Possibility of the High-T_c oxide Y-Ba-Cu-O as a Bardeen-Cooper-Schrieffer superconductor

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We present a theoretical analysis of experimental data for the magnetic penetration depth, the upper critical field, and the critical temperature of the high-T_c oxide Y-Ba-Cu-O using a BCS-like theory. The result is a unique set of normal-state parameters of the charge carriers. It is pointed out that an experimental and theoretical proof of these parameters will provide a distinctive step towards a proof of the validity of BCS-like theories in describing the superconducting properties of high-T_c superconductors. Aspects of the possibility of the standard electron-phonon-interaction model are also investigated.

The basic controversy in the theory of high-T_c superconductors—whether or not Fermi-liquid theory and local-density approximation (LDA) are appropriate in its description of the metallic ground state—is still unresolved. Nevertheless, there is growing evidence that some features of these materials are properly explained by LDA. Most striking of these is probably the good agreement between theory and experiment in the case of electric-field gradients[1] and in the case of Fermi surfaces.[2,3]

If one adopts the attitude that the Fermi-liquid theory *is* the proper explanation of the metallic ground state, a BCS-like model is the obvious choice for a description of the superconducting properties of high-T_c superconductors. Such a model features Cooper pairs as the microscopic element responsible for superconductivity. Such a pair consists of two fermionic charge carriers of equal sign which are coupled attractively by the exchange of a virtual boson. The effective coupling strength is described by the parameter g, which is constant up to a characteristic boson frequency ω_c and zero for all $\omega > \omega_c$. g and ω_c are certainly very important parameters for superconductivity but so are the normal-state parameters of the charge carriers, such as the effective mass $m^\star$, the density of states at the Fermi energy, $N(\varepsilon_F)$, and the Fermi velocity v_F.

It is the purpose of this study to show that three basic properties of superconductors—the critical temperature T_c, the upper critical field H_{c2}, and the magnetic penetration depth in the local approximation, λ_L—provide unique information on the normal-state properties of the charge carriers if a BCS-like theory is assumed to be valid. The calculation of these properties from experimental data does not even require assumptions on the nature of the exchange bosons or estimates of the values of g or ω_c. Thus, a verification of these normal-state parameters by experimental or theoretical means could provide the necessary proof of validity of a BCS-like theory for high-T_c superconductors with all its implications.

Our analysis considers two Fermi-surface models: a two-dimensional one characterized by a cylindrical Fermi surface with the cylinder axis perpendicular to the a-b plane and a three-dimensional one characterized by a spherical Fermi surface. (Band-structure calculations[4] indicate that the cylindrical-symmetric approach seems to be the more appropriate one.) It would not be necessary to use parabolic bands if we analyzed the magnetic penetration depth only, but the application of the theory of the upper critical field requires the explicit definition of an energy dispersion relation. At the moment we can only treat dispersion relations which are isotropic in the plane perpendicular to the direction of the external magnetic field. (It is possible to calculate the upper critical field renormalized to its slope at T_c for more complicated dispersion realtions[5] but this does not allow for an estimate of the Fermi velocity.) The analysis is then performed using experimental data for Y-Ba-Cu-O single crystals, which became very reliable recently.

The magnetic penetration depth is measured by a number of different techniques which agree very well in their extrapolated $T = 0$ value. There are differences, though in the temperature dependence, with muon spin relaxation experiments reporting data which are fitted by a two-fluid model,[6] while the other techniques report data which are better explained by a BCS local approximation.[7,8] Because of the small coherence length (~ 16 Å),[9,10] the local approximation seems to be more appropriate, and we use, for the magnetic penetration depth at $T = 0$,

$$\lambda_L(0) = \frac{1}{2}\frac{\hbar c}{e\, v_F}\left(\frac{2d}{m^\star}\right)^{1/2} \tag{1}$$

in the case of a cylindrical-symmetric Fermi surface (FS) and

$$\lambda_L(0) = \frac{\sqrt{3\pi}}{2} \frac{c}{m^\star e} \left(\frac{\hbar}{v_F}\right)^{3/2} \tag{2}$$

for the spherical one. Here, d is the average distance between two Cu-O planes; c, the velocity of light; e, the elementary charge; $m^\star$, the effective band mass; and v_F, the Fermi velocity.

