

Hole distribution and T_c suppression in $Y_{1-x}Pr_xBa_2Cu_3O_7$

Yabin Yu*

*Department of Physics, Zhejiang University, Hangzhou 310027, People's Republic of China
and Department of Physics, Yantai University, Yantai 264005, People's Republic of China*

Guanghan Cao and Zhengkuan Jiao

*Department of Physics, Zhejiang University, Hangzhou 310027, People's Republic of China
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A model Hamiltonian, which includes the components of the CuO_2 planes, CuO_3 chains, and the Pr-O hybridization, is considered to describe the electronic structure of $Y_{1-x}Pr_xBa_2Cu_3O_7$. We make the coherent-potential approximation calculation for the Hamiltonian to present the variation of the distribution of the holes against the Pr concentration. The results show that the hole transfer is mainly from the $pd\sigma$ band to the $p-f$ hybridization band, and a small reduction of the holes residing on the CuO_3 chains is caused by the Pr doping. A metal-nonmetal transition around $x=0.5$ can be obtained according to our calculation. We present a quantitative interpretation for the T_c suppression in terms of the combination of hole-transfer and magnetic scattering effects. Moreover, the enhancement of the magnetic pair breaking due to the presence of a normal-state pseudogap is also considered. Consequently, we give a satisfactory explanation of T_c suppression for the whole Pr-doping region. [S0163-1829(99)13701-9]

I. INTRODUCTION

Since the discovery of nonsuperconducting and nonmetallic $PrBa_2Cu_3O_7$ compounds,¹ many efforts have been made on the $Y_{1-x}Pr_xBa_2Cu_3O_7$ system in an attempt to understand the mechanism of the superconductivity suppression of Pr doping.²⁻¹² It has been experimentally shown that upon substituting Pr into the system, T_c decreases monotonically and vanishes at a critical concentration $x_{cr} \approx 0.55$, near the metal-nonmetal transition.^{1,2,8} As for $R_{1-x}Pr_xBa_2Cu_3O_7$ (R refers to the rare-earth elements) system, the T_c suppression is R -ion-size dependent: The larger the atomic size of the rare-earth elements in the host compounds is, the stronger the T_c suppression becomes.^{9,10}

The substitution effect of Y by Pr on T_c has been widely investigated theoretically, and many explanations have been proposed.¹²⁻¹⁴ Early explanations¹² involved either hole filling or the influence of Pr^{3+} spin on the CuO_2 planes. The former, assuming the valance state Pr^{4+} , considers that the itinerant holes in the CuO_2 planes are transferred to the Pr sites, leading to the quenching of superconductivity and a metal-nonmetal transition at x_{cr} . However, some direct experiments indicated that the Pr valance is mainly $+3$.²⁻⁴ The latter, assuming the valance state Pr^{3+} , considers that Pr^{3+} spins break the superconducting Cooper pairs. But this idea fails to explain the metal-nonmetal transition. The relatively satisfactory models for the explanation of the T_c suppression are that of Fehrenbacher and Rice (FR),¹³ and Liechtenstein and Mazin (LM).¹⁴ The FR model assumes hole depletion in the CuO_2 planes, not because of higher Pr valance, but because of transfer of the holes from the Cu-O $pd\sigma$ band into the O2p-Pr4f hybridization state. FR suggested that the $p-f$ hybridization bandwidth is small due to the orthogonality of the involved orbital on shared O sites of neighboring Pr cubes. The combination of the small bandwidth with a strong

