

SPIN SUSCEPTIBILITY IN HIGH - TC SUPERCONDUCTIVITY

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ABSTRACT

Spin- current loop fluctuations is proposed as the mechanism of holes pairing in high temperature superconductors using the assumption of the coexistence of short-ranged antiferromagnetism with superconductivity and the Anderson's superexchange theory. The spin-spin correlation function is calculated using the Kubo-Mori relaxation function and the magnetic susceptibility equation is derived in terms of force correlation. Also a Bardeen –Cooper-Schrieffer (BCS) type of equation is solved for the transition temperature (T_c).

KEY WORDS: Superconductivity, cuprates, superexchange, susceptibility.

INTRODUCTION

The problem of formation and stabilization of ferromagnets(FM) and antiferromagnets (AFM) was explained by Hubbard(Hubbard, 1963). According to Hund's rules the magnetic moments of the AFM sublattices exist as a result of intra atomic correlation of d-electrons as well as by their inter atomic hoppings.

The first high temperature superconductor was discovered in 1986 in the ceramic $La_{2-x}Sr_xCuO_4$, where the parent compound is AFM (Bednorz, Muller,1986).It was soon observed that it is actually the CuO plane that is responsible for the pairing of holes, coherence and superconductivity. The Cu and O atoms have electronic configurations:

$^{29}Cu = [Ar]3d^{10}4s^1$ and

$^{8}O = 1s^22s^22p^4$. With respect to the closed shell configurations ($3d^{10}$ or Cu^{1+} and $2p^6$ or O^{2-}),the ground state of the parent compound has electrons taken from or holes added to the Cu sites. An alternative configuration for copper ion is $[Ar]3d^9 = Cu^{2+}$. On doping Sr^{2+} in place of La^{3+} , charge balance requires that electrons be removed from the CuO plane or holes added to this plane. This electron deficiency can be compensated for by driving as many Cu atoms as the dopant concentration from Cu^{2+} to Cu^{3+} . Another possibility is the one in which the Cu^{2+} configuration remains unchanged as a result of which the oxygen site will remain deficient of electrons; this implies that holes are being added and localized at the oxygen sites. This

viewpoint has been widely used by many authors (Behera, 1989; Yu Lu, 1991; Eskes, et al, 1988). In this paper we shall consider the process in which Cu is in the $3d^{10}$ and the dopant holes go to the oxygen site. Due to strong Coulomb repulsion V_{pp} , one of the holes hops to the neighbouring Cu-A site resulting in Cu^{3+} ($3d^9$).The remaining hole is now in direct exchange with Cu-B ion with exchange integral J.This process is the superexchange mechanism and is based on Hund's rules. It portrays the AFM interaction between two sublattice Cu spins as due to mediation of the ligand oxygen. Superexchange as worked out by Anderson allows the ligand p-orbitals to engage in internal coupling(Anderson,1950), as well as enforce p-orbital exchange with Cu spins, enabling the system to be FM or AFM. Now in the case of AFM, the Cu spins are paramagnetically disoriented and then each of them pair with a p- hole. Here we make the assumption that the dopant holes affect the spin moments of the lattice just as the application of heat would. The applied heat would raise the temperature of the system above the Neel temperature T_N ; but since similar increase in temperature is not observed during doping, it means that doping leads to the system's increase in kinetic energy. To lower the kinetic energy, a hole's spin hooks up with the random Cu moment to form a quasiparticle, two such quasiparticles reach out to each other magnetically to form spin singlet pairs with d-wave symmetry. This process is made clearer in the quantum mechanics of entanglements, where for the AFM subsystems A,B the classical correlation for the density matrix $\hat{\rho}_{AUB}$ is given as

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$$\hat{\rho}_{A \cup B} = \sum_i p_i \rho_A^{(i)} \otimes \rho_B^{(i)} \quad 1$$

$$p_i > 0, \sum_i p_i = 1.$$

where the weight Recently it has been understood that once the entanglement is dynamical, the density matrix can be used to explain the phenomenon of entanglement swapping (Ilichev, 2001). This consists of the fact that for spin-half complexes the singlet state represents a state of maximum correlations of spin pairs. Thus the creation and recombination of pairs of spin-half quasiparticles establishes correlations of physical quantities in the singlet channels, and this correlations can be swapped.

The theory given in this paper allows for the formation and presence of stripes in high temperature superconductors. The occurrence of stripes was first predicted theoretically by Zaanen and Gunnarsson (Zaanen, Gunnarsson, 1989), and Machida (Machida, 1989).

