



PHOTOINDUCED SUPERCONDUCTIVITY IN CUPRATES

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ABSTRACT

The photoinduced superconducting phase transition temperature in high- T_C cuprates with two band Hamiltonian has been investigated. It is shown to possess two superconducting gaps. The superconductivity is caused by the interband repulsive electron-lattice and coulomb interaction. The photo- excitation produces a change of the hole doping (p) and as a result, the shift ΔT_C of T_C . The study of free energy, critical field and electronic specific heat based on this model is also presented.

Key words: Green's function, p and d holes, Gap parameter, Specific heat, Free energy, Critical field, Carrier concentration.

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INTRODUCTION

It is of fundamental importance to explain the doping dependence of the superconducting properties of high- T_C cuprates. Recent experimental investigations on high- T_C cuprates having compositions in the semiconductor regime, have shown light induced changes, which are indicative of photo-induced superconductivity¹⁻³. In some cases, there is an increase of the critical temperature T_C with radiation dosage⁴. The most interesting result is the growth of the absolute value of the diamagnetic moment almost linearly with radiation dosage, which saturates beyond a certain stage⁴. Yu et al.¹ have shown that the onset of transient photo-induced superconductivity, at high excitation levels is a real phenomenon.

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The Model Hamiltonian

The model Hamiltonian has the form⁵-

$$H = H_o^p + H_o^d + H_{pd} \quad \dots(1)$$

Where

$$H_o^p = \sum_p \epsilon_p (C_{p\sigma}^+ C_{p\sigma} + C_{-p\sigma'}^+ C_{-p\sigma'}) + \Delta_{pp}^+ \sum_p C_{p\sigma} C_{-p\sigma'} + \Delta_{pp} \sum_p C_{p\sigma}^+ C_{-p\sigma'}^+ \quad \dots(2)$$

$$H_o^d = \sum_d \epsilon_d (C_{d\sigma}^+ C_{d\sigma} + C_{-d\sigma'}^+ C_{-d\sigma'}) + \Delta_{dd}^+ \sum_d C_{-d\sigma'} C_{d\sigma} + \Delta_{dd} \sum_d C_{d\sigma}^+ C_{-d\sigma'}^+ \quad \dots(3)$$

and

$$H_{pd} = V_{pd} \langle C_{p\sigma}^+ C_{-p\sigma'}^+ \rangle \sum_d C_{-d\sigma'} C_{d\sigma} + V_{pd} \langle C_{d\sigma} C_{-d\sigma'} \rangle \sum_p C_{p\sigma}^+ C_{-p\sigma'}^+ \\ + V_{pd} \langle C_{d\sigma}^+ C_{-d\sigma'}^+ \rangle \sum_p C_{-p\sigma'} C_{p\sigma} + V_{pd} \langle C_{-p\sigma'} C_{p\sigma} \rangle \sum_d C_{d\sigma}^+ C_{-d\sigma'}^+ \quad \dots(4)$$

where p and d are momentum labels in the p and d bands, respectively with energies ϵ_p and ϵ_d ; μ is the common chemical potential. Each band has its proper pairing interaction V_{pp} and V_{dd} , while the pair interchange between the two bands is assured by V_{pd} term.

We have assumed $V_{pd} = V_{dp}$, and we define the following quantities :

$$\epsilon_p = \epsilon_p^0 - \mu \quad \epsilon_d = \epsilon_d^0 - \mu \\ \Delta_{pp}^+ = V_{pp} \langle C_{p\sigma}^+ C_{-p\sigma'}^+ \rangle \quad \Delta_{dd}^+ = V_{dd} \langle C_{d\sigma} C_{-d\sigma'} \rangle \\ \Delta_1^+ = V_{pd} \langle C_{p\sigma}^+ C_{-p\sigma'}^+ \rangle \quad \Delta_2^+ = V_{pd} \langle C_{d\sigma}^+ C_{-d\sigma'}^+ \rangle \quad \dots(5)$$

Now H_{pd} in equation (1) read as

$$H_{pd} = \Delta_1^+ \sum_d C_{-d\sigma'} C_{d\sigma} + \Delta_2^+ \sum_p C_{-p\sigma'}^+ C_{p\sigma}^+ + \Delta_2^+ \sum_p C_{-p\sigma'} C_{p\sigma} + \Delta_1 \sum_d C_{d\sigma}^+ C_{-d\sigma'}^+ \quad \dots(6)$$

We study the Hamiltonian (1) with the Green's function technique and following the equation of motion method.

Green's functions

In order to study the physical properties, we define the following normal and anomalous Green's functions⁶⁻¹⁵ :

$$\begin{aligned}
 \text{(a)} \quad G_p(p, \tau - \tau') &= -\langle T_\tau C_{p\sigma}(\tau) C_{p\sigma}^+(\tau') \rangle \\
 \text{(b)} \quad G_d(d, \tau - \tau') &= -\langle T_\tau C_{d\sigma}(\tau) C_{d\sigma}^+(\tau') \rangle \\
 \text{(c)} \quad f_p(p, \tau - \tau') &= \langle T_\tau C_{-p\sigma}(\tau) C_{p\sigma}(\tau') \rangle \\
 \text{(d)} \quad f_d(d, \tau - \tau') &= \langle T_\tau C_{-d\sigma}(\tau) C_{d\sigma}(\tau') \rangle \\
 \text{(e)} \quad f_p^+(p, \tau - \tau') &= \langle T_\tau C_{p\sigma}^+(\tau) C_{-p\sigma}^+(\tau') \rangle \\
 \text{(f)} \quad f_d^+(d, \tau - \tau') &= \langle T_\tau C_{d\sigma}^+(\tau) C_{-d\sigma}^+(\tau') \rangle \quad \dots(7)
 \end{aligned}$$

These Green's functions satisfy the following equations:

$$(\omega - \epsilon_p) \langle\langle C_{p\sigma}, C_{p\sigma}^+ \rangle\rangle = \delta_{pp'} - \Delta_p \langle\langle C_{p\sigma}^+, C_{-p\sigma}^+ \rangle\rangle \quad \dots(8)$$

$$(\omega - \epsilon_d) \langle\langle C_{d\sigma}, C_{d\sigma}^+ \rangle\rangle = \delta_{dd'} - \Delta_d \langle\langle C_{d\sigma}^+, C_{-d\sigma}^+ \rangle\rangle \quad \dots(9)$$

$$(\omega - \epsilon_p) \langle\langle C_{-p\sigma'}, C_{p\sigma} \rangle\rangle = -\Delta_p \langle\langle C_{p\sigma}^+, C_{p\sigma} \rangle\rangle \quad \dots(10)$$

$$(\omega - \epsilon_d) \langle\langle C_{-d\sigma'}, C_{d\sigma} \rangle\rangle = -\Delta_d \langle\langle C_{d\sigma}^+, C_{d\sigma} \rangle\rangle \quad \dots(11)$$

$$(\omega + \epsilon_p) \langle\langle C_{p\sigma}^+, C_{-p\sigma}' \rangle\rangle = -\Delta_p \langle\langle C_{p\sigma}, C_{p\sigma}^+ \rangle\rangle \quad \dots(12)$$

$$(\omega + \epsilon_d) \langle\langle C_{d\sigma}^+, C_{-d\sigma}' \rangle\rangle = -\Delta_d \langle\langle C_{d\sigma}, C_{d\sigma}^+ \rangle\rangle \quad \dots(13)$$

$$(\omega + \epsilon_p) \langle\langle C_{p\sigma}^+, C_{p\sigma} \rangle\rangle = \delta_{pp'} - \Delta_p \langle\langle C_{-p\sigma'}, C_{p\sigma} \rangle\rangle \quad \dots(14)$$

$$(\omega + \epsilon_d) \langle\langle C_{d\sigma}^+, C_{d\sigma} \rangle\rangle = \delta_{dd'} - \Delta_d \langle\langle C_{-d\sigma'}, C_{d\sigma} \rangle\rangle \quad \dots(15)$$

