Superconductive state of Cu-O metals

Y. Kuroda
Physics Department, Nagoya University, Nagoya, Japan

C. M. Varma
AT&T Bell Laboratories, Murray Hill, New Jersey 07974
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We present calculations for the superconductive state of Cu-O metals using as the pairing kernel the excitation spectrum necessary to understand their anomalous (marginal Fermi-liquid) normal-state properties. With parameters deduced from the normal state, we obtain s-state superconductivity with the right order of magnitude of T_c, a zero-temperature gap $2\Delta(0)\approx 8T_c$ and a sharply decreasing nuclear relaxation rate at T_c rather than the "coherence peak."

Bednorz and Müller's remarkable discovery[1] of high-temperature superconductivity in Cu-O—based materials has raised two important related theoretical questions. What is the mechanism for pairing and what is the nature of the normal state in these materials? As is well known, most of their normal-state properties are unlike any other metal. It has been shown[2] that these normal-state anomalies follow from a single hypothesis about the excitation spectrum, and that the same hypothesis implies an effective particle-particle attraction in the s-wave channel at low energies. We take the point of view here that the normal-state anomalies and superconductivity arise from the same physics, and present calculations of the properties in the superconductive state that follow from the same excitation spectrum.

In contrast to the normal state, the superconductive state of the Cu-O's presents few *qualitatively* new phenomena. London penetration depth measurements[3] yield a superfluid density that has zero slope as $T\rightarrow 0$; this is consistent with s-wave pairing. A direct measurement of the low-temperature one-particle spectrum by photoemission[4] is consistent with s-wave pairing[5] with an unusually large gap: $2\Delta(0)/T_c\approx 8$. The most surprising effect discovered[6] is the absence of the BCS "coherence peak" in the nuclear relaxation rate, T_1^{-1} just below T_c; in fact T_1^{-1} sharply decreases in $YBa_2Cu_3O_{6.9}$ with $(d\ln T_1^{-1}/d\ln T)_{T_c}\approx 5$.

We will show that the excitation spectrum that leads to the normal-state anomalies also leads the observed behavior of T_1^{-1}. We also find that the ratio $2\Delta(0)/T_c$ is enhanced while at the same time the mean-field jump in the specific heat is reduced and its slope below T_c enhanced when compared to traditional superconductivity.

Our calculation is just the familiar strong-coupling modification of BCS theory; only the spectrum of excitations exchanged by the electrons is unusual. The hypothesis[2] about the excitation in the normal state is that there exists a contribution to the polarizability [see Fig. (1)], over most of the range of momentum, both for charge and spin excitation of the form

$$\begin{aligned}\mathrm{Im}\tilde{P}(q,\omega) &\sim N(0)\omega/T, \quad |\omega| \ll T \\ &\sim N(0) sgn\,\omega, \quad |\omega| \gg T\ ,\end{aligned} \tag{1}$$

with a cutoff $|\omega_c|$. If Eq. (1) is multiplied by a smooth function of $\mathbf{q}$, none of the results for the normal state or those calculated here for the superconductive state change qualitatively.

Equation (1) leads to a single-particle self-energy in the normal state whose leading frequency dependence is

$$\Sigma(q,\omega)\approx(\lambda_\rho+\lambda_\sigma)\left[\omega\ln\frac{x}{\omega_c}-i\frac{\pi}{2}x\right] . \tag{2}$$

Here $x=\max(|\omega|,T)$ and $\lambda_{\rho,\sigma}$ are dimensionless coupling constants for charge and spin fluctuations.

