{n}} dS_i(\mathbf{n}) d\psi_\alpha^+(\mathbf{n}, \tau) d\psi_\alpha(\mathbf{n}, \tau) \exp\left(- \int_0^\beta d\tau L(\tau, \mu = g = 0) \right) .$$

Using the method of bilocal operator[8] for the calculation of the big statistical sum in the approximation of weak coupling (lowest order in g^2), the Schwinger–Dyson equation and equation for free energy are obtained. The detailed calculations were given in Refs. 9 and 10.

The Schwinger–Dyson equation

$$G^{-1} = G_0^{-1} - \Gamma^0\Gamma_5\mu + \frac{g^2}{18}(\Gamma^i \mathrm{Tr}\, \Gamma^j G\chi_{ij} - 2\Gamma^i G \Gamma^j \chi_{ij}) , \tag{7}$$

where $\Gamma_0\Gamma^i$ are the Dirac matrices. From Eq. (7) the gap equation can be easily obtained[2] (Fig. 1).

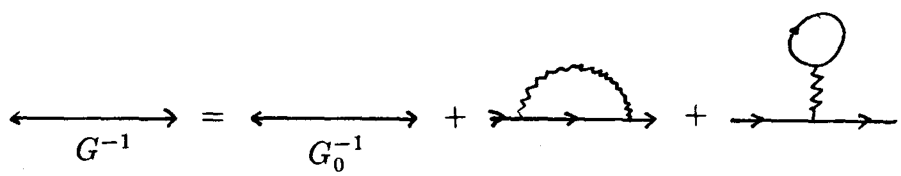

Fig. 1. Graphic depiction of the Schwinger–Dyson equation.

The free energy equation

$$F_1 = -\frac{g^2}{32} \mathrm{Tr}(\Gamma^i G \mathrm{Tr}\, \Gamma^j G - 2G\Gamma^i G \Gamma^j)\chi_{ij} \tag{8}$$

(where G and χ_{ij} are the fermion and spin Green functions, respectively) corresponds to the contribution of two vacuum diagrams (Fig. 2).

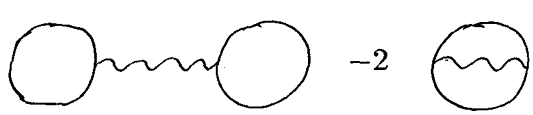

Fig. 2. Graphic depiction of Eq. (2). Here the solid line corresponds to the Green function of fermion, G, and the wave line corresponds to the spin Green function.

3. Gap Equation

From Eq. (7) it is easy to obtain the gap equation which is given in Ref. 2. Realizing now a Fourier transformation

$$G(x,\tau)=\sum_{n=-\infty}^{\infty}\int_{-\pi/a}^{\pi/a}\frac{d^2k}{(2\pi)^2}G(\mathbf{k},\omega_n)e^{i\omega_n\tau-i\mathbf{kx}}\left.\begin{matrix}\omega_n=\frac{(2n+1)\pi}{\beta} & \text{for fermions},\\ \omega_n=\frac{2\pi n}{\beta} & \text{for bosons},\end{matrix}\right\}$$

we rewrite Eq. (7) in pulse space:

$$\begin{aligned}G^{-1}(\mathbf{k},i\omega_n)=G_0^{-1}(\mathbf{k},i\omega_n)+\frac{g^2}{4\beta}\sum_{m=-\infty}^{\infty}\int_{-\pi/a}^{\pi/a}\frac{d^2p^2}{2\pi}[\Gamma^i\Gamma_5\mathrm{Tr}\,\Gamma^i\Gamma_5G(\mathbf{p},i\omega_m)\\ -2\Gamma^i\Gamma_5G(\mathbf{p},\omega_m)\Gamma^i\Gamma_5]\chi(\mathbf{k}-\mathbf{p},i\omega_n-i\omega_m),\end{aligned}\tag{9}$$

where we set $\chi_{ij}=\delta_{ij}\chi$,

$$\begin{aligned}G_0^{-1}(\mathbf{k},i\omega_n)&=\begin{pmatrix}0 & \{i\omega_n-[\varepsilon(\mathbf{k})-\mu]\}I\\ [i\omega_n+\varepsilon(\mathbf{k})-\mu]I & 0\end{pmatrix}\\ &\equiv\Gamma^0i\omega_n-\Gamma^0\Gamma_5[\varepsilon(\mathbf{k})-\mu],\\ \varepsilon(\mathbf{k})&=-2t(\cos k_xa+\cos k_ya).\end{aligned}\tag{10}$$