To solve the above equations, we have assumed

$$(\Delta_{pp} + \Delta_2) = \Delta_p \quad \text{and} \quad \Delta_p^+ \cong \Delta_p$$

$$(\Delta_{dd} + \Delta_1) = \Delta_d \quad \text{and} \quad \Delta_d^+ \cong \Delta_d$$

Then

$$(\Delta_{pp}^+ + \Delta_2^+) = \Delta_p^+ \cong \Delta_p$$

$$(\Delta_{dd}^+ + \Delta_1^+) = \Delta_d^+ \cong \Delta_d \quad \dots(16)$$

Finally, one obtains the Green's functions by solving coupled equations (8) to (15) as :

Green's function for p-holes

$$\langle\langle C_{p\sigma}^+ , C_{-p\sigma'}^+ \rangle\rangle = \frac{-\Delta_p}{(\omega^2 - E_p^2)} \quad \dots(17)$$

$$\langle\langle C_{p\sigma}^+ , C_{p\sigma} \rangle\rangle = \frac{(\omega - \epsilon_p)}{(\omega^2 - E_p^2)} \quad \dots(18)$$

Green's function for d-holes

$$\langle\langle C_{d\sigma}^+ , C_{-d\sigma'}^+ \rangle\rangle = \frac{-\Delta_d}{(\omega^2 - E_d^2)} \quad \dots(19)$$

$$\langle\langle C_{d\sigma}^+ , C_{d\sigma} \rangle\rangle = \frac{(\omega - \epsilon_d)}{(\omega^2 - E_d^2)} \quad \dots(20)$$

The Correlation Functions

We obtain the correlation functions for the Green's functions given by equations (17) and (18) as¹⁰⁻¹⁴ -

$$\langle C_{p\sigma}^+ C_{-p\sigma'}^+ \rangle = \frac{-\Delta_p}{(\alpha_1 - \alpha_2)} [f(\alpha_1) - f(\alpha_2)] \quad \dots(21)$$

Where

$$\alpha_1 = +\sqrt{\epsilon_p^2 + \Delta_{pp}^2 + \Delta_2^2 + \Delta_{pp}^+ \Delta_2 + \Delta_2^+ \Delta_{pp}} = +\sqrt{\epsilon_p^2 + \Delta_p^2},$$

$$\alpha_2 = -\sqrt{\epsilon_p^2 + \Delta_{pp}^2 + \Delta_2^2 + \Delta_{pp}^+ \Delta_2 + \Delta_2^+ \Delta_{pp}} = -\sqrt{\epsilon_p^2 + \Delta_p^2} \quad \dots(22)$$

and $f(\alpha_1)$ and $f(\alpha_2)$ are Fermi functions.

$$\langle C_{p\sigma}^+ C_{p\sigma} \rangle = f(\alpha_2) + \left[\frac{\alpha_1 - \epsilon_p}{(\alpha_1 - \alpha_2)} \right] [f(\alpha_1) - f(\alpha_2)] \quad \dots(23)$$

Similarly, correlation functions for Green's functions (19) and (20) for d holes are obtained.

One can define the two superconducting order parameters related to the correlation functions corresponding to Green's functions $\langle\langle C_{p\sigma}^+, C_{-p\sigma'}^+ \rangle\rangle$ and $\langle\langle C_{d\sigma}^+, C_{-d\sigma'}^+ \rangle\rangle$ for p and d holes, respectively. In a similar manner, free energy and critical magnetic field can also be defined related to both p and d holes.

Superconducting Order Parameters

Gap parameter Δ is the superconducting order parameter, which can be determined self consistently from the gap equation. We obtained the superconducting order parameter for p and d holes as below:

(1) For p holes

$$\frac{1}{|V_{pp}|N(0)} = \int_0^{\hbar\omega_p} d\epsilon_p \frac{1}{(\alpha_1 - \alpha_2)} \left[\tanh\left(\frac{\beta\alpha_1}{2}\right) - \tanh\left(\frac{\beta\alpha_2}{2}\right) \right] \quad \dots(24)$$

(2) For d holes: In a similar manner, we can obtain the expression for superconducting order parameter for d holes.

$$\frac{1}{|V_{dd}|N(0)} = \int_0^{\hbar\omega_d} d \in_d \frac{1}{(\alpha_1 - \alpha_2)} \left[\tanh\left(\frac{\beta\alpha_1}{2}\right) - \tanh\left(\frac{\beta\alpha_2}{2}\right) \right] \quad \dots(25)$$

We observe that expressions (24) and (25) reduces to standard BCS¹⁶.

$$\alpha_1 = +\sqrt{\epsilon_d^2 + \Delta_{dd}^2 + \Delta_1^2 + \Delta_{dd}^+ \Delta_1 + \Delta_1^+ \Delta_{dd}} = +\sqrt{\epsilon_d^2 + \Delta_d^2}$$

and

$$\alpha_2 = -\sqrt{\epsilon_d^2 + \Delta_{dd}^2 + \Delta_1^2 + \Delta_{dd}^+ \Delta_1 + \Delta_1^+ \Delta_{dd}} = -\sqrt{\epsilon_d^2 + \Delta_d^2} \quad \dots(26)$$

Where α_1 and α_2 for p holes is given by (22) and for d holes is given by (26).

Using equations (24) and (25), one can study the behavior of superconducting order parameter with temperature for both; p and d holes.

Dependences of Superconducting Gaps on

Temperature (T) and Carrier Concentration on (T_C)

One can study the dependence of T_C on the hole concentration n_h and chemical potential (μ) for the system YBa₂Cu₃O_{7-x} from this model. The effective chemical potential (μ) corresponds to the average carrier concentration (n_h). The maximum of T_C (n_h) corresponds to chemical potential (μ) lying in the common region of both bands roughly in the middle between E_o and E_c.

From two band model, one can study the dependence of the superconducting transition temperature on the hole concentration determined by chemical potential (μ) by studying:

- (a) Dependence of chemical potential (μ) on critical temperature T_C.
- (b) Variation of hole concentration (n_h) with T_C.

Dependence of Chemical Potential (μ) on Critical Temperature T_C

We calculate the superconducting transition temperature T_C for E_o < μ < E_c,

In Matrix form, superconducting order parameter can be written as⁵ -

$$\bar{\Delta}_i = \sum_j V_{ij} G(\bar{\Delta}_j) \bar{\Delta}_j \quad \dots(27)$$

Where i and j represent p and d holes. There are two superconducting gaps for p and d holes in our interband model.

The expressions for the dependence of superconducting gaps at $T \rightarrow T_C$ on the hole concentration can be derived.