coupling to spin degree of freedom and with a potential disorder renders the $p-f$ band localized. They assumed that the CuO_3 chains are intrinsically metallic, and ascribed the absence of metallic conductivity to oxygen disorder. This has been supported by experiments.¹¹ Although the FR model has been supported by many experiments, and resolves the controversy on the different valance values of the Pr ion obtained from different measurements,² it still fails to explain some experimental observations. One of the failures of the FR model is that it cannot explain the R -ion-size dependence of the T_c suppression.¹⁴ In addition, an important conclusion of FR is that there are only two stable solutions for the hole distribution in their model: $n_p=0$ or $n_p=(1-n_{ch})/2$ (n_p is the hole density in the CuO_2 planes, and n_{ch} is the hole density in the CuO_3 chains). They suggested that the parameters of their model are favorable for the solution $n_p=0$ in the $PrBa_2Cu_3O_7$ and for the solution $n_p=(1-n_{ch})/2$ in $RBa_2Cu_3O_7$. However, when the FR model is applied to the intermediate doping regime of $Y_{1-x}Pr_xBa_2Cu_3O_7$, one immediately find that there should be a critical value of x , below which the hole density in the CuO_2 planes is not affected by the Pr doping. This is not in agreement with the experiments. Liechtenstein and Mazin¹⁴ extended the FR model, and showed that the R -O hybridization forms a dispersive band (called the FR band in Ref. 14). They concluded that only in $PrBa_2Cu_3O_7$ does this FR band disperse across the Fermi level and hence compete for holes with the Cu-O $pd\sigma$ band. For the different rare-earth elements in $R_{1-x}Pr_xBa_2Cu_3O_7$, the position of the FR band varies with the atomic number of the rare earth through the 4f energy level. Using their extended model, LM presented the number of the holes grabbed by the FR band as a function of the Pr concentration in $Y_{1-x}Pr_xBa_2Cu_3O_7$, and $Nd_{1-x}Pr_xBa_2Cu_3O_7$, and explained the fact that Pr doping suppresses T_c in $Nd_{1-x}Pr_xBa_2Cu_3O_7$ more strongly than in $Y_{1-x}Pr_xBa_2Cu_3O_7$.

Another important fact is that the amount of holes in the CuO_3 chains does not change with the increasing Pr doping, which is phenomenologically assumed in both the FR and LM models. According to the LM model, the number of states above the Fermi level in the FR band is the number of depleted holes in the CuO_2 planes. However, based on band-calculation^{15,16} and x-ray-absorption measurement,^{17,18} it has been shown that the O $2p$ holes near the Fermi level in $\text{YBa}_2\text{Cu}_3\text{O}_7$ are distributed in the CuO_2 planes and the CuO_3 chains. So, the hole depletion takes place not only in the CuO_2 planes but also in the CuO_3 chains. In fact, recent experiments^{19–21} indicated that a small reduction of the hole concentration is caused by Pr doping in $\text{Y}_{1-x}\text{Pr}_x\text{Ba}_2\text{Cu}_3\text{O}_7$.

The aim of this paper is to investigate the hole-density distribution among the CuO_2 planes, CuO_3 chains and the FR band, and then study the suppression of T_c in the $\text{Y}_{1-x}\text{Pr}_x\text{Ba}_2\text{Cu}_3\text{O}_7$ system. To do this, we consider a model Hamiltonian in which the electronic structure of the CuO_2 planes and CuO_3 chains, and the Pr-O hybridization are all included. Here, following LM we describe the FR band by employing a three-band model; using the planar singlet-hole spectrum given by Dagotto *et al.*,²² we describe the electronic structure of the $pd\sigma$ band in the CuO_2 planes; according to Ref. 15 we give the electronic structure in the CuO_3 chains. In Ref. 14, Liechtenstein and Mazin already suggested that the coherent-potential approximation calculation should be made to study the behavior of the system at the intermediate Pr doping, by assuming disorder on the R sites (for $R = \text{Y}$, the $4f$ energy level is to be taken infinity). Following from this idea we make the coherent-potential approximation calculation for our model Hamiltonian to give the Pr-doping dependence of the hole distribution. In the study of the T_c suppression, following our previous work,²³ we consider the combination of hole depletion with the magnetic pair breaking of Pr ions. With increasing Pr concentration the system would evolve into the under-hole-doping region, so we also consider that the pair breaking is enhanced by the appearance of the normal-state pseudogap.²⁴ Therefore, we succeed in quantitatively understanding the whole T_c suppression in the $\text{Y}_{1-x}\text{Pr}_x\text{Ba}_2\text{Cu}_3\text{O}_7$ system.

By the way, several authors^{25–27} reported the observation of superconductivity in $\text{PrBa}_2\text{Cu}_3\text{O}_7$. But it has not been confirmed widely, and the experimental data²⁵ indicated that the superconducting samples are strong inhomogeneous. The difference of the crystal structure between the superconducting and nonsuperconducting samples is not yet clear. On the other hand, recently, Pieper *et al.*²⁸ have made nuclear magnetic resonance experiment to study the nature of the doped hole in the CuO_2 planes of $\text{Pr}_{1-x}\text{Ba}_{2+x}\text{Cu}_3\text{O}_7$ single crystals, and found that there exist mobile holes in the rich-Ba $\text{Pr}_{1-x}\text{Ba}_{2+x}\text{Cu}_3\text{O}_7$ samples. This suggests that the appearance of the superconductivity in $\text{PrBa}_2\text{Cu}_3\text{O}_7$ might be because the p - f hybridization is depressed by the Ba residing on Pr sites. So, our attention is paid to the study of the T_c suppression in the $\text{Y}_{1-x}\text{Pr}_x\text{Ba}_2\text{Cu}_3\text{O}_7$ based on p - f hybridization.