As discussed earlier,[2] Eq. (1) implies a negative contribution to the density correlation $\mathrm{Re}[\epsilon^{-1}(\mathbf{q},\omega)-1]$ and therefore to an attractive interaction in the s-wave, particle-particle channel for $\omega\lesssim\omega_c$. We calculate the *normal* and the *pairing* self-energies Σ_1 and Σ_2, respectively, in the superconductive state, using Eq. (1), as the kernel in the customary fashion[7]

$$\begin{aligned}i\tilde{\epsilon}_n &\equiv i\epsilon_n-\Sigma_1(i\epsilon_n)\ ,\\ \tilde{\Delta}_n &\equiv \Delta_n-\Sigma_2(i\epsilon_n)\ .\end{aligned} \tag{3}$$

Here n denote the Matsubara frequencies, and Δ_n is the contribution of the pairing (or pair-breaking) self-energies due to excitations not included in (1). It is useful to

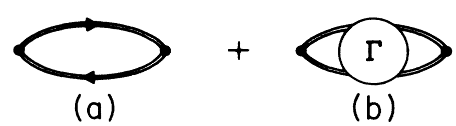

FIG. 1. The polarizability can, in general, be divided into two parts, as shown. The lines represent renormalized propagators. Equation (1) is assumed to represent the leading frequency dependence of the second graph of this figure.

define[7]

$$u(i\epsilon_n)\equiv\tilde{\epsilon}_n/\tilde{\Delta}_n\ , \tag{3a}$$

in terms of which most of the physical quantities in the superconducting state can be calculated. u is found to be given by the integral equation

$$u(\epsilon_n)=\frac{\epsilon_n}{\Delta_n}+\frac{\pi\lambda_\rho}{2\Delta_n}T\sum_{\omega_m}F(i\omega_m)\frac{u(\epsilon_n+\omega_m)-u(\epsilon_n)}{[1+u^2(\epsilon_n+\omega_m)]^{1/2}}+\frac{\pi\lambda_\sigma}{2\Delta_n}T\sum_{\omega_m}F(i\omega_m)\frac{u(\epsilon_n+\omega_m)+u(\epsilon_n)}{[1+u^2(\epsilon_n+\omega_m)]^{1/2}}\ . \tag{4}$$

$F(i\omega_m)$ is the Green's function for the excitations whose absorptive part in the *normal state* is given by Eq. (1):

$$F(i\omega_m)=\int_{-\infty}^{\infty}\frac{dx}{\pi}\frac{\text{Im}\tilde{P}(x)}{i\omega_m-x}\ . \tag{5}$$

For simplicity, the calculations in this paper use the parametrization[8]

$$\text{Im}\tilde{P}(\omega)=\begin{cases}N(O)\tanh\omega/2T, & |\omega|<\omega_c,\\ 0, & |\omega|>w_c\ .\end{cases} \tag{6}$$

It is important to note that, if $\tilde{P}$ is part of the excitation spectrum of the particles that undergo the superconductive instability, it is modified strongly at low frequencies. This effect produces only a small correction, proportional to T_c/E_F, for the determination of T_c. But it is very important for all properties for $T\ll T_c$, and for some properties like T_1^{-1} even near T_c.

First we look for a solution of Eq. (4) near T_c in powers of $\Delta(\epsilon)$ on the real axis. The details of this involved analysis will be given elsewhere. With $\lambda_\pm=\lambda_\rho\pm\lambda_\sigma$ the result is that for $\lambda_+\ln(\omega_c/T_c)\gg 1$ and $\lambda_+/\lambda_-\gg 1$, T_c is given by

$$\ln\left|\frac{\omega_c}{2T_c}\right|\simeq\frac{1+\alpha^2}{2\lambda_-}\left\{\lambda_1+\left[\lambda_1^2+4\lambda_-\left[\frac{1-\pi}{2a_1\lambda_0}\right](1+\alpha^2)^{-1}\right]^{1/2}\right\}, \tag{7}$$

where

$$\lambda_1\equiv\lambda_+-a_1\lambda_--\pi/2\lambda_0(1+\alpha^2)\ ,$$

$$a_1\equiv(1+\alpha^2)^{-1}\ln(4\gamma/\pi)-\Delta\bar{A}_0(\alpha)\ ,$$

$$\Delta\bar{A}_0(\alpha)\equiv\int_0^1 dx\tanh x/2[x^{-1}(1+\alpha^2)^{-1}-x(x^2+\alpha^2)^{-1}]\ .$$

and α is the all important pair-breaking parameter,

$$\alpha=(\pi/2)\lambda_+(1+\lambda_+\ln\omega_c/2T_c)^{-1}\ . \tag{8}$$

In Eq. (7), λ_0 is the coupling constant for excitations not included in (1), suitably renormalized to have an upper cutoff ω_c.