One can write the equations for superconducting gaps for p and d holes as follows -

$$\Delta_p = V_{pd} N_d(0) \Delta_d \int \frac{d \epsilon_d}{\sqrt{\epsilon_d^2 + \Delta_d^2}} \tanh \frac{\sqrt{\epsilon_d^2 + \Delta_d^2}}{2k_B T_C} \quad \dots(28)$$

$$\Delta_d = V_{dp} N_p(0) \Delta_p \int \frac{d \epsilon_p}{\sqrt{\epsilon_p^2 + \Delta_p^2}} \tanh \frac{\sqrt{\epsilon_p^2 + \Delta_p^2}}{2k_B T_C} \quad \dots(29)$$

Where V_{pp} and V_{dd} are pairing interaction of p and d bands, respectively, while the pair interchange between the two bands is assured by the V_{pd} term. The quantity V_{pd} has been supposed to be operative and constant in the energy interval for higher band and lower band, keeping in mind the integration ranges, the gap order parameter satisfy the system.

Since $-V_{pp} \sim V_{dd} \ll V_{pd}$, so V_{pp} and V_{dd} can be neglected.

On further simplification of equations (28) and (29), one obtains

$$V_{pd} V_{dp} N_p(0) N_d(0) \int \frac{d \epsilon_d}{\sqrt{\epsilon_d^2 + \Delta_d^2}} \tanh \frac{\sqrt{\epsilon_d^2 + \Delta_d^2}}{2k_B T_C} \times \int \frac{d \epsilon_p}{\sqrt{\epsilon_p^2 + \Delta_p^2}} \tanh \frac{\sqrt{\epsilon_p^2 + \Delta_p^2}}{2k_B T_C} = 1 \quad \dots(30)$$

At $T = T_C$ $\Delta_{p,d}(T_C) = 0$, so equation (30) takes the form

$$V_{pd} V_{dp} N_p(0) N_d(0) \int \frac{d\epsilon_d}{\epsilon_d} \tanh \frac{\epsilon_d}{2k_B T_C} \times \int \frac{d\epsilon_p}{\epsilon_p} \tanh \frac{\epsilon_p}{2k_B T_C} = 1$$

We have assumed that $V_{pd} = V_{dp}$

$$V_{pd}^2 N_p(0) N_d(0) \int \frac{d\epsilon_d}{\epsilon_d} \tanh \frac{\epsilon_d}{2k_B T_C} \times \int \frac{d\epsilon_p}{\epsilon_p} \tanh \frac{\epsilon_p}{2k_B T_C} = 1 \quad \dots(31)$$

Dependence of Hole Concentration (n_h) on Critical Temperature (T_C)

Konsin and coworkers^{3,17-20} studied the dependence of carrier concentration on T_C .

For studying the doping dependence on the chemical potential, we have [3, 21]—

$$\rho_1 \int_0^{E_1} f(E) dE + \rho_2 \int_{E_0}^{E_C} f(E) dE = p \quad \dots(32)$$

Here $f(E) = \{\exp [(E-\mu)/k_B T] + 1\}^{-1}$, p is the number of holes per cell and E_1 is the width of the broad band.

Using the condition of electroneutrality, we obtain the equation for the chemical potential as³-

$$\rho_1 \left[E_1 - k_B T \log \left(\frac{1 + \exp\left(\frac{E_1 - \mu}{k_B T}\right)}{1 + \exp\left(\frac{-\mu}{k_B T}\right)} \right) \right] + \rho_2 \left[E_C - E_0 + k_B T \log \left(\frac{1 + \exp\left(\frac{E_0 - \mu}{k_B T}\right)}{1 + \exp\left(\frac{E_C - \mu}{k_B T}\right)} \right) \right] = p \quad \dots(33)$$

Where p is the total number of holes per cell.

The relation connecting n_h and p reads as

$$n_h = p - p_0, \text{ where } p_0 = \rho_1 \left(\frac{E_1}{2} \right).$$

Dependence of Chemical Potential Shift ($\Delta\mu$) on Hole Concentration (n_h)

We have calculated the hole concentration dependence of the chemical potential shift $\Delta\mu$ for our system $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ with the same fitting parameters used in calculation of hole concentration.

According to Konsin and Sorkin²¹, the pseudogap E_{pg} induces the shift of the chemical potential through the dependence of the density of states ρ_1 on E_{pg} . As a result, the electron chemical potential shift with doping is obtained as -

$$\Delta\mu(n_h) = \mu(n_h) + \frac{E_1}{2} \quad \dots(34)$$

The chemical potential equals -

$$\mu(n_h) = -\mu_0(n_h) - E_{pg}(n_h) + E_{pg}(0) \quad \dots(35)$$

Where

$$\mu_0(n_h) = \frac{1}{(\rho_1 + \rho_2)} \left(n_h + \rho_2 E_0 + \frac{1}{2} \rho_1 E_1 \right) \quad \dots(36)$$

$$E_{pg}(n_h) = 0.13 (1 - n_h/n_{hcr}) \text{ eV at } 0.19 \leq n_h \leq 2.058 \quad \dots(37)$$

The dependence of $E_{pg}(n_h)$ is derived from electronic specific heat. We obtained critical concentration for our system $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ is $n_{hcr} \approx 2.058$ and $E_{pg}(0) \sim 0.3$ eV.

The calculated doping dependences of the chemical potential shifts $\Delta\mu(n_h)$ for our system $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ is presented in Figure 5 and theoretical predicted values are shown in Table 6.

In under-doped and optimally-doped regions, the chemical potential shift $\Delta\mu(n_h)$ is strongly suppressed by the pseudogap $E_{pg}(n_h)$ up to $n_{hcr} \approx 2.058$.

The parameters are model dependent for the calculation of $\Delta\mu(n_h)$ and $T_C(n_h)$, but the good agreement of the theoretical and experimental curves of $T_C(n_h)$ and $\Delta\mu(n_h)$ for $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ is obtained.

As follows from our calculations at low temperatures, the shift $\Delta\mu(n_h)$ in $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ is unaffected by the pseudogap. The influence of the pseudogap $E_{pg}(0)$ on the superconducting transition temperature is weak because the contributions of $E_{pg}(0)$ to the chemical potential μ and to the gaps $\Delta_{p,d}$ are approximately compensated for in the equation of T_C .

Physical Properties of Superconductors

Electronic Specific heat (C_{es})

The electronic specific heat per atom of a superconductor is determined.^{10-15,22}

For p holes

We obtain –

$$C_{es}^p = \frac{2N(0)}{N} \int_0^{\hbar\omega_p} d\epsilon_p \left\{ \frac{\beta \epsilon_p \alpha_2 \exp(\beta\alpha_2)}{T \{\exp(\beta\alpha_2) + 1\}^2} + \frac{\beta(\alpha_1 - \epsilon_p) \epsilon_p}{2T \sqrt{\epsilon_p^2 + \Delta_{pp}^2 + \Delta_2^2 + \Delta_{pp}^+ \Delta_2^+ + \Delta_2 \Delta_{pp}^+}} \right. \\ \left. \left[\frac{\alpha_1 \exp(\beta\alpha_1)}{\{\exp(\beta\alpha_1) + 1\}^2} - \frac{\alpha_2 \exp(\beta\alpha_2)}{\{\exp(\beta\alpha_2) + 1\}^2} \right] \right\} \quad \dots(38)$$

Where α_1 and α_2 are given by equation (22).