The existence of stripes was first determined experimentally by Tranquada and collaborators (Tranquada, et al, 1995) and since then more experimental and theoretical findings have been made (Seibold, et-al, 2012; Vojta, 2012; Avella, et al, 2011; Abbamonte, et-al, 2012; Valla, 2012). In the present paper we consider the stripes as being formed right below the bridging oxygen of Cu-O-Cu in such a way as to be able to feed the oxygen vacancies in a conveyor-belt fashion. As already stated the oxygen holes have antiparallel spins, when these

spins arrive at the Cu-3d¹⁰ sites, Cu-3d⁹ are formed and the holes pair up through the agency of the intersite effective interaction V_{eff} . As the conveyor-belt slots in the next pair of oxygen holes, their spins directions are both opposite to those of the previous hole pair. These newly arrived spins according to the Kanamori-Goodenough-Anderson (KGA) rules (Suzuki, Suzuki, 2009) will upturn the Cu spins. It turns that this process introduces the now measurable spin fluctuations in the cuprates. The AFM sublattices contain two spin magnetic moments as we know and according to basic theory of magnetism, equal and opposite spin currents link the moments. Let us denote the currents as J^+ and J^- . When the AFM system is doped, the new currents become $\langle J^+ \rangle$ and $\langle J^- \rangle$ and the correlation in the spin-current deviations is given by $\langle \Delta J^+ \Delta J^- \rangle = (J^+ - \langle J^+ \rangle)(J^- - \langle J^- \rangle)$. Thus the survival of some form of short-range magnetic order in the doped AFM allows spin-current loops to spring up, each loop connecting two holes of opposite spins together in a singlet state in such a way that the orbital part of the wave function of the pair obviously forms a $d_{x^2-y^2}$ symmetry beginning in the underdoped region of the phase diagram. Correlations of two physical quantities A , B shall be denoted by $\langle \langle AB \rangle \rangle$ everywhere in this work and we shall study the spin-current loops and their fluctuations using the mathematical techniques developed by Zubarev (Zubarev, 1960).

The double-time Green function

The retarded double-time Green function is defined for two operators A and B as

$$G_{ij}(t, t') = \langle \langle A(t); B(t') \rangle \rangle = -i\theta(t-t') \langle \langle [A(t), B(t')] \rangle \rangle \quad 2$$

where $\theta(t)$ is the step function and $\langle \dots \rangle$ denotes statistical averaging. The equation of motion for the Green function is

$$\frac{d}{dt} \langle \langle A(t); B(t') \rangle \rangle = \delta(t-t') \langle \langle [A(t); B(t')] \rangle \rangle + \langle \langle [A(t), H]; B(t') \rangle \rangle \quad 3$$

where H is the Hamiltonian of the system. The Fourier transform of equation (2) is given as

$$G_{ij}(t, t') = \frac{1}{2\pi} \int_0^\infty G_{ij}(\omega) e^{-i\omega(t-t')} d\omega \quad 4$$

That is

$$\langle \langle A(t); B(t') \rangle \rangle = \frac{1}{2\pi} \int_0^\infty \langle \langle [A|B] \rangle \rangle_\omega e^{-i\omega(t-t')} d\omega \quad 5$$

And we can write for $t' = 0$,

$$\langle \langle [A|B] \rangle \rangle_\omega = -i \int_0^\infty \langle \langle [A(t); B] \rangle \rangle e^{i\omega t} dt \quad 6$$

The Fourier transform of the equation of motion is

$$\omega \langle \langle [A|B] \rangle \rangle_\omega = \langle \langle [A, B] \rangle \rangle_\omega + \langle \langle [A, H]|B \rangle \rangle_\omega \quad 7$$

When the operators A,B are Fermi-like, the anticommutator(+ sign) is used; the commutator (lower sign) is taken for Bose-like operators, or at least when one of the two operators is Bose-like.

