Physica C 161 (1989) 88–90
North-Holland, Amsterdam

DILUTE ANNEALED MAGNETISM AND HIGH TEMPERATURE SUPERCONDUCTIVITY

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Received 12 July 1989

We calculate the critical temperature as a function of doping using a BCS formalism and a mean field approach to the annealed diluted quasi-two-dimensional antiferromagnet. We find reasonable agreement with the experimental data of Torrance et al. on $La_{2-x}Sr_xCuO_4$.

It has become increasingly appreciated that the strong antiferromagnetic coupling between in-plane Cu atoms in most of the high-temperature superconductors is not merely fortuitous [1–4]. However a coherent understanding of exactly how the magnetic interactions influence the observed superconductivity has been elusive.

Here we focus on the prototype compound, $La_{2-x}Sr_xCuO_4$ ("2-1-4"). We present calculations suggesting that the BCS parameter λ scales with the effective strength of the magnetic interactions, and that these weaken with progressive dilution. In particular, we show that this decrease of magnetic interactions produces the characteristic decrease of the curve $T_c(x)$ with x, where $0<x<2$ is the number of ferromagnetic bonds per plaquette.

We begin by considering the BCS equation in the weak coupling limit [5],

$$k_B T_c = A\omega_c e^{(-1/\lambda)} \quad [\omega_c < E_F] \,. \tag{1}$$

Here ω_c is a characteristic frequency which plays the role of a cutoff in the BCS equation and which also sets the energy scale, E_F is the Fermi energy and A is a constant with order of magnitude unity. Here $\lambda = N(0)V$, where $N(0)$ is the density of states at the Fermi level and V is the strength of the pairing interaction. In ordinary BCS theory, where the electron–phonon interaction is responsible for pairing, ω_c is the Debye frequency ω_D.

If $\omega_D \approx 10^2$ and $\exp(-1/\lambda) \approx 10^{-1}$–$10^{-2}$, then $T_c \approx 1$–10 K. Thus an electron–phonon interaction is not expected to produce T_c of the order of 10–100 K.

If mechanisms other than the electron–phonon interaction are present, however, ω_c may be larger than the Fermi energy E_F. In this case, the cutoff in (1) would be replaced by E_F [2,6]. For two dimensions we can use the expression

$$E_F = \frac{\pi\hbar^2}{m^*}\rho \,, \tag{2}$$

where $\rho = \rho(x)$ is the carrier density and m^* is the effective mass. Thus (1) becomes

$$k_B T_c = A E_F e^{-1/\lambda} \quad [\omega_c > E_F] \,. \tag{3}$$

There is considerable experimental evidence [2] that $T_c \propto \rho(x)$, so from (2) $T_c \propto E_F$. In 2-1-4, E_F is of the order of 10^3 k_B, so if $\exp(-1/\lambda) \sim 10^{-1}$ to 10^{-2}, then T_c ranges between 15 and 150. Thus, if ω_c is larger than E_F, an explanation for the HTSC phenomenon could be given by the BCS equation (3).

It is becoming increasingly believed that magnetism can play a dominant role in the pairing mechanism [1–4]. Due to the large antiferromagnetic interaction J_A (≈ 1300 K) between nearest neighbor Cu ions, it is plausible that the characteristic frequency should be larger than E_F. Hence (3) should

0921-4534/89/$ 03.50

apply. Indeed, eq. (3) has been used in ref. [4] to calculate $T_c(x)$. Specifically, ref. [4] assumes $V(x)=V_0\exp(-r_0/\xi(x))$, where $\xi(x)$ is the correlation length. Ref. [4] then advances arguments for choosing $r_0=6A$ and interprets experimental data to justify the choice $\xi(x)=3.8/\sqrt{x}$. When (3) is compared with experimental data, the agreement is encouraging. Here we take a different approach. Specifically, we consider annealed magnetism instead of quenched magnetism, since superconductivity occurs only in the metallic phase. Second, we evaluate $V(x)$ in terms of the microscopic exchange interactions J_A and J_F instead of the phenomenological form used in ref. [4].

We begin by partitioning V into two terms, $V=V_1+V_2$, where V_1 is related to the magnetic interactions and V_2 is everything else (zero-point energy, Coulomb interactions, etc.). For simplicity, we assume V_2 to be negligible [4]. The magnetic pairing interaction could be explained by assuming that the effect of doping the pure compound is to create a hole on the oxygen in the plane [3]. In the non-metallic region at small values of x, the hole is localized. Due to the presence of this hole, the oxygen couples ferromagnetically with two nearest neighbor Cu, with a coupling strength J_F. Since $J_F>J_A$, the two neighboring Cu interact via an effective ferromagnetic interaction. This effective ferromagnetic interaction creates a polarization; as a consequence, two holes can attract each other via a dipole–dipole interaction, where the strength of the interaction is proportional to J_A [3].