For d holes

Similarly, one can write the expression for electronic specific heat C_{es}^d for d holes, as-

$$C_{es}^d = \frac{2N(0)}{N} \int_0^{\hbar\omega_d} d\epsilon_d \left\{ \frac{\beta \epsilon_d \alpha_2 \exp(\beta\alpha_2)}{T \{\exp(\beta\alpha_2) + 1\}^2} + \frac{\beta(\alpha_1 - \epsilon_d) \epsilon_d}{2T \sqrt{\epsilon_d^2 + \Delta_{dd}^2 + \Delta_1^2 + \Delta_{dd}^+ \Delta_1^+ + \Delta_1 \Delta_{dd}^+}} \right. \\ \left. \left[\frac{\alpha_1 \exp(\beta\alpha_1)}{\{\exp(\beta\alpha_1) + 1\}^2} - \frac{\alpha_2 \exp(\beta\alpha_2)}{\{\exp(\beta\alpha_2) + 1\}^2} \right] \right\} \quad \dots(39)$$

Where α_1 and α_2 are given by equation (26).

The jumps of specific heat at $T = T_C$ is obtained as -

$$C_{es} - C_{en} = \Delta C = 9.42 R k_B^2 T_C \quad \dots(40)$$

Where R is given by

$$R = \frac{1}{2} [\rho_1 \gamma_1^2 + \rho_2 \gamma_2^2] \quad \Gamma_3 < \mu < \Gamma_{2,4}$$

$$\gamma_1 = \left\{ \frac{1 + \kappa \log^2 [(\mu - \Gamma_1)(\Gamma_2 - \mu) 4\gamma^2 (k_B T_C \pi)^{-2}]}{1 + \kappa^2 \beta \log^4 [(\mu - \Gamma_1)(\Gamma_2 - \mu) 4\gamma^2 (k_B T_C \pi)^{-2}]} \right\}^{1/2}$$

$$\gamma_2 = \left\{ \frac{1 + \kappa \log^2 [(\mu - \Gamma_3)(\Gamma_4 - \mu) 4\gamma^2 (k_B T_C \pi)^{-2}]}{1 + \kappa^2 \beta^{-1} \log^4 [(\mu - \Gamma_3)(\Gamma_4 - \mu) 4\gamma^2 (k_B T_C \pi)^{-2}]} \right\}^{1/2} \quad \dots(41)$$

With $\beta = \rho_1 / \rho_2$ $\kappa = \frac{1}{4} V_{pd}^2 \rho_1 \rho_2$

The specific heat in the normal phase is obtained as

$$C_{en} = \frac{2\pi^2}{3} R_0 k_B^2 T \quad \dots(42)$$

Where R_0 is given by -

$$R_0 = \frac{1}{2} [\rho_1 + \rho_2] \quad \Gamma_3 < \mu < \Gamma_{2,4}$$

One can easily show that the relative jump of the specific heat at $T = T_C$ equals

$$\frac{\Delta C}{C_{en}} = 1.43 \frac{R}{R_0} \quad \dots(43)$$

The ratio $\frac{R}{R_0}$ characterizes the possible deviation of the relative jump of the specific heat in the present model from the BCS one²⁰.

Free Energy

It is well established that the thermal properties of a metal changes sharply as the temperature is allowed to decrease through the transition temperature to a superconducting

state. The entropy decreases remarkably on cooling the superconductors below the critical temperature. The free energy can easily be defined for the superconducting transition as it is related by the entropy, hence it also exhibit a similar behaviour²³. Obviously, the entropy as well as the free energy difference in the normal state is always greater than the entropy in the superconducting state.

$$\frac{F_S - F_N}{V} = \int_0^{\Delta} d\Delta (\Delta^2) \frac{d}{d\Delta} \left(\frac{1}{|V'|N(0)} \right) \quad \dots(44)$$

Where F_S is free energy in superconducting state and F_N is free energy in normal state and V is the volume per unit cell and V' is pairing interaction.

One can write expressions for the free energy difference for p-holes and d-holes separately.

One obtains the final expression for free energy difference as

$$\begin{aligned} \frac{F_S - F_N}{V} = & \frac{\Delta^2}{2|V_{pp}|} - \frac{4N(0)}{2\beta} \int_0^{\hbar\omega_p} d \in_p \left[\log \left(1 + \frac{\beta}{2} \sqrt{\in_p^2 + \Delta_p^2} \right) + e^{-\frac{\beta \sqrt{\in_p^2 + \Delta_p^2}}{2}} \right] \\ & + \frac{2N(0)}{\beta} \int_0^{\hbar\omega_p} d \in_p \left[\log \left(1 + \frac{\beta \in_p}{2} + e^{-\frac{\beta \in_p}{2}} \right) \right] \quad \dots(45) \end{aligned}$$

With the help of the above relation, we can calculate the free energy difference for p-holes.

Similarly, one obtains the free energy difference for d holes as

$$\begin{aligned} \frac{F_S - F_N}{V} = & \frac{\Delta^2}{2|V_{dd}|} - \frac{4N(0)}{2\beta} \int_0^{\hbar\omega_d} d \in_d \left[\log \left(1 + \frac{\beta}{2} \sqrt{\in_d^2 + \Delta_d^2} \right) + e^{-\frac{\beta \sqrt{\in_d^2 + \Delta_d^2}}{2}} \right] \\ & + \frac{2N(0)}{\beta} \int_0^{\hbar\omega_d} d \in_d \left[\log \left(1 + \frac{\beta \in_d}{2} + e^{-\frac{\beta \in_d}{2}} \right) \right] \quad \dots(46) \end{aligned}$$

Where $\alpha_1 = +\sqrt{\in_d^2 + \Delta_d^2}$ and $\alpha_2 = -\sqrt{\in_d^2 + \Delta_d^2}$

Critical Field (H_C)

The critical field H_C (T) called the thermodynamic field for the transition between the normal to superconducting state and is related to the free energy difference is given as,

$$F_S - F_N = \frac{1}{8\pi} \left[\frac{dH_c^2}{dT} \right] \quad \dots(47)$$

Hence, the low temperature critical field is obtained as -

$$H_c = \left[8\pi \left| \left\{ \frac{F_S - F_N}{V} \right\} \right| \right]^{1/2} \quad \dots(48)$$

One can obtain the relation for critical field for both types of holes.

Numerical Calculations

Values of various parameters appearing in equation are given in Table 1. Using these values, we have made study of various parameters for the system $Y Ba_2Cu_3O_{7-x}$.

Table 1: Values of various parameters for $Y Ba_2Cu_3O_{7-x}$

Parameter	Value
*Superconducting transition temperature (T_c)	88 K
* Phonon energy ($\hbar\omega_p$)	$1.6 \times 10^{-21} J$
* Phonon energy ($\hbar\omega_d$)	$1.3 \times 10^{-21} J$
*Density of states at the Fermi surface $N(0)$	$\cong 4.95 \times 10^{19} J/atom$
* Pairing interaction for p holes	$0.32 \times 10^{-19} J/atom$
* Pairing interaction for d holes	$0.38 \times 10^{-19} J/atom$
*Number of electrons per unit cell (n)	$\sim 5 \times 10^{22}$
* Boltzmann constant (k_B)	$1.38 \times 10^{23} J$

Superconducting Order Parameter (Δ)

To study the behavior of superconducting order parameter for the system $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$, one finds following two different situations:

- The superconducting order parameter due to p-holes only,
- The superconducting order parameter due to d-holes only.