The Kubo-Mori functions

The Kubo-Mori relaxation function (Plakida, 2006) is defined as

$$\langle\langle A|B \rangle\rangle_{\omega} = -i \int_0^{\infty} \langle A(t), B \rangle e^{i\omega t} dt \quad 8$$

where $\langle A(t), B \rangle$ is the scalar function given by

$$\langle A(t), B \rangle = \int_0^{\beta} \langle A(t - i\lambda) B \rangle d\lambda \quad 9$$

$$\beta = 1/T, \hbar = k_B = 1.$$

If we substitute equation(9) in (8), we then obtain the following expression

$$\omega \langle\langle A|B \rangle\rangle_{\omega} = -i \langle AB \rangle \quad 10$$

From equation (6) we see that

$$\langle\langle A|B \rangle\rangle_{\omega} = -i \langle [A, B] \rangle \quad 11$$

Thus ,

$$\langle\langle A|B \rangle\rangle_{\omega} = \omega \langle\langle A|B \rangle\rangle_{\omega} + i \langle BA \rangle \quad 12$$

Since

$$\langle AB \rangle = \langle BA \rangle e^{-\beta\omega} \quad 13$$

then equation (12) yields

$$\langle\langle A|B \rangle\rangle_{\omega=0} = i \langle BA \rangle \quad 14$$

Then we obtain the very useful equation(15) below

$$\omega \langle\langle A|B \rangle\rangle_{\omega} = \langle\langle A|B \rangle\rangle_{\omega} - \langle\langle A|B \rangle\rangle_{\omega=0} \quad 15$$

Other relations that can be arrived at in a similar way are

$$\langle\langle i\dot{A}|B \rangle\rangle_{\omega} = \langle\langle A|-i\dot{B} \rangle\rangle_{\omega} = \langle\langle A|B \rangle\rangle_{\omega} \quad 16$$

$$\langle iA, B \rangle = \langle A, -iB \rangle = \langle [A, B] \rangle \quad 17$$

$$\langle A, B \rangle = -\langle\langle A|B \rangle\rangle_{\omega=0} \quad 18$$

Let us now consider the idea of spin susceptibility of the AFM system. From linear response theory the spin susceptibility Green function is defined as

$$\chi(q, \omega) = -\langle\langle S_q^+ | S_q^- \rangle\rangle_{\omega} = -\sum_{R_{ij}} \langle\langle S_i^+ | S_j^- \rangle\rangle_{\omega} e^{-iqR_{ij}} \quad 19$$

where q is the momentum, ω is the frequency, S_i^+, S_j^- are the spin raising and spin lowering operators respectively. Using equation (15) and following Jackeli (Jackeli and Plakida,1999) we write the last expression in the form

$$\chi(q, \omega) = \chi(q, 0) - \omega \langle\langle S_q^+ | S_q^- \rangle\rangle_{\omega} = \chi(q, 0) - \omega \Phi_q(\omega) \quad 20$$

Here $\chi(q, 0) = \chi_q$ is the static spin susceptibility, $\Phi_q(\omega) = \langle\langle S_q^+ | S_q^- \rangle\rangle_{\omega}$ is the spin-spin relaxation function. Let us introduce the idea of the memory function by

$$\Phi_q(\omega) = \frac{\chi_q}{\omega - \frac{M(q, \omega)}{\chi_q}} \quad 21$$

where $M(q, \omega)$ is the memory function. In terms of spins we write (15) in the form

$$\omega \langle (S_q^+ | S_q^-) \rangle_\omega = -\langle (S_q^+ | S_q^-) \rangle_{\omega=0} + \langle (iS_q^+ | S_q^-) \rangle_\omega = \chi(q, \mathbf{0}) + \frac{1}{\omega} \langle (i\dot{S}_q^+ | -\dot{S}_q^-) \rangle_\omega \quad 22$$

Substituting the last expression in equation (20) yields the dynamical susceptibility as

$$\chi(q, \omega) = -\frac{1}{\omega} \langle (iS_q^+ | -iS_q^-) \rangle_\omega \quad 23$$

On the two-dimensional lattice such as we have in the doped La_2CuO_4 the exchange of spin fluctuations between two quasiparticles of spins σ_1, σ_2 is considered the basis for the formation of the nearly antiferromagnetic Fermi liquid by Pines and co-workers (see Plakida, 2006). The interaction between the quasiparticles is then described by

$$V_{eff}(q, \omega) = g^2 \chi(q, \omega) \sigma_1 \sigma_2 \quad 24$$

where the dynamical spin susceptibility $\chi(q, \omega)$ fitted to experimental data is

$$\chi(q, \omega) = \frac{a\xi^2}{1 + \xi^2(Q_{AF} - q)^2 - i\omega/\omega_{sf}} \quad 25$$

Here $\xi(T)$ is the AFM correlation length, $\hbar\omega_{sf}$ is the AFM fluctuation energy and g is the coupling constant. It is noted that strong enhancement of the spin susceptibility near the

$Q_{AF} = (\pi, \pi)$ can bring about high T_c .