The mean-field jump in the specific heat, normalized to the normal-state specific heat at T_c is calculated to be,

$$\frac{\Delta C_s}{C_N}\simeq\frac{12}{\pi^2}[(1+\alpha^2)^2 b_1(\alpha)\lambda_+\ln(\omega_c/2T_c)]^{-1}\ , \tag{9}$$

where $b_1(\alpha)$ in a slowly varying function of α, which varies between 0.22 and 0.27 for the relevant range of α between 0 and 1. In Fig. (2), we plot $(\Delta C_x/C_N)\lambda_+\ln(\omega_c/2T_c)$ as a function of α.

Consider next the nuclear relaxation rate T_1^{-1}. In the normal state the low-frequency spin-fluctuation contributions of the usual form [from the first graph of Fig. (1)] and those of Eq. (1) [from the second graph of Fig. (1)] both contribute[2] to T_1^{-1}. The former leads to $T_1^{-1}\sim T$ (with logarithmic corrections) and the latter leads to a temperature-independent term, whose magnitude at T_c, for in-plane Cu nuclei in $YBa_2Cu_3O_{6.9}$, should be about five times the former to fit experiments. It is now necessary to consider the modification of Eq. (1) due to superconductivity. Figure (1b) represents a (reducible) ladder diagram in the particle-hole channel with an (unknown) vertex at every rung of the ladder. We wish to calculate the change in it, to leading order in Δ^2. There are two kinds of changes: changes in the vertices and changes in the particle-hole lines connecting them. In the absence of a microscopic theory, we cannot calculate the former.

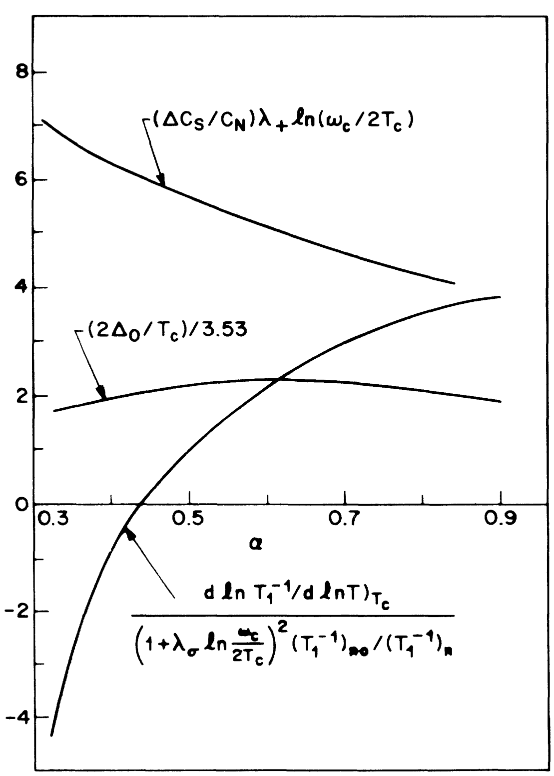

FIG. 2. The specific-heat discontinuity at T_c and the logarithmic derivative of the nuclear relaxation rate, T_1^{-1}, at T_c, suitably normalized, are shown as a function of the pair-breaking parameter α. The normalized zero-temperature gap is also shown as a function of α with the choice $\lambda_+/\lambda_-=3$.