The SC Order Parameter for p-Holes

One obtains the expression for Δ_p as -

$$\frac{1}{|V_{pp}|N(0)} = \frac{1}{2} \int_0^{\hbar\omega_p} \frac{d\epsilon_p}{\sqrt{\epsilon_p^2 + \Delta_p^2}} \tanh \frac{\sqrt{\epsilon_p^2 + \Delta_p^2}}{2k_B T_C} \quad \dots(49)$$

Using the following changes in variables $\Delta_p = x \times 10^{-21} \text{ J}$, $\epsilon_p = \hbar\omega_p y$, $d\epsilon_p = \hbar\omega_p dy$ and after simplification, one obtains -

$$0.6302 = \int_0^1 \frac{dy}{\sqrt{y^2 + 0.3906x^2}} \left[\frac{1}{e^{\frac{-116}{T}\sqrt{y^2 + 0.3906x^2}} + 1} - \frac{1}{e^{\frac{116}{T}\sqrt{y^2 + 0.3906x^2}} + 1} \right] \quad \dots(50)$$

Solving equations (50) numerically, one can study the variation of SC order parameter with temperature in the absence of d-holes. The values obtained from equations (50) are depicted in Table 2 and the behavior is shown in Figure 1 for p holes.

Table 2: Dependence of superconducting order parameter (Δ_p) (p-holes) with temperature

S. No	Temperature (K)	$\Delta_p = x \times 10^{-21} \text{ J}$
1	10	2.37
2	20	2.35
3	30	2.33
4	40	2.30

Cont...

S. No	Temperature (K)	$\Delta_p = x \times 10^{-21} J$
5	50	2.20
6	60	2.00
7	70	1.70
8	80	1.20
9	88	0.00

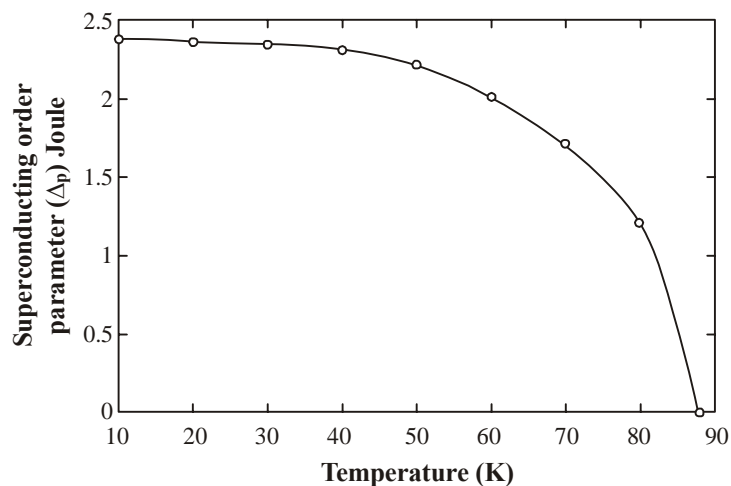


Fig. 1: Behavior of superconducting order parameter (Δ_p) with temperature for p- holes

The SC Order Parameter for d-Holes

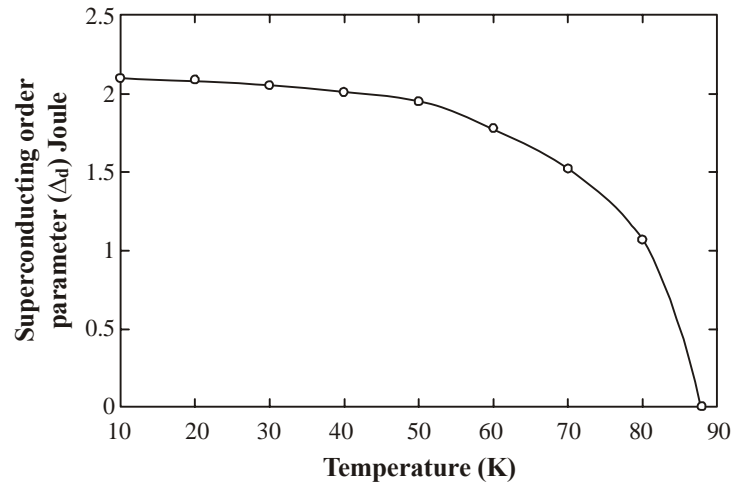
Similarly, one obtains the following expression for superconducting order parameter for d holes -

$$0.5203 = \int_0^1 \frac{dy}{\sqrt{y^2 + 0.7692x^2}} \left[\frac{1}{e \frac{-94.4}{T} \sqrt{y^2 + 0.7692x^2 + 1}} - \frac{1}{e \frac{-94.4}{T} \sqrt{y^2 + 0.7692x^2 + 1}} \right] \dots(51)$$

Solving equation (51), one can study the variation of SC order parameter with temperature in the absence of p-holes. The values obtained from equation (51) are depicted in Table 3 and the behaviour is shown in Figure 2 for d holes.

Table 3: Dependence of superconducting order parameter (Δ_d) (d-holes) with temperature

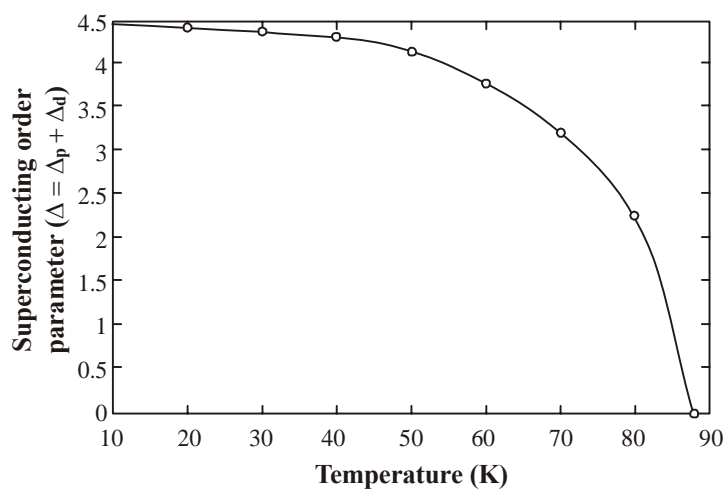
S. No.	Temperature (K)	$\Delta_d = x \times 10^{-21} J$
1	10	2.09
2	20	2.08
3	30	2.05
4	40	2.00
5	50	1.94
6	60	1.77
7	70	1.51
8	80	1.06
9	88	0.00

**Fig. 2: Behavior of superconducting order parameter (Δ_d) with temperature for d – holes.**

One can study the variation of SC order parameter of both; p-holes and d-holes with temperature. The values are depicted in Table 4 and the behaviour is shown in Figure 3 for both p and d holes.

Table 4: Dependence of superconducting order parameter ($\Delta = \Delta_p + \Delta_d$) (for p & d holes) with temperature

S. No.	Temperature (K)	$(\Delta = \Delta_p + \Delta_d) = x \times 10^{-21} J$
1	10	4.46
2	20	4.43
3	30	4.38
4	40	4.30
5	50	4.14
6	60	3.77
7	70	3.21
8	80	2.26
9	88	0.00

**Fig. 3: Behavior of superconducting order parameter ($\Delta = \Delta_p + \Delta_d$) with temperature for p and d – holes**

Electronic Specific Heat

On the basis of equation (40) and (42), one can show that the relative jump of the specific heat at $T = T_C$ equals

$$\frac{\Delta C}{C_{en}} = 1.43 \frac{R}{R_0}$$

The ratio $\frac{R}{R_0}$ characterizes the possible deviation of the relative jump of the specific heat in the present model from the BCS one. The function R reveals only a weak dependence on n_h , it is understandable that the curve ΔC vs n_h is mainly determined by the function $T_C(n_h)$ standing outside the R in the formula for ΔC (40). The resemblance between the dependence of ΔC and T_C on n_h on (c.f. Figure 4 and Figure 6) reflects also this circumstance.