As x increases, the concentration of the ferromagnetic bonds increases. This results in a decrease of the effective antiferromagnetic interaction J_{eff} between neighboring Cu. Since the polarization decreases when J_{eff} decreases, the holes become more mobile as x increases. When a threshold x_c is reached, the system becomes metallic and therefore superconductivity can set in. Although the dipole–dipole interaction was for the *non-metallic* region where the holes are localized [3], in the *metallic* region we assume that two holes still interact via a potential proportional to the effective interaction J_{eff}. To calculate J_{eff} in the metallic phase, since the holes are free to move, we cannot require that they be localized and therefore the annealed [7] approach is more appropriate, so we start with the Hamiltonian for a single bond,

$$\mathcal{H}_{ij}=J_F t\sigma(S_i+S_j)+J_A S_i S_j\,, \tag{4}$$

where $t=0$ or 1 depending on whether a hole is present or not.

We first consider the case where σ, S_i and S_j are Ising spin variables. Since the temperatures involved are low, we use a mean field approximation for which t is substituted with its mean field value p, where $0<p<1$ is the density of holes per bond – so $x=2p$.

To obtain J_{eff}, we sum over the σ variables,

$$\sum_{\sigma} e^{-\beta\mathcal{H}_{ij}}=Ae^{+\beta J_{eff}S_iS_j}\,. \tag{5}$$

Hence

$$\beta J_{eff}=\tfrac{1}{2}\ln\cosh(2p\beta J_F)+\beta J_A\,. \tag{6}$$

Since the temperature that we will consider satisfies $kT\ll J_F$, J_A, we obtain from (6)

$$J_{eff}=pJ_F+J_A=(p+\alpha)J_F\,, \tag{7}$$

where $J_A/J_F\equiv\alpha$. For an XY model using a small angle approximation, namely that the angle between S_1 and S_2 is close to the equilibrium value π, we obtain the same result.

We need some idea of the interactions involved. There is experimental evidence that these interactions are quite strong indeed, with $|J_A|\approx 1300$ K and J_F even larger, with $\alpha\equiv J_A/J_F\approx -0.36$ [8]. Using the fact that $V=CJ_{eff}$, where C is a constant, we have

$$\lambda=CN(0)\,|J_{eff}|\,. \tag{8}$$

In order to compare with experimental data on $T_c(x)$, we must evaluate the Fermi energy E_F. Using [9] $m^*=5m_e$, where m_e is the electron mass, and $\rho=x/[2a_0^2]$, *where* $a_0\approx 3.8$ Å is the lattice constant, we find $E_F/k_B=3818x$. Substituting this expression for the Fermi energy and eq. (8) into eq. (3), we finally obtain

$$T_c=3818x\exp[-1/CN(0)\,|J_{eff}|\,]\,. \tag{9}$$

If we regard $CN(0)$ as an adjustable parameter, we obtain the curve in fig. 1. Also shown are the data of Torrance et al. [10]. We note the curve could be improved if we take into account the insulator-to-metal transition which occurs at the value $x_c\simeq 0.05$. This can be accounted for either by assuming that

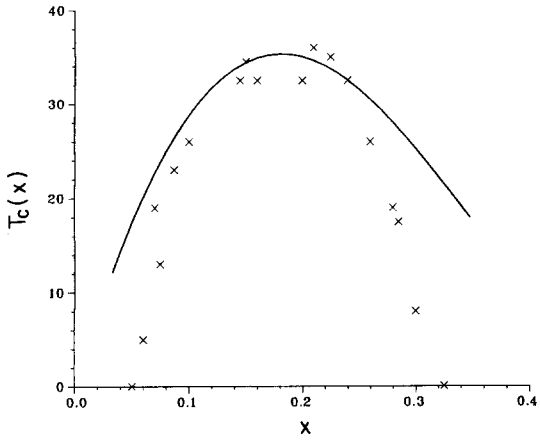

Fig. 1. Comparison between eq. (9) with $m^* = 5m_e$ and the experimental data of ref. [10]. The one adjustable parameter $CN(0)J_F$ is chosen to be 0.80.

the density of mobile holes goes appropriately to zero [4] as $x \to x_c$ or by assuming that the mass $m^* \to \infty$ at x_c. In both cases, the calculated curve would go to zero at x_c.

There is also the V_2 term that we have neglected; it should shift the value of x where T_c drops toward lower values. We note that the first part of the curve could also be explained by assuming that the pairs form bound bosons, which undergo Bose condensation. In this case T_c is still proportional to x, but the effective mass should assume a rather large value.

Just as BCS does not pretend to explain low-T_c superconductivity exactly and for all materials, so also our extension of BCS theory does not pretend to explain high-T_c superconductivity exactly. Our two main points are that eq. (1) of ordinary BCS is replaced with eq. (3), and the mechanism for pairing is due to magnetism and therefore λ is given by (8). In particular, we have assumed that the pairing occurs only in two-dimensional Cu–O sheets; a straightforward extension to three dimensions results in qualitatively similar behavior of $T_c(x)$.

Acknowledgements

We wish to thank R. Vasconcelos dos Santos and I. Fittipaldi for very helpful discussions and pertinent remarks. We also thank A. Aharony, R.J. Birgeneau, V.J. Emery and M.A. Kastner for helpful discussion on the connection between magnetism and superconductivity. Finally, we thank NATO for financial support, and the Boston University Academic Computing Center for machine time.

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