II. MODEL AND COHERENT-POTENTIAL APPROXIMATION

As mentioned above, the model Hamiltonian describing electronic structure of the system may be given by

$$H = H_{pf} + 2H_{ps} + H_{ch}, \quad (1)$$

where

$$H_{pf} = \sum_{\mathbf{k}\alpha} \varepsilon_p p_{\mathbf{k}\alpha}^+ p_{\mathbf{k}\alpha} + \sum_{\mathbf{k}} \varepsilon_f f_{\mathbf{k}}^+ f_{\mathbf{k}} - t_{pp} \sum_{\mathbf{k}\alpha \neq \beta} S_{\alpha} S_{\beta} p_{\mathbf{k}\alpha}^+ p_{\mathbf{k}\beta} + t_{pf} \sum_{\mathbf{k}\alpha} S_{\alpha} (f_{\mathbf{k}}^+ p_{\mathbf{k}\alpha} + \text{H.c.}) + \sum_j \varepsilon_j f_j^+ f_j, \quad (2)$$

is the R -O hybridization Hamiltonian given by LM,¹⁴ in which the hole notation is used, and α, β refer to x or y , and $S_{x,y} = 2 \sin(k_{x,y}/2)$;

$$H_{ps} = \sum_{\mathbf{k}} E_{\mathbf{k}}^s a_{\mathbf{k}}^+ a_{\mathbf{k}}, \quad (3)$$

and

$$H_{ch} = \sum_{\mathbf{k}\sigma} E_{\mathbf{k}}^c c_{\mathbf{k}\sigma}^+ c_{\mathbf{k}\sigma}, \quad (4)$$

describe parts of the holes in the CuO_2 planes and the CuO_3 chain, respectively. In Eq. (2) j labels the Pr (or Y) site, and $\varepsilon_j = 0$ or ∞ for the Pr or Y site; according to LM we take the parameters $\varepsilon_p = \varepsilon_f = 1.9$ eV (where we use the hole notation). $E_{\mathbf{k}}^s$ and $E_{\mathbf{k}}^c$ represent the energy spectra of the holes in the CuO_2 planes and CuO_3 chains, respectively. Following Dagotto *et al.*²² we give $E_{\mathbf{k}}^s$ as

$$E_{\mathbf{k}}^s = E_0^s + 1.33J \cos k_x \cos k_y + 0.37J(\cos 2k_x + \cos 2k_y), \quad (5)$$

where $J = 0.125$ eV. According to Oles and Grzelka,¹⁵ we can describe the electronic structure in the chains using a tight-binding band

$$E_{\mathbf{k}}^c = E_0^c + \frac{w}{2} \cos(k), \quad (6)$$

where w is the bandwidth, and $w \approx 2.0$ eV.¹⁵ Here, we measure energy from the initial Fermi level of holes (i.e., that in $\text{YBa}_2\text{Cu}_3\text{O}_7$), and E_0^s and E_0^c are determined by the initial hole concentration in the CuO_2 planes and in the CuO_3 chains.

In order to investigate the behavior of the system at the intermediate doping, we make the coherent-potential approximation (CPA) for the Hamiltonian (2). According to the CPA,²⁹ we can write the following effective Hamiltonian:

$$H_{\text{CPA}} = \sum_{\mathbf{k}\alpha} \varepsilon_p p_{\mathbf{k}\alpha}^+ p_{\mathbf{k}\alpha} - t_{pp} \sum_{\mathbf{k}\alpha \neq \beta} S_{\alpha} S_{\beta} p_{\mathbf{k}\alpha}^+ p_{\mathbf{k}\beta} + t_{pf} \sum_{\mathbf{k}\alpha} S_{\alpha} (f_{\mathbf{k}}^+ p_{\mathbf{k}\alpha} + \text{H.c.}) + \sum_{\mathbf{k}} \Sigma_f f_{\mathbf{k}}^+ f_{\mathbf{k}}, \quad (7)$$

where Σ_f is the CPA self-energy of the f hole and can be self-consistently given by

$$\Sigma_f = \varepsilon_f - (1-x)(G_f)^{-1}, \quad (8)$$

in which G_f is the local Green's function of f holes, and x is the Pr concentration. By introducing the Green's-function matrix