The upper-critical-magnetic-field measurements using untwinned single crystals and magnetization techniques[9] no longer exhibit an upward curvature of $H_{c2}(T)$ in the vicinity of T_c. This, of course, suggests the application of the standard Werthamer, Helfand, and Hohenberg (WHH) theory[11] and we use

$$T_c \sum_{n=0}^{n_0(T_c)} [\chi^{-1}(\tilde{\omega}_n(T_c), 0) - t_+]^{-1} = T \sum_{n=0}^{n_0(T)} [\chi^{-1}(\tilde{\omega}_n(T), H_{c2}) - t_+]^{-1} , \tag{3}$$

with the arbitrary cutoff

$$\hbar\omega_0 = [2n_0(T) + 1]\, \pi k_{\rm B} T \tag{4}$$

and the Matsubara frequencies $\tilde{\omega}_n(T)$ renormalized by the charge-carrier–impurity interaction.[12] $t_+ = \hbar/(2\pi\tau_{\rm tr})$ with $\tau_{\rm tr}$ the transport relaxation time. The Werthamer function $\chi(\omega_n, H)$ is defined as

$$\chi(\omega_n, H) = 2 \int_0^\infty d\rho\, \rho\, \exp\left(-\frac{e\hbar}{4m^\star c} H \rho^2\right) \times \left| K_0(\rho\sqrt{-(\varepsilon_F + i\hbar\omega_n)})\right|^2 \tag{5}$$

in the two-dimensional FS model ($\varepsilon_F = m^\star v_F^2/2$), and by

$$\chi(\omega_n, H) = \frac{2\pi}{\hbar\sqrt{\alpha}} \int_0^\infty d\rho\, \exp(-\rho^2) \tan^{-1}\left(\frac{\rho\sqrt{\alpha}}{|\omega_n|}\right) \tag{6}$$

in the three-dimensional FS model. $K_0(x)$ is the modified Bessel function of zeroth order and $\alpha = eHv_F^2/(2\hbar c)$. It was observed by Pint,[12] using numerical analysis, that in the two-dimensional model H_{c2} does not explicitly depend on ε_F and $m^\star$. It scales instead, as in the three-dimensional model, as $1/v_F^2$. This allows one to determine the Fermi velocity directly from H_{c2} experiments.

Thus, Eqs. (1), (3), and (5) define uniquely $m^\star$ and v_F for the cylindrical FS and Eqs. (2), (3), and (6) for the spherical FS. The density of states per spin is then given by

$$N(\varepsilon) = \frac{m^\star}{2\pi\hbar^2 d} \left(\text{or } N(\varepsilon) = \frac{m^\star}{2\pi^2\hbar^3}\sqrt{2m^\star\varepsilon}\right) , \tag{7}$$

with the formula in large parentheses for the three-dimensional model. This, finally, determines the number of charge carriers per unit volume,

$$n = 2 \int_0^{\varepsilon_F} d\varepsilon\, N(\varepsilon), \tag{8}$$

the Drude plasma frequency

$$\omega_p^2 = \frac{4\pi n e^2}{m^\star} = \left(\frac{c}{\lambda_L(0)}\right)^2 , \tag{9}$$

and the Sommerfeld constant

$$\gamma = \frac{2\pi^2 k_B^2}{3} N(\varepsilon_F). \tag{10}$$

As in standard BCS theory, we made no assumptions about a possible "dressing" of the normal-state properties by the exchange interaction responsible for superconductivity.

If $\lambda_L(0) = 140$ nm, $\mu_0 dH_{c2}(T)/dT|_{T=T_c} = -1.8$ T/K,[9] with the external magnetic field perpendicular to the a-b plane and $T_c = 93$ K, we find the normal-state properties listed in Table I. The impurity parameter t_+ is assumed to be equal to zero because the experimental data of Scheidt *et al.*[8] suggest a rather long mean free path ($\ell \sim 1.6$ μm), which justifies a calculation of the upper critical field using the clean limit of the WHH theory.

We see that the normal-state parameters for the two FS models differ, but it is questionable whether these differences will be significant enough to allow a clear answer on which of the two symmetries is more likely. Nevertheless, the data are different enough from the normal-state properties found for the charge carriers in "classical" superconductors. We find an effective mass of the order of six bare-electron masses, a value which is in the scope of the theoretical study by Wu, Ting, and Xing,[13] who investigated the extrapolated residual resistivity in high-T_c oxides in terms of fermionic and bosonic charge carriers. It is one of the major results of that analysis that fermionic charge carriers are more likely than bosonic

TABLE I. Summary of normal-state parameters of charge carriers in Y-Ba-Cu-O. The effective mass $m^\star$ is given in units of the bare-electron mass, the Fermi velocity in 10^6 m s^{-1}, the number of charge carriers per unit volume n in 10^{27} m^{-3}, the charge-carrier density of states $N(\varepsilon_F)$ in 10^{25} states/(meV m^3 spin), the plasma frequency ω_p in eV, and the Sommerfeld constant γ in mJ/(mol K^2).