Making use of the formula for spectral representation of correlations, then

$$\langle J^+(t)J^-(t') \rangle = -\frac{1}{\pi} \int_{-\infty}^{\infty} \frac{e^{-i\omega(t-t')}}{1 + e^{\beta\omega}} \text{Im} \langle J^+ J^- \rangle_\omega d\omega \quad 26$$

We can differentiate the last expression to obtain

$$i^2 \langle J^+(t)J^-(t') \rangle = -\frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\omega^4}{1 + e^{\beta\omega}} \langle J^+(t)J^-(t') \rangle d\omega dt dt' \quad 27$$

The force acting on the particle is defined as $F = iJ^+$, so that the last expression is written in terms of forces as

$$\begin{aligned} \langle F^+(t)F^-(t') \rangle &= -\frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\omega^4 (1 - e^{\beta\omega})}{1 + e^{\beta\omega}} \langle J^+(t)J^-(t') \rangle d\omega dt dt' \\ &= -\frac{1}{\pi} \int_{-\infty}^{\infty} \omega^2 \langle J^+ J^- \rangle \tanh \beta\omega d\omega \end{aligned} \quad 28$$

One can obtain from (20) the expression

$$\chi(q, \omega) - \chi(q, \mathbf{0}) = \frac{1}{\omega^3} \langle F^+ F^- \rangle \quad 29$$

Substitute this in eqn.(28) to have

$$\chi(q, \omega) - \chi(q, \mathbf{0}) = -\frac{1}{\pi} \int_{-\infty}^{\infty} \frac{1}{\omega} \langle J^+ J^- \rangle \tanh \beta\omega d\omega \quad 30$$

The last equation be transformed into a gap equation for the spin fluctuating superconductor. In order to do that we make the following assumptions: the left hand side of eqn (30) is proportional to $N(\mathbf{0})J_{exch}^2 \delta\Delta_0$ and the spin current fluctuation on the right side is proportional to $\delta\Delta_0 J_{exch}$, where $N(\mathbf{0})$ is the density of

states, J_{exch} is the exchange integral, J_{exch}^2 comes from the two vertices of spin current diagram, δ is the dopant concentration and Δ_0 is the d-wave energy gap. The assumptions come as the result of experimental observation of a resonance peak at 41 meV in doped YBCO. This peak already exists in the normal state of this

superconductor at 25 meV and doping progressively shifts the peak to the right towards higher energies where it becomes vanishingly small at higher doping.

In the superconducting state the resonance peak also shifts (Kulic,2004) to the right diminishing in height and width until it becomes very sharp and small at 41 meV, near 90K(close to T_c). Since the resonance occurs in the normal state and merely shifts with sharpening profile and diminishing shape in the superconducting state, then the pair could signify unoccupied pair states that are progressively occupied during doping until it can

$$1 = -\frac{1}{N(0)V_{eff}} \int_0^{\omega_s} \frac{1}{\omega} \tanh \beta \omega d\omega \quad 31$$

Finally,

$$T_c = 1.14 \omega_s e^{\frac{1}{N(0)V_{eff}}} \quad 32$$

Here $V_{eff} = 2Z_c J_{exch}$, ω_s is the spin wave fluctuation frequency, Z_c is a renormalization factor which is material dependent, and the density of states $N(0) = 1(\text{eV} \cdot \text{spin})^{-1}$. We shall take the following values (Hayden et al, 1991; Plakida et al, 2001): for LaCuO, $J_{exch} = 0.13\text{eV}$, $Z_c = 1.1$, $\omega_s = 0.12\text{eV}$, and for YBCO, $J_{exch} = 0.14\text{eV}$, $Z_c = 1.2$, $\omega_s = 0.15\text{eV}$.

The BCS-like formula (32) yields $T_c = 47\text{K}$ for $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ and $T_c = 95\text{K}$ for $\text{YBa}_2\text{Cu}_3\text{O}_7$. The experimental critical temperature values for these cuprates are $\sim 40\text{K}$ and $\sim 93\text{K}$ (see for example, Manske, 2004; Villarreal and Llano, 2010). The difference in the experimental and theoretical values of T_c of each cuprate is due mainly to the almost approximate values of the quantities used in the calculation of T_c in equation (32).

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