$$G_{\mathbf{k}}(E) = (E - H_{\mathbf{k}}^{\text{CPA}})^{-1}, \quad (9)$$

we can obtain the Green's functions $G_{p\mathbf{k}}^{\alpha}(E)$ and $G_{f\mathbf{k}}(E)$, which correspond to the three components of the holes. $H_{\mathbf{k}}^{\text{CPA}}$ is the matrix form of Hamiltonian (7). Then the Green's function G_f in Eq. (8) is given by

$$G_f(E) = \frac{1}{N} \sum_{\mathbf{k}} G_{f\mathbf{k}}(E). \quad (10)$$

Now, we arrive at the following self-consistent equations for the hole-densities;

$$n_p = \frac{1}{N} \int_{-\infty}^{\mu} \sum_{\alpha\mathbf{k}} G_{p\mathbf{k}}^{\alpha}(E+0^+) dE, \quad (11a)$$

$$n_f = \frac{1}{N} \int_{-\infty}^{\mu} \sum_{\mathbf{k}} G_{f\mathbf{k}}(E+0^+) dE, \quad (11b)$$

$$n_{ps} = \frac{1}{N} \int_{-\infty}^{\mu} \sum_{\mathbf{k}} \rho_{ps\mathbf{k}}(E) dE, \quad (11c)$$

and

$$n_{ch} = \frac{1}{N} \int_{-\infty}^{\mu} \sum_{\mathbf{k}\sigma} \rho_{ch\mathbf{k}}(E) dE, \quad (11d)$$

$$n_p + n_f + 2n_{ps} + n_{ch} = n_0 + n_{ch0}, \quad (11e)$$

where μ is the chemical potential of the holes and also can be self-consistently obtained in Eq. (11); $\rho_{ps}(E)$ and $\rho_{ch}(E)$ are densities of states in the CuO_2 planes and CuO_3 chains, which are obtained through Eqs. (3) and (4). n_p and n_f are densities of the O $2p$ hole and the Pr $4f$ hole in the FR state, respectively; n_{ps} and n_{ch} are the hole densities in the CuO_2 and in the CuO_3 chains; n_0 is the initial value of hole density in the bilayer CuO_2 planes, and according to Ref. 14 we will take $n_0 = 0.39$; n_{ch0} is the initial value of hole density in the CuO_3 chains. The band-structure calculations^{15,30} showed that the hole filling in the chains of $\text{YBa}_2\text{Cu}_3\text{O}_7$ is close to 1.5 holes per unit cell, so we will assume that the initial value of n_{ch} is 1.5 in our calculations, i.e., $n_{ch0} = 1.5$.

III. DOPING DEPENDENCE OF HOLE DENSITY DISTRIBUTION

In our picture, according to Eq. (11), we can calculate the hole-distribution among the CuO_2 planes, CuO_3 chains, and the FR state, for various doping densities. First, we calculate the hole density in the CuO_2 planes. According to LM, the O-O hopping t_{pp} and t_{pf} are taken as 0.2 and 0.75 eV, respectively, and other parameters are taken as in Sec. II. The result is presented in Fig. 1 (dashed line). One can notice that for $t_{pf} = 0.75$ the decrease of the holes with increasing x is so slow that up to $x = 1.0$ the hole concentration is still 0.07. This is not in accordance with the Hall measurement,³¹ which shows a reduction by about 90% of the carrier density. In addition, for $x = 0.55$ the curve gives the hole density $n_{ps} \approx 0.12$, which cannot explain the metal-nonmetal transition near this point. In fact, for $x > 0.5$ the $\text{Y}_{1-x}\text{Pr}_x\text{Ba}_2\text{Cu}_3\text{O}_7$ system displays a semiconducting-type behavior at low

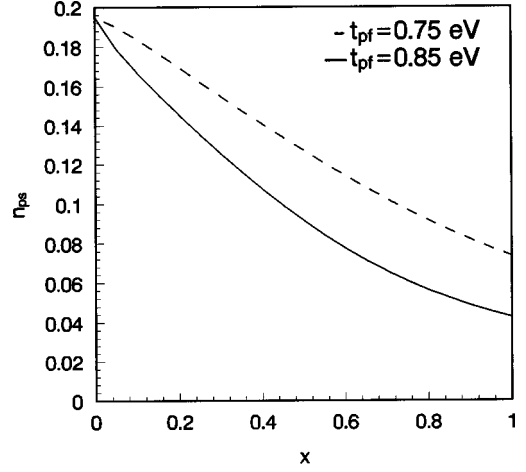


FIG. 1. Hole density in CuO_2 planes as a function of Pr concentration for $t_{pf} = 0.75$ (dashed) and 0.85 eV (solid).