Model	$m^\star$	v_F	n	$N(\varepsilon_F)$	ω_p	γ
Cylindrical	6.48	0.105	9.34	2.32	1.41	19.0
Spherical	5.60	0.128	8.08	2.31	1.41	18.9

ones and this would be in support of a BCS-like model. A similar value for the effective mass was reported by Kresin and Wolf[14] for the system $La_{1.8}Sr_{0.2}CuO_4$ in an analysis of data on the Hall effect and the Sommerfeld constant.

The Drude plasma frequency ω_p of 1.4 eV is inside the experimental range of 0.9–2.7 eV.[15–17] The density of states at the Fermi surface of 2.3×10^{25} states/(meV m^3 spin) is certainly above the band-structure results of 1.6×10^{25} quoted by Krakauer, Pickett, and Cohen[18] and of 1.95×10^{25} calculated by Massidda *et al.*[19] (This last value is found if one assumes that the original value of Massidda *et al.* is the single-spin density of states, as was commented by Pickett.[4]) The reported experimental error of about ± 20 nm in the magnetic penetration depth results in a change of the plasma frequency of about ∓ 0.24 eV, which still keeps it at the bottom of the experimental range. The same error causes a change in $N(\varepsilon_F)$ of about $\mp 0.35 \times 10^{25}$ states/(meV m^3 spin), which would bring it closer to the theoretical value of Massidda *et al.* if the penetration depth were larger than 140 nm. The Sommerfeld constant γ is also at the lower end of the experimental range reported by Junod.[20]

In a more realistic approach we will have to "dress" all normal-state properties by the charge-carrier–phonon interaction, which certainly plays some role in the high-T_c superconductors. Thus we have to introduce the temperature-dependent mass enhancement factor $\lambda(T)$, the temperature dependence of which was studied extensively by Grimval[21] and by Kresin and Zaitsev.[22] According to this renormalization of the effective mass, the observed magnetic penetration depth $\lambda'_L(0)$ is related to the "naked" $\lambda_L(0)$ of Eq. (1,2) by

$$\lambda'_L(0) = \frac{\lambda(0)}{\sqrt{1+\lambda(0)}} , \tag{11}$$

where $\lambda(0)$ is the mass renormalization at $T = 0$. The dressed Fermi velocity is found from

$$v'_F = v_F\,[1+\lambda(T_c)] , \tag{12}$$

with $\lambda(T_c)$ the mass enhancement factor at $T = T_c$. This, finally, results in a renormalization of all the other normal-state parameters according to

$$m'^\star = \frac{m^\star[1+\lambda(0)]}{[1+\lambda(T_c)]^2} \left\{ \text{or } m'^\star = \frac{m^\star}{1+\lambda(T_c)}\sqrt{\frac{1+\lambda(0)}{1+\lambda(T_c)}} \right\},$$
$$N'(\varepsilon'_F) = \frac{N(\varepsilon_F)[1+\lambda(0)]}{[1+\lambda(T_c)]^2}; \qquad \varepsilon'_F = m'^\star\,(v'_F)^2/2, \tag{13}$$
$$\gamma' = \frac{\gamma[1+\lambda(0)]}{[1+\lambda(T_c)]^2},$$
$$n' = n\left(\frac{1+\lambda(0)}{1+\lambda(T_c)}\right)^2 .$$

($\{\cdots\}$ refers to the spherical FS.)

In the next step of this analysis we adopt a more speculative attitude and assume that the mediating bosons in the Cooper pairs are presented by phonons. [There is one theoretical study by Fung and Kwok[23] in which the very small isotope effect observed for Y-Ba-Cu-O (Refs. 24–26) is explained by a modified BCS-type theory which includes the local volume change at vacancy sites caused by compressional phonon modes. This gives at least some justification of our hypothesis.]