Let us define an eigenenergy part $\sum(\mathbf{k},i\omega_n)$ as

$$G^{-1}(\mathbf{k},i\omega)=G_0^{-1}(\mathbf{k},i\omega_n)-\Sigma(\mathbf{k},i\omega_n).\tag{11}$$

Equation (9) is then an equation for $\sum$. The solution for $\sum$ will be in the form

$$\sum=\Gamma^0A+\Gamma^0\Gamma_5B+\Delta+\Gamma^0\Gamma_5\Gamma^i\Delta_i\tag{12}$$

(A, B, Δ, and Δ_i are functions of $\mathbf{k}$ and $i\omega_n$). Then finding a matrix inverse to Eq. (11) we will get

$$G(\mathbf{k},i\omega_n)=\frac{\Gamma^0(\omega-A)-\Gamma^0\Gamma_5[\varepsilon(\mathbf{k})-\mu+B]+\Delta+\Gamma^0\Gamma_5\Gamma^i\Delta_i}{(\omega-A)^2-[\varepsilon(\mathbf{k})-\mu+B]^2-\Delta^2-\Delta_i^2}.\tag{13}$$

Substituting Eqs. (12) and (13) into Eq. (9) for functions A, B, Δ, and Δ_i, we get a system of equations

$$A(\mathbf{k},i\omega_n)=\frac{3g^2}{4\beta}\sum_m\int\frac{d^2p}{(2\pi)^2}\frac{i\omega_m-A(\mathbf{p},i\omega_m)}{\mathcal{D}(i\omega_m,\mathbf{p})}\chi(\mathbf{k}-\mathbf{p},i\omega_n-i\omega_m),\tag{14}$$

$$B(\mathbf{k},i\omega_n)=\frac{3g^2}{4\beta}\sum_m\int\frac{d^2p}{(2\pi)^2}\frac{\varepsilon(\mathbf{p})-\mu+B(\mathbf{p},i\omega_m)}{\mathcal{D}(i\omega_m,\mathbf{p})}\chi(\mathbf{k}-\mathbf{p},i\omega_n-i\omega_m),\tag{15}$$

$$\Delta(\mathbf{k},i\omega_n)=\frac{3g^2}{4\beta}\sum_m\int\frac{d^2p}{(2\pi)^2}\frac{\Delta(\mathbf{p},i\omega_m)}{\mathcal{D}(i\omega_m,\mathbf{p})}\chi(\mathbf{k}-\mathbf{p},i\omega_n-i\omega_m),\tag{16}$$

$$\Delta_i(\mathbf{k},i\omega_n)=-\frac{g^2}{4\beta}\sum_m\int\frac{d^2p}{(2\pi)^2}\frac{\Delta_i(\mathbf{p},i\omega_m)}{\mathcal{D}(i\omega_m,\mathbf{p})}\chi(\mathbf{k}-\mathbf{p},i\omega_n-i\omega_m),\tag{17}$$

where $\mathcal{D}(i\omega_m,\mathbf{p})=(i\omega_m-A)^2-[\varepsilon(p)-\mu+B]^2-\Delta^2-\Delta_i^2$.

Equation (16) corresponds to a singlet pairing and (17) to a triplet pairing. Moreover, in a singlet channel, we have a repulsion, and in a triplet, an attraction. That is why it is necessary to take a trivial solution $\Delta = 0$ of Eq. (16). In what follows we will neglect a contribution of A and B functions, which leads only to a renormalization of the wave function and chemical potential, and we will consider only Eq. (17). Neglecting Δ_i^2 in a denominator we come to a linearized equation for $\Delta_i(\mathbf{k})$, which defines a critical temperature T_c. For the correlation function $\chi(q, i\omega_n)$ we use a variance ratio

$$\begin{aligned}\chi(q, i\omega_n) &= -\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{d\omega'\,\mathrm{Im}\,\chi(q, \omega')}{i\omega_n - \omega'}\\ &= -\frac{1}{\pi}\left(\int_0^{\infty}\frac{d\omega'\mathrm{Im}\,\chi(q, \omega')}{i\omega_n - \omega'} + \int_0^{\infty}\frac{d\omega'\mathrm{Im}\,\chi(q, -\omega')}{i\omega_n + \omega'}\right). \end{aligned} \tag{18}$$

For a realization of a summation over m in Eq. (18) we consider a contour $C = C_1 + C_2$ (Fig. 3).