temperature.³² So, we repeat the calculation for $t_{pf} = 0.85$ eV, and the result is also shown in Fig. 1 (solid line). This makes the result in rather good agreement with experiments. First, for $x = 0.55$ the result gives a reasonable hole density, i.e., $n_{ps} \approx 0.084$, lying in the region of metal-nonmetal transition (< 0.1).³³ Second, for $x = 1.0$ the curve gives the hole density $n_{ps} \approx 0.04$. So, about 80% of the holes in $\text{YBa}_2\text{Cu}_3\text{O}_7$ are grabbed by the FR band, which is roughly in agreement with the result of Hall measurement. Therefore, in the following calculations, we will choose $t_{pf} = 0.85$ eV. But it should be pointed out that the value $t_{pf} = 0.75$ eV finally chosen by LM is already taken larger than the value of the local density approximation (LDA) calculation, i.e., 0.65 eV, and our value $t_{pf} = 0.85$ eV is a further departure from the LDA value.

In order to investigate the change of the holes in the CuO_3 chains, in Fig. 2, we present the reduction of the hole density $\delta n_{ch} = n_{ch}(x=0) - n_{ch}(x)$ in the chains as a function of Pr-doping density x . As a comparison, we also present the reduction of hole density δn_{ps} in Fig. 2. One can find that the reduction of the hole density in the chains is small. For $x = 1.0$ the result shows $\delta n_{ch} \approx 0.08$, i.e., the hole density in

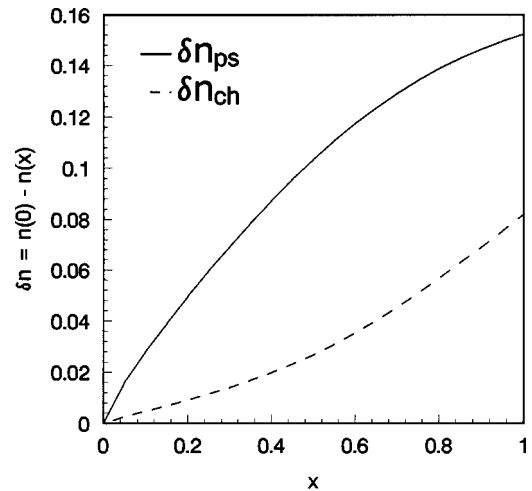


FIG. 2. Reduction of the hole densities in the CuO_2 planes (δn_{ps}) and CuO_3 chains (δn_{ch}) against Pr concentration.

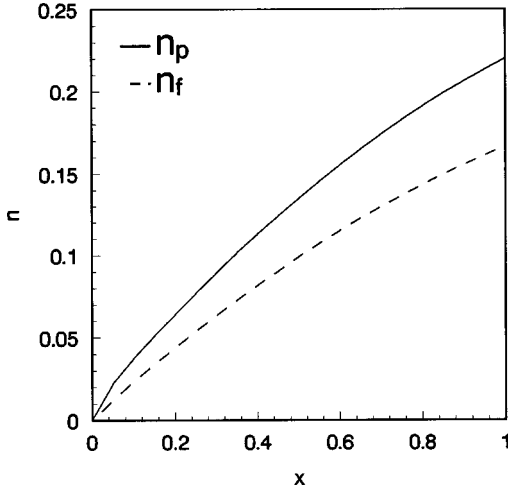


FIG. 3. Component of the holes in the p - f hybridization band. The solid line represents $2p$ hole densities (n_p), and the dashed line represent $4f$ hole densities (n_f).

the chain decreases from 1.5 to 1.42. The calculations of Oles *et al.* showed that about 54% of the holes in the chains of $\text{YBa}_2\text{Cu}_3\text{O}_7$ is oxygen holes. This indicates that the oxygen hole density in the chains decreases only by 0.043. So, our calculation can explain the experimental fact that no obvious reduction of the O holes residing on the CuO_3 chains is caused by the Pr doping.^{19–21} In fact, for $\text{YBa}_2\text{Cu}_3\text{O}_7$, strongly coupled to the antiferromagnetic fluctuation, the holes in the CuO_2 planes form a spin-polaron band with small bandwidth, and the Fermi level is near the van Hove singularities. While on the CuO_3 chains the bandwidth is wider. So, on doping Pr into the system, the p - f hybridization states mainly grab the holes in the planes.