The latter can be calculated by changing the particle-hole propagators from those of the normal state to those of the superconducting state. This procedure is similar to the calculation[9] of the change of the paramagnon spectrum in ^{3}He due to superconductivity. The contribution to T_1^{-1} of both Figs. (1a) and (1b), to leading order in Δ^2, can then be added together. The result of this calculation is

$$(T_1^{-1})_s \simeq (T_1^{-1})_n + \left[1+\lambda_\sigma^{1/2}\ln\left[\frac{\omega_c}{T_c}\right]\right]^2 (T_1^{-1})_{so} + \ldots , \qquad (10)$$

Here $(T_1^{-1})_n$ is the value of the total relaxation rate at T_c and $(T_1^{-1})_{so}$ is the contribution to order Δ^2 of Fig. (1a) alone. $(T_1^{-1})_{so}$ is given by[10]

$$\frac{(T_1^{-1})_{so}}{(T_1^{-1})_{no}} = \int_0^\infty \frac{d\omega}{2T}\cosh^{-2}\left[\frac{\omega}{2T}\right] \times \left[\left[\mathrm{Im}\frac{u}{(1-u^2)^{1/2}}\right]^2 + \left[\mathrm{Im}\frac{1}{(1-u^2)^{1/2}}\right]^2\right] . \qquad (11)$$

Here $(T_1^{-1})_{no}$ is the contribution of the first graph of Fig. (1) at T_c. We evaluate Eq. (11) using our solution for Eq. (4):

$$(T_1^{-1})_{so}/(T_1^{-1})_{no} \approx \left[1-\frac{4}{1+\alpha^2}b_1^{-1}(\alpha)F(\alpha)\ln|T_c/T|\right] . \qquad (12)$$

Here $F(\alpha)$ is a rapidly varying function of the pair-breaking parameter α. In Fig. (2), the quantity

$$\frac{4}{1+\alpha^2}b_1^{-1}(\alpha)F(\alpha) = \left[\frac{d\ln T_{1s}^{-1}}{d\ln T}\right]_{T_c} \times \frac{(T_1^{-1})_n}{(T_1^{-1})_{no}}\left[1+\lambda_\sigma^{1/2}\ln\frac{\omega_c}{T_c}\right]^{-2} \qquad (13)$$

is plotted, from which the logarithmic derivative of the relaxation rate at T_c^- can be deduced. For $\alpha \gtrsim 0.44$, the coherence peak is eliminated, and a sharply decreasing relaxation rate can be obtained if the factor $[1+\lambda_\sigma^{1/2}\ln(\omega_c/T_c)]^2$ is large. This factor, related to the real part of Eq. (1), comes about due to the change in $\tilde{P}(q,\omega)$ below T_c. The physics is that, there is large amplitude for pair breaking near T_c, due to spin-fluctuations and due to inelastic scattering since Eq. (1) leads to an appreciable scattering at thermal energies.[11] The latter is of course responsible for the normal-state transport relaxation rate $\tau^{-1} \sim \lambda_+ T$. (The idea that the transport relaxation rate and the pair-breaking rate are the same has been verified.[12]) There is a rapid diminution of spin-fluctuations and of the inelastic scattering just below T_c. This leads to a rapid change in T_1^{-1}.

The change in $P(\mathbf{q},\omega)$ is especially important for the density of states in the superconducting state at low temperatures. A gap in the density of states Δ_0 at $T=0$ must be self-consistently accompanied by a gap $2\Delta_0$ in $\mathrm{Im}P(\mathbf{q},\omega)$. The latter eliminates an important source of pair breaking at low temperatures thereby increasing Δ_0. Such a self-consistent solution is indeed found from Eq. (4) with

$$(2\Delta_0/T_c) \simeq (2\Delta_0/T_c)_{BCS}G(\alpha,\alpha_s) , \qquad (14)$$

where

$$\alpha_s \equiv \frac{\pi}{2}\lambda_+/(1+\lambda_+\ln|\omega_c/\Delta_0|) , \qquad (15)$$

and $G(\alpha,\alpha_s)$ is an enhancement factor plotted (for a given ratio λ_+/λ_-) in Fig. (2) as a function of α and $(2\Delta_0/T_c)_{BCS} \approx 3.528$.