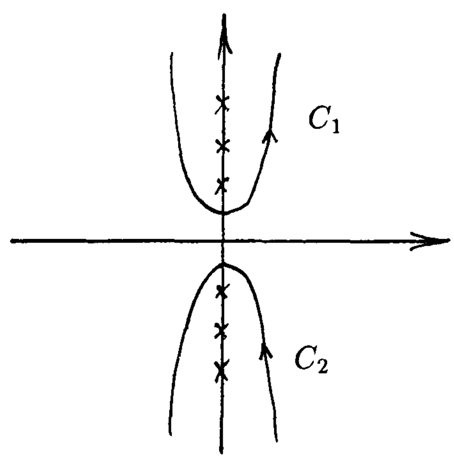

Fig. 3. The contour of integration.

Then the next formula (for $\omega_n = (2n+1)\pi/\beta$) takes place:

$$\sum_{n=-\infty}^{\infty} F(i\omega_n) = -\frac{\beta}{2\pi i}\int_C \frac{F(\omega)d\omega}{e^{\beta\omega}+1} = -\frac{\beta}{2\pi i}\int_C \frac{F(\omega)d\omega}{e^{-\beta\omega}+1} \tag{19'}$$

or

$$\sum_{n=-\infty}^{\infty} F(i\omega_n) = -\frac{\beta}{2\pi i}\,\frac{1}{2}\int_C F(\omega)\tanh\frac{\beta\omega}{2}\,d\omega\,.$$

After some calculations we arrive at the gap equation from Ref. 2:

$$\Delta(\mathbf{k}) = \frac{g^2}{8}\int \frac{d^2p}{(2\pi)^2}\left(\operatorname{Re}\chi[\mathbf{k}-\mathbf{p},\,\varepsilon(\mathbf{p})-\mu]\,\frac{\tanh\{[\varepsilon(\mathbf{p})-\mu]\beta/2\}}{\varepsilon(\mathbf{p})-\mu} + 2\int_0^\infty \frac{d\nu}{\pi}\right.$$
$$\left.\times\coth\frac{\beta\nu}{2}\operatorname{Im}\chi(\mathbf{k}-\mathbf{p},\,\nu)\,\frac{[\varepsilon(\mathbf{p})-\mu]^2-\nu^2+\delta^2}{\{[\varepsilon(\mathbf{p})-\mu]^2-\nu^2+\delta^2\}+4\delta^2\nu^2}\right)\Delta(\mathbf{p})\,. \tag{19''}$$

This confirms the validity of our approach.

4. Thermodynamic Potential of Antiferromagnetic Spin Fluctuations

For the free energy we have from Eq. (8)

$$\beta\Omega = \Gamma(G) = -\frac{1}{2}\operatorname{Tr}\left[\ln G_0 G^{-1} + (G_0^{-1}+\Gamma^0\Gamma_5\mu)G^{-1}\right]$$
$$-\frac{g^2}{32}\operatorname{Tr}(\Gamma^i G \operatorname{Tr}\Gamma^j G\chi_{ij} - 2G\Gamma^i G\Gamma^j\chi_{ij})\,, \tag{19}$$

where G satisfies Eq. (7). Let us multiply Eq. (7) by G and take Tr. This allows us to express

$$\frac{g^2}{8}\operatorname{Tr}(\Gamma^i G\operatorname{Tr}\Gamma^j G\chi_{ij} - 2G\Gamma^i G\Gamma^j\chi_{ij}) = -\operatorname{Tr}[(G_0^{-1}+\Gamma^0\Gamma_5\mu)G-1]\,. \tag{20}$$

Using Eq. (20) we can rewrite expression (19) for the functional of free energy calculated on the solutions of the Schwinger–Dyson equation in the form

$$\beta\Omega = -\frac{1}{2}\operatorname{Tr}\left(\ln G_0\Gamma^{-1} + \frac{1}{2}(G_0^{-1}+\Gamma^0\Gamma_5\mu)G - \frac{1}{2}\right)\,. \tag{21}$$

Making Fourier transformation we find

$$\Omega = \frac{1}{2\beta}V\sum_{n=-\infty}^{\infty}\int_{-\pi/a}^{\pi/a}\frac{d^2k}{(2\pi)^2}\operatorname{Tr}\Big(\ln G_0(\mathbf{k},\,i\omega_n)G^{-1}(\mathbf{k},\,i\omega_n)$$
$$+\frac{1}{2}\left[G_0^{-1}(\mathbf{k},\,i\omega_n)+\Gamma^0\Gamma_5\mu\right]G(\mathbf{k},\,i\omega_n) - \frac{1}{2}\Big)\,, \tag{22}$$

where V is a two-dimensional volume (an area of cuprate plane) and Tr is a matrix trace.