In Fig. 3, we present the component of FR holes (i.e., Pr hole or O hole). From the figure we find that the weight of O hole (n_p) larger than that of the Pr hole (n_f). So, a large part of the FR holes is of oxygen character. When $x=1$, we obtain $n_f \approx 0.17$, this indicates that the valance of Pr in $\text{PrBa}_2\text{Cu}_3\text{O}_7$ is roughly +3. Because the Pr $4f$ electrons in the FR state are dispersive, the local magnetic moment of Pr ion is that of $4f^1$ as observed experimentally.

In order to obtain the reasonable hole depletion, we have enhanced the Pr-O hybridization t_{pf} in our calculations. Of course, we may also adjust the other parameters such as t_{pp} and ε_p to obtain a good result. In fact, the increase of t_{pp} and ε_p also can raise the hole depletion. However, as in Ref. 14, we choose enhancing t_{pf} . Perhaps, one notice that $t_{pf} = 0.85$ eV seems to be too large in comparison with the value of $t_{pf} = 0.4$ – 0.5 eV given by FR. This is not surprising. First, FR's value was estimated based on their pure local model. Second, the meaning of t_{pf} is different between the two models. In the FR model, t_{pf} represents the hybridization between one Pr site and one O site, but in the LM model, t_{pf} is a effective hybridization between one Pr site and two O sites in the bilayer planes.

IV. QUANTITATIVE DISCUSSION FOR THE T_c SUPPRESSION

There are at least two consequences of the Pr-O hybridization: one is the hole transfer from the $pd\sigma$ band to the p - f

band, as discussed above; the other is the modification to the magnetic state of CuO_2 planes, since the CuO_2 planes are antiferromagnetically correlated in $\text{PrBa}_2\text{Cu}_3\text{O}_7$ below ~ 300 K.² Hall angle measurements^{34,35} in the $\text{Y}_{1-x}\text{Pr}_x\text{Ba}_2\text{Cu}_3\text{O}_7$ system have indicated that Pr doping change the slope α as well as the intercept C in the linear $\cot \Theta_H - T^2$ equation ($\cot \Theta_H = \alpha T^2 + C$). Experimentally, α varies only depending on the carrier concentration as shown in $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$,^{34,36} while C is directly related to the $\text{Cu}(2)$ -site substitution such as in $\text{YBa}_2\text{Cu}_{3-x}\text{Zn}_x\text{O}_7$.³⁷ Moreover, according to Anderson's theory,³⁸ α is predicted to be sensitive to carrier concentration, and C is due to magnetic impurity scattering. Therefore, it is reasonable and necessary to consider the two effects simultaneously.

If one does not consider the effect of magnetic interaction, it is plausible that the holes residing on the $pd\sigma$ band support the superconductivity. As we know, T_c obeys phenomenologically a parabolic relation dependent of the hole concentration,³⁹ which can be written as

$$T_c(n_{ps}) = T_{c,\max} \left[1 - \frac{(n_{\text{opt}} - n_{ps})^2}{(n_{\text{opt}} - n_{\text{zero}})^2} \right], \quad (12)$$

where n_{ps} is the hole concentration of $pd\sigma$ band in the CuO_2 planes. n_{opt} is the optimal hole density that gives the maximum of T_c ($T_{c,\max}$) in $\text{YBa}_2\text{Cu}_3\text{O}_7$, and n_{zero} is the zero- T_c hole density at which T_c vanishes.

Now, we may introduce the magnetic effect of Pr doping. We do not think that the Pr-ion magnetic moment itself will break Cooper pairs, since most “123” compounds with large rare-earth magnetic moments are still superconductors. However, the Pr-O hybridization does affect the pairing environment, or Pr-O hybridization may induce a kind of magnetic scattering. Generally, it can be treated, at least phenomenologically, by the Abrikosov-Gorkov pair-breaking theory,^{24,41}

$$\ln \frac{T_c(x)}{T_{c0}} = \Psi \left(\frac{1}{2} \right) - \Psi \left(\frac{1}{2} + 0.14 \frac{\Gamma}{\Gamma_c} \frac{T_{c0}}{T_c(x)} \right), \quad (13)$$

where $T_c(x) = T_c[x, n_{ps}(x)]$, and $T_{c0} = T_c[0, n_{ps}(x)]$. $\Gamma = x\pi N_0 V^2$ is magnetic scattering rate, N_0 is the density of state at the Fermi level, and V represents the scattering potential. Here, we use the Born approximation because the scattering is weak. Γ_c is the critical scattering rate. We can write Eq. (13) as