Having decided on the maximum phonon frequency ω_c, we can calculate the coupling constant g from

$$k_B T_c = 1.13\,\hbar\omega_c \exp\left(-\frac{1}{N(\varepsilon_F)g}\right) , \tag{14}$$

the standard BCS T_c equation. It is valid for both FS symmetries and is a very good approximation even in cases where $\omega_c \lesssim \varepsilon_F$ and $T_c < \omega_c$ (Ref. 27) (error $\sim 7\%$ for $\omega_c = \varepsilon_F$). The weak-coupling limit of the Eliashberg theory[28] finally provides a simple relation between the product $N(\varepsilon_F)g$ and the charge-carrier mass enhancement factor λ,

$$\frac{\lambda(0)-\mu^\star}{1+\lambda(0)} = N(\varepsilon_F)g, \tag{15}$$

with the Coulomb interaction pseudopotential $\mu^\star$. Table II demonstrates how $N(\varepsilon_F)g$ depends on the choice of ω_c for a given T_c of 93 K and how this in turn affects $\mu^\star$ for a given value of $\lambda(0)$. For instance, an ω_c of 90 meV which corresponds to the maximum phonon frequency of Y-Ba-Cu-O (Ref. 29) and a λ of 1.0 would result in a $\mu^\star$ of about 0.2, which is not all that unusual. It is also not too far from the threshold value of $\lambda = 0.7$ calculated by Gor'kov and Kopnin,[30] which allows for a linear temperature dependence of the resistivity under a standard charge-carrier–phonon interaction. Furthermore, $\lambda(T_c)$ is just about one-third of $\lambda(0)$ and, as a result, Table III lists the normal-state properties of a *phononic* high-T_c superconductor Y-Ba-Cu-O. We note that this renormalization procedure had almost no effect on the Sommerfeld constant γ, which is still at the lower end of the experimental range.

It is interesting to point out, in a final remark, that the two "classical" BCS values

$$\frac{\Delta C}{\gamma T_c} = 1.43 \quad \text{and} \quad \frac{2\,\Delta(0)}{k_B T_c} = 3.53 \tag{16}$$

are also valid in the case of the cylindrical-symmetric FS. [ΔC is the jump in the specific heat at T_c and

TABLE II. Connection between ω_c, $\lambda(0)$, and $\mu^\star$ according to Eq. (14) for a T_c of 93 K.

ω_c	$N(\varepsilon_F)g$	λ	$\mu^\star$
50	0.511	1.2	0.076
60	0.468	1.0	0.065
		1.2	0.171
90	0.393	0.7	0.032
		1.0	0.214
		1.2	0.335

TABLE III. Same as Table I but for a *phononic* superconductor.

Model	m'^*	v'_F	n'	$N'(\varepsilon'_F)$	ω'_p	γ'
Cylindrical	7.29	0.140	21.0	2.61	1.99	21.4
Spherical	5.15	0.171	14.9	2.60	1.99	21.3

$\Delta(0)$ is the zero-temperature energy gap of the superconductor.] For a λ of 1, strong-coupling Eliashberg theory would change these two numbers to about 2 and 4, respectively.[28] Very recent tunneling measurements by Wang, He, and Wang,[31] which show a high degree of reproducibility, suggest that $2\Delta(0)/(k_BT_c)$ is in the range 4–5.8, with the maximum probability at the value 4.8. Thus, our rather crude analysis is at the lower end of the latest experimental results but still inside the experimental range of the rather huge body of experimental data. Nevertheless, it is definitely too early to conclude from this last part of our analysis that the high-T_c superconductors are phononic systems.

In conclusion, we want to emphasize that the presented theoretical analysis of experimental data of the critical temperature, of the magnetic penetration depth, and of the upper critical field for the system Y-Ba-Cu-O in terms of a BCS-like model provides a unique set of normal-state properties of the charge carriers. This analysis does *not* require any assumptions about the nature of the mediating bosons responsible for the attractive interaction between the two fermionic charge carriers of the Cooper pair. Those properties are distinctively different from the data usually found in "classical" superconductors. For two parameters, namely the Drude plasma frequency and the charge-carrier density of states at the Fermi energy, good agreement between experimental and theoretical data is found. This agreement is certainly not sufficient for a proof beyond doubt of the validity of BCS-like models in a description of the superconducting properties of high-T_c superconductors. But a verification of *all* the normal-state properties reported here for the system Y-Ba-Cu-O by experimental and theoretical means will certainly be a distinctive step towards such a proof for at least one of the high-T_c oxides.

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