Table 5: Variation of hole concentration (n_h) with critical temperature (T_C) and chemical potential (μ)

S. No	Chemical potential (μ)	Critical temp. (T_C) K	p	$P_0 = \rho_1 \left(\frac{E_1}{2} \right)$	Hole concentration $n_h = p - p_0$
1	1.1	88.30	2.005	1.815	0.19
2	1.2	88.50	2.210	1.815	0.395
3	1.3	88.60	2.415	1.815	0.6
4	1.4	88.50	2.620	1.815	0.805
5	1.5	88.20	2.825	1.815	1.01
6	1.6	87.69	3.030	1.815	1.215
7	1.7	87.00	3.235	1.815	1.42
8	1.8	86.10	3.440	1.815	1.625
9	1.9	85.10	3.645	1.815	1.83
10	2.0	83.70	3.841	1.815	2.026
11	2.1	82.20	3.873	1.815	2.058

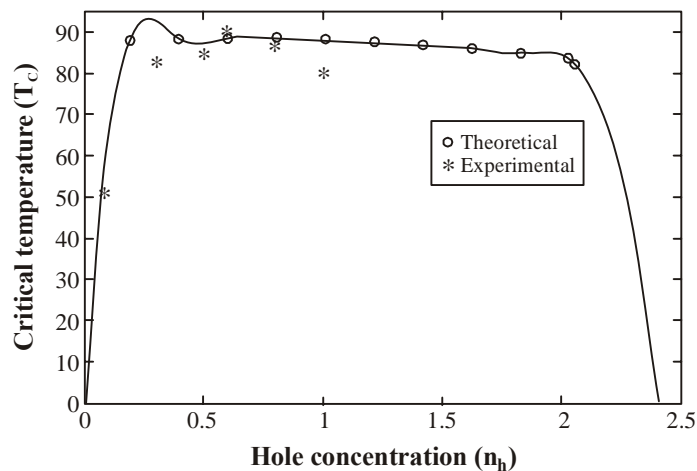


Fig. 4: Variation of hole concentration (n_h) with critical temperature (T_C)

Table 6: Dependence of chemical potential shift $\Delta\mu$ on hole concentration n_h

S. No.	Hole concentration (n_h)	$\mu_o(n_h)$	$E_{pg}(n_h)$	$E_{pg}(O)$	$\mu(n_h)$	$\Delta\mu = \mu(n_h) + \frac{E_1}{2}$
1	0.19	1.183	0.1180	0.3	-1.00	+0.100
2	0.395	1.291	0.1050	0.3	-1.096	+0.0040
3	0.6	1.399	0.0921	0.3	-1.19	-0.090
4	0.805	1.507	0.0791	0.3	-1.286	-0.186
5	1.01	1.614	0.0662	0.3	-1.380	-0.280
6	1.215	1.722	0.0533	0.3	-1.475	-0.3750
7	1.42	1.830	0.0403	0.3	-1.570	-0.4700
8	1.625	1.938	0.0274	0.3	-1.665	-0.5650
9	1.83	2.046	0.0144	0.3	-1.760	-0.6600
10	2.026	2.149	0.0020	0.3	-1.851	-0.7510
11	2.058	2.166	0.00	0.3	-1.866	-0.7660

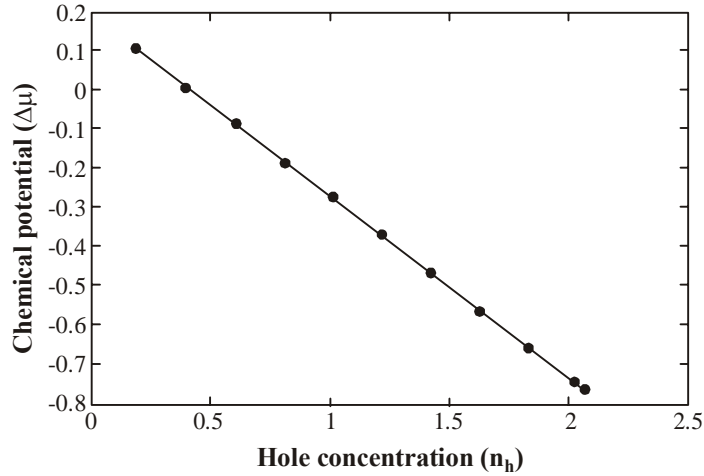


Fig. 5: Dependence of chemical potential shift ($\Delta\mu$) on hole concentration (n_h)

To carry out numerical estimates, we utilize the same sets of fitting parameters as used in T_C calculation written in critical field. The theoretical dependence of ΔC on hole concentration (n_h) for $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ is depicted in Table 7 and behaviour is shown in Fig. 6.

Table 7: Dependence of ΔC with hole concentration n_h

S. No.	Critical temperature (K)	Hole concentration $n_h = p - p_0$	$\Delta C = 9.42 R k_B^2 T_C \times 10^{-6}$	$C_{en} = \frac{2\pi^2}{3} \times R_0 k_B^2 T \times 10^{-6}$
1	88.30	0.19	6.18	4.101
2	88.50	0.395	6.20	4.111
3	88.60	0.6	6.20	4.115
4	88.50	0.805	6.20	4.111
5	88.20	1.01	6.18	4.097
6	87.69	1.215	6.14	4.073
7	87.00	1.42	6.09	4.041
8	86.10	1.625	6.03	3.999
9	85.10	1.83	5.96	3.953
10	83.70	2.026	5.86	3.8880
11	82.20	2.058	---	3.818

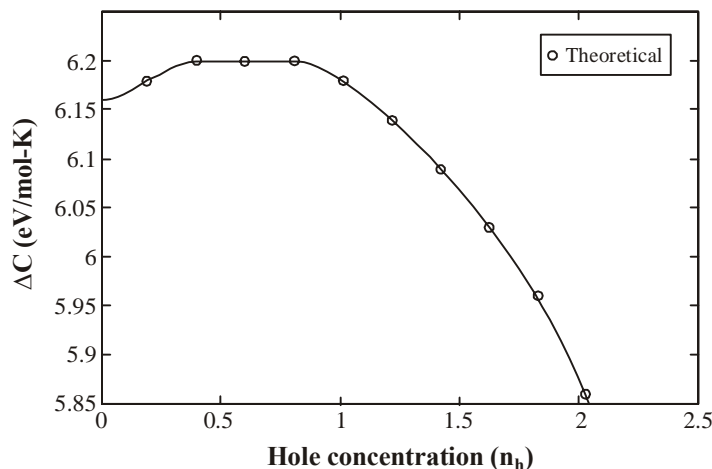


Fig. 6: Dependence of ΔC with hole concentration n_h

Free Energy

The free energy difference for p holes is given in equation (45), making the use of $\epsilon_p = \hbar\omega_p y$, $d\epsilon_p = \hbar\omega_p dy$ and following values from Table 1, one obtains for p holes

$$\begin{aligned} \left(\frac{F_S - F_N}{V}\right)_p &= (1.562 \times 10^{19}) \Delta_p^2 - 0.00011 \times T \int_0^1 1.6 \times 10^{-21} \left[\log \left(1 + \frac{\sqrt{2.56 \times 10^{-42} y^2 + \Delta_p^2}}{2.760 \times 10^{-23} \times T} \right) \right] dy \\ &- (0.00011 \times T) \int_0^1 1.6 \times 10^{-21} \left[\log \left(e^{\frac{\sqrt{2.56 \times 10^{-42} y^2 + \Delta_p^2}}{2.760 \times 10^{-23} \times T}} \right) \right] dy \\ &+ (0.00011 \times T) \int_0^1 1.6 \times 10^{-21} \left[\log \left(1 + 57.9710 \frac{y}{T} + e^{-57.9710 \frac{y}{T}} \right) \right] dy \end{aligned} \quad \dots(52)$$