$$\ln \frac{T_c(x)}{T_{c0}} = \Psi \left(\frac{1}{2} \right) - \Psi \left(\frac{1}{2} + 0.14 \frac{x}{x_c^m} \frac{T_{c0}}{T_c(x)} \right), \quad (14)$$

where x_c^m is the magnetic scattering critical Pr content at which T_c becomes zero if there were *only* pair-breaking interactions (x_c^m can be larger than 1.0). Let $P(x) = T_c(x)/T_{c0}$, we can obtain the numerical solution of $P(x)$. So, $T_c(x)$ can be calculated by

$$T_c(x) = T_{c,\max} \left[1 - \frac{[n_{\text{opt}} - n_{ps}(x)]^2}{(n_{\text{opt}} - n_{\text{zero}})^2} \right] P(x). \quad (15)$$

We should still consider the variation of x_c^m under different hole doping. Kluge *et al.*⁴⁰ found that T_c suppression of Cu-site substitution was basically unchanged in the optimal and overdoped regime, but became serious in the underdoped

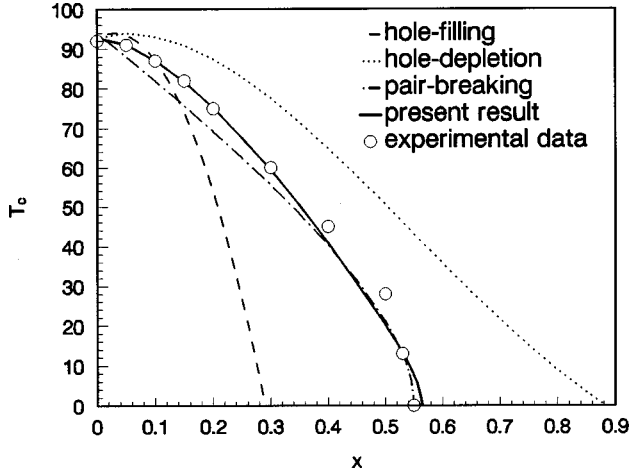


FIG. 4. Comparison of calculated $T_c(x)$ curves according to different models with the typical experimental data [from Maple's group (Ref. 35)].

regime. This indicates that the strength of pair breaking increases with the decreasing carrier density in the underdoped regime. So, x_c^m should be decreased with the increasing Pr doping. Recently, the authors of Ref. 24 gave a reasonable explanation for the T_c suppression induced by Zn substitution. They ascribed the increase of the pair-breaking effect in the underdoping region to the presence of the normal-state pseudogap. Tallon *et al.*²⁴ presented the critical scattering rate Γ_c as a function of the pseudogap $E_g(p)$,

$$\Gamma_c = \Gamma_{c0}(1-z^2)^{5/4}, \quad (16)$$

in which $z = E_g(p)/\Delta_{00}$ where $\Delta_{00} = \sqrt{E_g^2 + \Delta'_{00}{}^2}$, and Δ'_{00} is the superconducting order parameter at zero temperature in the absence of impurity; p is hole concentration (i.e., here n_{ps}), and Γ_{c0} is the critical scattering rate in the absence of E_g . On the other hand, according to Williams *et al.*²⁴ $N_0 \propto (1-z)^{0.5}$. Therefore, we can obtain

$$x_c^m = x_{c0}^m(1-z^2)^{3/4}, \quad (17)$$

where x_{c0}^m is the magnetic scattering critical Pr concentration in the absence of E_g . Tallon *et al.*²⁴ used $z = 3.08 - 15.4p$ to describe the observed linear dependence of E_g on hole concentration, but it seems unreasonable because $z > 1$ as long as $p < 0.135$. Here, we will use $z = 7.14(0.19 - p)$ to satisfy $E_g(0.19) = 0$,²⁴ and $\Delta'_{00}(p = n_{zero} = 0.05) = 0$. Whereas x_{c0}^m can be reasonably estimated by comparing the magnetic-scattering-induced reduction of T_c ($\Delta T_{c,m}$) in $Y_{1-x}Pr_xBa_2Cu_3O_7$ (Ref. 34) and $YBa_2Cu_{3-x}Zn_xO_7$ (Ref. 37) systems. The intercept C of the equation ($\cot \Theta_H = \alpha T^2 + C$) indicates the magnetic scattering, thus it should correspond to $\Delta T_{c,m}$. Comparing the experimental data of C (Refs. 34 and 37) in the two systems, we obtain $\Delta T_{c,m} \approx 40$ K for $Y_{0.4}Pr_{0.6}Ba_2Cu_3O_7$. We give $x_{c0}^m = 1.1$ in the following numerical calculation, so that $\Delta T_{c,m}$ for $Y_{0.4}Pr_{0.6}Ba_2Cu_3O_7$ is just around 40 K.