It is convenient to compare the value Ω, calculated at $\Delta \neq 0$, with the corresponding values of free energy at $\Delta = 0$. For the difference $\Omega(\Delta) - \Omega(\Delta = 0)$, we have

$$\Omega(\Delta) - \Omega(\Delta=0) = -\frac{1}{2\beta}V\sum_{n=-\infty}^{\infty}\int\frac{d^2k}{(2\pi)^2}\operatorname{Tr}\Big(-\ln\{G(\mathbf{k},\,i\omega_n)[G_0^{-1}(\mathbf{k},\,i\omega_n)$$
$$+\Gamma^0\Gamma_5\mu]\} + \frac{1}{2}\left[G_0^{-1}(\mathbf{k},\,i\omega_n)+\Gamma^0\Gamma_5\mu\right]G(\mathbf{k},\,i\omega_n) - \frac{1}{2}\Big)\,. \tag{23}$$

After some calculations we obtained the jump for the thermodynamical potential near T_c:

$$\Omega(\Delta) - \Omega(0) = \frac{V}{8} \int \frac{d^2k}{(2\pi)^2} \frac{\Delta_i^4(\mathbf{k})}{[\varepsilon(\mathbf{k}) - \mu]^2} \left[\frac{\beta}{2} \left(1 - \tanh^2 \frac{\beta[\varepsilon(\mathbf{k}) - \mu]}{2} \right) - \frac{1}{[\varepsilon(\mathbf{k}) - \mu]} \tanh \frac{[\varepsilon(\mathbf{k}) - \mu]}{2} \right] , \qquad (24)$$

where $\varepsilon(k)$ describes the spectrum of two-dimensional electrons, the free energy F is connected with the thermodynamical potential Ω by $F = \beta\Omega$, and $\Omega(\Delta)$ and $\Omega(0)$ are the thermodynamical potentials at $T < T_c$ and $T > T_c$, respectively.

In spite of the presence of the factors $[\varepsilon(\mathbf{k}) - \mu]$ in the denominator of formula (24), it is not difficult to test that the singularity on the Fermi surface $\varepsilon(\mathbf{k}) - \mu$ is absent. Equation (24) (at $T \sim T_c$) can be a basis for the calculation of different thermodynamic quantities.

The jump of specific heat was calculated by

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

At the present time we have provided the qualitative evaluations of the parameter $\Delta C/\gamma T_c$. The parameters of spin fluctuations were taken from Ref. 2. For $YBa_2Cu_3O_{6.63}$ at $\Delta_{max}(0)/kT_c = 3.4$, we got $\Delta C/\gamma T_c = 1.43$, and for $La_{1.85}Sr_{0.15}CuO_4$ at $\Delta_{max}(0)/kT_c = 4.3$, we got $\Delta C/\gamma T_c = 1.9$. At the present time we provide detailed computer calculations.

5. Conclusion

Using the method of functional integration to the problem of antiferromagnetic spin fluctuations allows us to solve the problem of their thermodynamics. We plan to calculate the thermodynamic properties using the second order of perturbative theory.

A similar method of calculation was elaborated by S. Weinberg.[11]

References

1. D. Pines, *Physica* **C185–189**, 120 (1991).
2. P. Monthoux, A. V. Balatsky, and D. Pines, *Phys. Rev. Lett.* **67**, 3448 (1991).
3. T. Moriya, V. Takahashi, and K. Ueda, *Physica* **C185–189**, 114 (1991).
4. B. G. Levi, *Phys. Today* **N5**, 17 (1993).
5. K. Miyake and S. Schmitt-Rink, *Phys. Rev.* **B34**, 6554 (1986).
6. P. Monthoux and D. Pines, *Phys. Rev.* **B46**, 10 (1993).
7. Y. N. Popov, *Functional Integrals and Collective Excitations* (Cambridge Univ. Press, 1987), p. 216.
8. J. Conwall, R. Jackiw, and E. Tomhoulis, *Phys. Rev.* **D10** (1974).
9. S. P. Kruchinin, preprint ITP-94-20E (Kiev, 1994), p. 11.
10. S. P. Kruchinin, in *Proc. M^2S-HTSC-IV Conference*, Grenoble, France, 5–9 July 1994.
11. S. Weinberg, preprint UTTG-18-93, p. 17.