Similarly for d holes, We obtain form equation (46),

$$\begin{aligned} \left(\frac{F_S - F_N}{V}\right)_d &= (1.315 \times 10^{19}) \Delta_d^2 - 0.00011 \times T \int_0^1 1.6 \times 10^{-21} \left[\log \left(1 + \frac{\sqrt{1.69 \times 10^{-42} y^2 + \Delta_d^2}}{2.760 \times 10^{-23} \times T} \right) \right] dy \\ &- (0.00011 \times T) \int_0^1 1.6 \times 10^{-21} \left[\log \left(e^{\frac{\sqrt{1.69 \times 10^{-42} y^2 + \Delta_d^2}}{2.760 \times 10^{-23} \times T}} \right) \right] dy \\ &+ (0.00011 \times T) \int_0^1 1.3 \times 10^{-21} \left[\log \left(1 + 47.1014 \frac{y}{T} + e^{-47.1014 \frac{y}{T}} \right) \right] dy \end{aligned} \quad \dots(53)$$

The values of free energy difference at various temperatures, obtained from equation (52) are shown in Table 8 and Figure 7 for p holes and obtained from equation (53) shown in Table 9 and Figure 8 for d holes.

Table 8: Variation of free energy difference $\left(\frac{F_S - F_N}{V}\right)_p$ for p-holes with temperature

S. No.	Temperature (K)	$\left(\frac{F_S - F_N}{V}\right)_p \times 10^{-23}$ Joule/mole
1	10	10.21
2	20	9.98
3	30	9.80
4	40	9.58
5	50	8.87
6	60	7.55
7	70	5.80
8	80	3.50
9	88	1.20

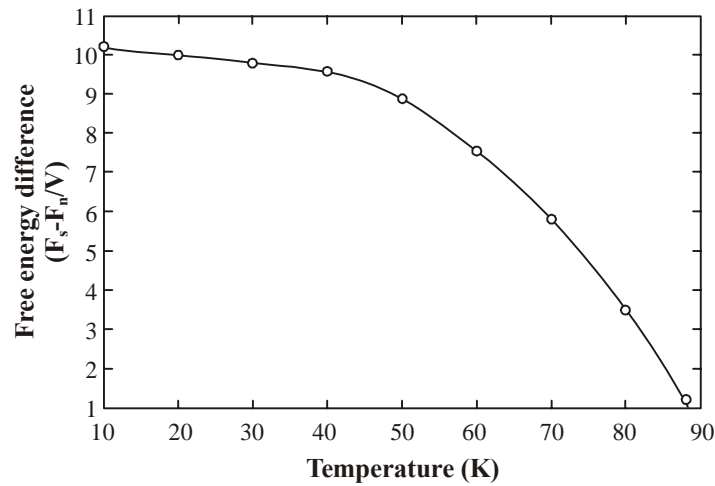


Fig. 7: Variation of free energy difference with temperature for p holes.

Table 9: Variation of free energy difference $\left(\frac{F_S - F_N}{V}\right)_d$ for d-holes with temperature

S. No.	Temperature (K)	$\left(\frac{F_S - F_N}{V}\right)_d \times 10^{-23}$ Joule/mole
1	10	6.752
2	20	6.638
3	30	6.455
4	40	6.193
5	50	5.905
6	60	5.084
7	70	3.968
8	80	2.441
9	88	0.946

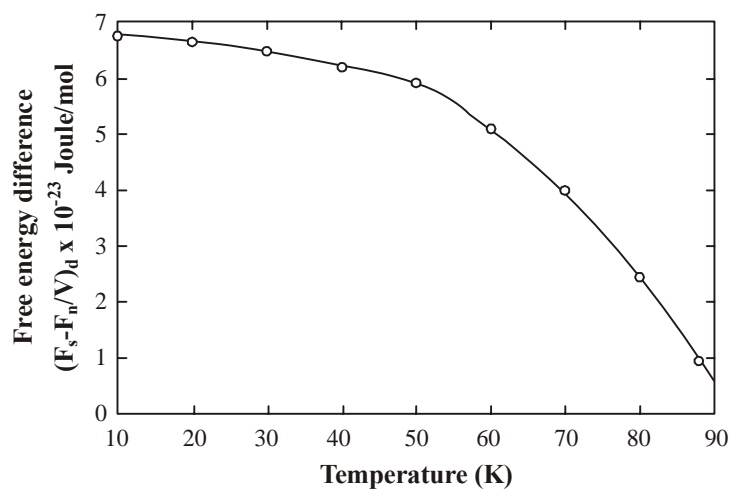


Fig. 8: Variation of free energy difference with temperature for d holes

Critical Field (H_C)

Using the relation (48) and substituting the value of free energy difference from Eq. (52) and (53), one can obtain the relation for critical field for both types of holes.

For p holes, it is

$$(H_c)_p = 8\pi \left[\frac{\Delta^2}{2|V_{pp}|} - \frac{4N(0)}{2\beta} \int_0^{\hbar\omega_p} d \epsilon_p \left[\log \left(1 + \frac{\beta}{2} \sqrt{\epsilon_p^2 + \Delta_p^2} \right) + e^{-\frac{\beta\sqrt{\epsilon_p^2 + \Delta_p^2}}{2}} \right] + \frac{2N(0)}{\beta} \int_0^{\hbar\omega_p} d \epsilon_p \left[\log \left(1 + \frac{\beta \epsilon_p}{2} + e^{-\frac{\beta \epsilon_p}{2}} \right) \right] \right]^{\frac{1}{2}} \dots(54)$$

and for d holes,

$$(H_c)_d = 8\pi \left[\frac{\Delta^2}{2|V_{dd}|} - \frac{4N(0)}{2\beta} \int_0^{\hbar\omega_d} d \epsilon_d \left[\log \left(1 + \frac{\beta}{2} \sqrt{\epsilon_d^2 + \Delta_d^2} \right) + e^{-\frac{\beta\sqrt{\epsilon_d^2 + \Delta_d^2}}{2}} \right] + \frac{2N(0)}{\beta} \int_0^{\hbar\omega_d} d \epsilon_d \left[\log \left(1 + \frac{\beta \epsilon_d}{2} + e^{-\frac{\beta \epsilon_d}{2}} \right) \right] \right]^{\frac{1}{2}} \dots(55)$$

The relation (54) and (55) are reducible to standard BCS relation.

The values of critical field at various temperatures, obtained from equation (54) are shown in Table 10 and Figure 9 for p holes and obtained from equation (55) are shown in Table 11 and Figure 10 for d holes.