Using the above equations, we can calculate the $T_c(x)$. For the $Y_{1-x}Pr_xBa_2Cu_3O_7$ system, we chose the typical values: $T_{c,max} = 94$ K, $n_{opt} = 0.18$, and $n_{zero} = 0.05$. It is found that the calculated $T_c(x)$ is quite in accordance with most

experimental data.^{2,35} This can be clearly seen in Fig. 4, in which the experimental $T_c(x)$ values are taken from the result of Maple's group.³⁵

To our knowledge, other existing models cannot give a good explanation for the whole T_c suppression so far. In Fig. 4 we also shows the comparison between the results of various scenarios. In the hole-filling case (i.e., Pr ion is Pr^{4+}), the hole density of the $pd\sigma$ band will be decreased by $0.5x$ (x is the Pr content). So, $pd\sigma$ hole density is $0.5(n_0 - x)$. We find that the hole-filling mechanism would give a sharp T_c drop (see dashed curve). The dotted curve is obtained by only considering hole-depletion effect. It shows a more steady T_c decrease than the experimental result. Even if one may adjust the values of some parameters such as n_0 , n_{opt} , and n_{zero} to elucidate the $T_c(x)$ behavior for lower x , it is still difficult to understand the abrupt drop of T_c at $x = 0.5 - 0.55$. The pure pair-breaking theory gives the dash-dotted curve, as we know, it can basically account for the latter point, but fails to explain the "plateau" of $T_c(x)$ for $x < 0.1$.² Neumeier *et al.*⁵ already proposed the combination of hole filling and pair breaking, but they could interpret the $T_c(x)$ curve only for $x \leq 0.2$.

It is worth noticing that the experimental data of $T_c(x)$ just implies the mechanisms. $T_c(x)$ values decrease slowly for $0 \leq x \leq 0.1$; then go down more rapidly and nearly linearly for $0.1 \leq x \leq 0.5$; finally drop sharply to zero at $x \sim 0.55$.^{2,35} The first stage mainly reflects a crossover from overdoping to underdoping; and the second stage reflects the combination of hole depletion and pair breaking; the last stage suggests that pair breaking plays a significant role due to the opening of the pseudogap. Therefore, the $T_c(x)$ behavior strongly suggests that there are two mechanisms coexisting in the systems: hole depletion and magnetic scattering, and the former strengthens the latter.

V. CONCLUSION

We have considered a model Hamiltonian to investigate the hole-density distribution in the $Y_{1-x}Pr_xBa_2Cu_3O_7$ system. In the Hamiltonian the electronic structure of the CuO_2 planes and CuO_3 chains, and the Pr-O hybridization are all included. In our picture, with the increasing Pr content, the transfer of holes into the $p-f$ hybridized states appears not only in CuO_2 planes but also in the CuO_3 chains. We made the coherent-potential approximation calculations for this model Hamiltonian to study the behavior of the system at the intermediate Pr doping, and presented the Pr-doping dependent distribution of the holes. Our calculation shows that no obvious reduction of the hole residing on the CuO_3 chains is caused by the Pr doping, and the oxygen hole in the chains decreases only by about 0.043 per unit cell. So, the hole transfer is mainly from the $pd\sigma$ band of the CuO_2 planes to the $p-f$ hybridization band. We presented a hole-depletion behavior in the CuO_2 planes, which is coincident with the experimental results. A metal-nonmetal transition around $x = 0.5$ was predicted based on the calculation for the reasonable parameters.

Combining the hole-depletion effect with pair breaking, and considering the enhancement of the pair breaking due to the appearance of the normal-state pseudogap, we have given a good explanation for the whole T_c suppression in

$Y_{1-x}Pr_xBa_2Cu_3O_7$. For small x , it is mainly hole depletion that controls that T_c variation. For intermediate x , the combination of the hole depletion with the pair breaking renders the T_c depression. When x is near x_{cr} , a pair-breaking-like mechanism plays a significant role, resulting in the fast drop of T_c . We thus conclude that there are two mechanisms

coexisting in the systems: hole transfer and magnetic scattering.

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*Electronic address: yhren@public1.hz.zj.cn

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