Figure (2) and Eq. (7) for T_c contain the central results of this paper. We can use it to see if a consistent comparison with experiments may be made. We need three parameters ω_c, λ_+, and λ_-, which are all obtainable from the normal-state properties, to within factors of about 2.

With $\omega_c \approx 3\times10^3$ K, consistent with the fit[2] to Raman and reflectivity measurements $\lambda_+ \approx 3$ consistent with normal-state resistivity and reflectivity and $\lambda_\sigma \approx 0.8$ consistent with the constant contribution to the Cu II nuclear relaxation in the normal state, we get $2\Delta(0)/T_c \approx 7.7$, $(d\ln T_1^{-1}/d\ln T)_{T_c} \approx 2.6$, and $T_c \approx 110$ K; the last by using Eq. (7) with $\lambda_0 \approx 0$. These are to be compared with the experimental numbers of approximately 8, 5, and 90 K, respectively. With $\omega_c \approx 2\times10^3$ K and λ_+, λ_σ as before, we get 7.9 and 3.4, for $2\Delta(0)/T_c$ and $(d\ln T_1^{-1}/d\ln T)_{T_c}$, respectively, and $T_c \approx 75$ K. One may wish to ascribe the smaller slope of the calculated T_1^{-1} compared to experiment to the absence of any renormalization of the vertex in Fig. (1) due to superconductivity in the theory. It is also possible to fiddle with the parameters in the permitted range to get the nuclear relaxation rate as well as T_c and Δ_0 to agree with experiment. But that would be an empty exercise. We should note, however, that within a sensible range of parameters $2\Delta_0/T_c$ is rather insensitive, $\ln|\omega_c/2T_c|$ depends on the ratio λ_+/λ_- rather than individually on λ_+ and λ_- and T_1^{-1} does not have a coherence peak. To get a large $d\ln T_1^{-1}/d\ln T$, we need to pick a larger λ_σ.

The mean-field jump in the specific heat, with the two set of parameters above, is predicted to be $\Delta C/C_N(T_c) \approx 0.7$, and 0.64, respectively, less than the BCS value 1.43. Since the normal-state electronic specific heat in the high-temperature superconductors is not known accurately at present, direct comparison with experiment is not possible. Specific-heat measurements in good quality single-layer Bi compound $T_c \approx 10$ K are suggested to test this prediction as well as the logarithmic correction to the normal-state specific heat. For the same reasons as the rapid diminution of T_1^{-1} below T_c, we expect to find an unusually large $(dC_v/dT)_{T_c^-}$. This is as found in experiment but higher order (in Δ^2) calculations than done here are needed for quantitative comparison.

The quantitative success above should be tempered with the following reservations. The approximations $\lambda_+\ln(\omega_c/2T_c)$, $\lambda_+/\lambda_- \gg 1$, made for obtaining analytical results may not be very good but this can be remedied by numerical calculations we shall present elsewhere. Our lack of knowledge of the vertex[13] in Fig. (1) is, in principle, the essential missing link. Small quantitative changes will occur because $\text{Im}\tilde{P}$ at $T \approx 0$ will be larger just above $2\Delta_0$ than assumed, as also due to vertex corrections as the small parameter for the validity of the Migdal approximation, is $\omega_c/E_F \approx 10^{-1}$, not $\approx 10^{-2}$ as typically for the electron-phonon problem.

What has been shown is that the excitation spectrum, which explains the normal-state properties gives s-wave superconductivity, as observed, with crucial quantitative features like a very large enhancement of $2\Delta(0)/T_c$ over the BCS value and the sharp diminution of T_1^{-1} just below T_c rather than a coherence peak. This encourages one to further study microscopic models[14] designed to give s-wave attraction through electron-electron scattering. The main unsolved problem would appear to be to obtain $\tilde{P}(\mathbf{q},\omega)$ from attractive interaction models.

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