Table 10: Variation of critical field (H_C) for p-holes

S. No.	Temperature (K)	Critical field ($H_C \times 10^{-11}$) _p Tesla
1	10	5.064
2	20	5.006
3	30	4.961
4	40	4.905
5	50	4.720
6	60	4.354
7	70	3.817
8	80	2.965
9	88	1.736

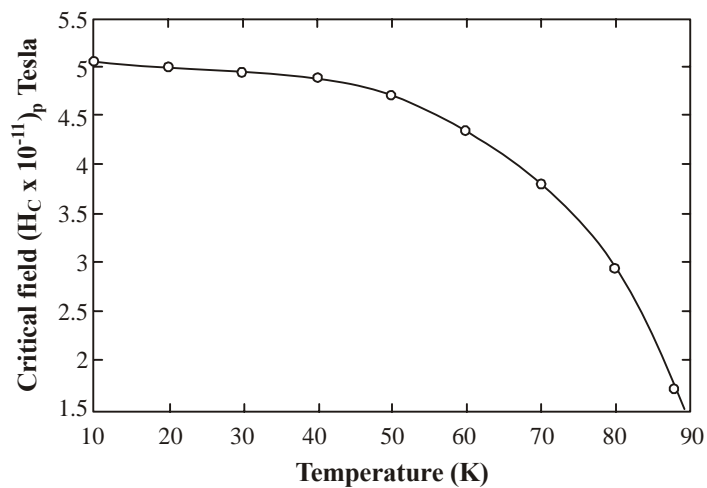


Fig. 9: Variation of critical field with temperature for p holes

Table 11: Variation of critical field (H_C) for d-holes

S. No.	Temperature (K)	Critical Field ($H_C \times 10^{-11}$) _d Tesla
1	10	4.118
2	20	4.083
3	30	4.026
4	40	3.947
5	50	3.851
6	60	3.573
7	70	3.157
8	80	2.476
9	88	1.541

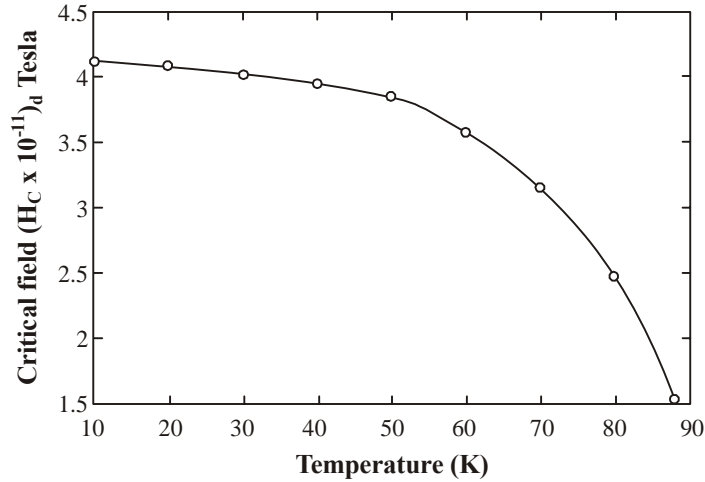


Fig. 10: Variation of critical field with temperature for d holes

Dependence of Chemical Potential (μ) on Critical Temperature (T_C):

For $YBa_2Cu_3O_{7-x}$ superconductors, we used the best fitting parameters value for numerical estimation:

$$N_p(0) = \text{Density of states for p holes} = 1.65 \text{ eV}^{-1},$$

$$N_d(0) = \text{Density of states for d holes} = 0.25 \text{ eV}^{-1},$$

$$V_{pd} = \text{The pair interchange between the two bands} = 1.80 \text{ eV},$$

$$E_c = \text{Cut-off energy of lower band} = 2.1 \text{ eV},$$

$$E_1 = \text{Top energy of higher band} = 2.2 \text{ eV},$$

$$E_0 = \text{Top energy of lower band} = 1.0 \text{ eV},$$

$$\hbar\omega_p = 1.6 \times 10^{-21} \text{ Joule} = 0.01 \text{ eV},$$

$$\hbar\omega_d = 1.3 \times 10^{-21} \text{ Joule} = 0.00812 \text{ eV}.$$

The small difference between E_c and E_0 is taken keeping in mind the uncertainty in defining the effective bottom of the band E_c .

The parameters are model dependent for the calculation of T_C (n_h). These quantitative characteristic seem to be reasonable at least they are of the order proposed^{3,21} for high T_C cuprates.

Making use of $\epsilon_p = \hbar\omega_p y$, $d \epsilon_p = \hbar\omega_p dy$ and $\epsilon_d = \hbar\omega_d y$, $d \epsilon_d = \hbar\omega_d dy$, with above parameters and limits of integration on equation (31), for dependence of critical temperature (T_C) on chemical potential dependence (μ), one obtains

$$1.336 \int_{-\mu}^{2.1-\mu} \frac{dy}{y} \tanh\left(\frac{0.01}{2 \times 0.00008625 \times T_C}\right) \times \int_{1.0-\mu}^{2.1-\mu} \frac{dy}{y} \tanh\left(\frac{0.00812}{2 \times 0.00008625 \times T_C}\right) = 1 \quad \dots(56)$$

Solving numerically equation (56), we get Table 5 for critical temperature (T_C) with respect to different doping parameters (μ) in interval $E_o < \mu < E_C$.

Dependence of Carrier Concentration (n_h) with Critical Temperature T_C

By substituting numerical values of chemical potential μ and critical temperature T_C in equation (33) with fitting parameters, we get dependence of carrier concentration n_h on critical temperature T_C .

The calculated dependence of carrier concentration (n_h) on critical temperature T_C for system $YBa_2Cu_3O_{7-x}$ is shown in Table 5 and depicted in Fig. 4.

DISCUSSION AND CONCLUSIONS

We have made a study of photo-induced high T_C cuprate superconductivity by canonical two-band BCS Hamiltonian containing a Fermi surface of p and d holes. Following Green's function techniques and equation of motion method, we have shown that the system possess two superconducting gaps. It is also evident from the study that the system admits a precursor phase of Cooper pair droplets that undergoes a phase locking transition at a critical temperature below the mean field solution⁵.

In the two-component model, the superconductivity is caused by the interband repulsive electron-lattice and Coulomb interaction. The photoexcitation produces a change of the hole doping (p) and as a result, there is shift ΔT_C of the high temperature cuprate superconductors.

We have made self-consistent studies of the doping dependences of superconducting transition temperature (T_C) and chemical potential (μ) shift in $YBa_2Cu_3O_{7-x}$. Study reveals that the phase space for pair-transfer scattering between the overlapping bands is governed by the position of chemical potential, i.e. the dependence of the electron chemical potential shift of n_h regulates the phase shift for pair transfer scattering between the overlapping band and narrow bands and leads to the observed doping dependences of T_C . Experiments clearly

lend support to the proposed doping dependence of $\Delta\mu(n_h)$ and $T_C(n_h)$ in the compound $YBa_2Cu_3O_{7-x}$. The fitting of the theory with experimental data shows one of the participating hole bands to be narrow, as expected from theory.

According to our model, there are two superconducting gaps on the system $YBa_2Cu_3O_{7-x}$ and temperature dependences of these gaps are of BCS type.

We have also obtained the free energy expression and critical magnetic field, which shows that in the interband model, the superconducting state is stable at $T > T_C$. The model fairly explains the observed features in $YBa_2Cu_3O_{7-x}$.

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