Pressure effect on T_c for the rare-earth series $RBa_2Cu_3O_{7-\delta}$

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The pressure dependence of the superconducting transition temperature T_c in $RBa_2Cu_3O_{7-\delta}$ (R=Y and rare earths) series has been investigated systematically on the basis of the t-t'-t''-J model with d-wave pairing by taking into account the variations of the hole concentration in the CuO₂ planes and the effective interaction with pressure. It is shown that the pressure-induced change of hole concentration increases with the trivalent rare-earth ion radius. The calculated T_c and its pressure derivative dT_c/dP are found to be the increasing functions of the radius of the R^{3+} ions for the fully oxygenated $RBa_2Cu_3O_7$. Good agreement with experiments suggests that the rare-earth ion size effect on dT_c/dP in $RBa_2Cu_3O_7$ mainly originates from the pressure-induced change transfer from the charge reservoir CuO chain to the conducting CuO₂ planes. The change of dT_c/dP with hole concentration and the pressure dependence of T_c in the recently discovered superconducting PrBa₂Cu₃O_y are well reproduced in this simple model. We have arrived at the conclusion that the unusually large T_c enhancement in PrBa₂Cu₃O_y under pressure results from its underdoped nature. Further experiments are proposed to enhance T_c at ambient pressure in PrBa₂Cu₃O_y.

I. INTRODUCTION

Substitution with rare-earth elements on the Y site of the high-temperature superconductors (HTSCs) $YBa_2Cu_3O_{7-\delta}$ is an important method for understanding the mechanism of the occurrence of superconductivity. Recent measurements^{1,2} show that the superconducting transition temperature T_c increases systematically with the ionic radius of trivalent rareearth ions in the fully oxygenated $RBa_2Cu_3O_7$ (R = Y and rare earths) compounds. $PrBa_2Cu_3O_{\nu}$ has been believed as the exceptional material being nonsuperconducting among the isostructural $RBa_2Cu_3O_{7-\delta}$ compounds for a long time.³ However, very recently, Zou *et al.*⁴ reported that PrBa₂Cu₃O_v grown by the traveling-solvent floating zone (TSFZ) method is superconductive with $T_c = 85$ K. The long-standing search for the chemical pressure and the origin of the intrinsic pressure effect on T_c is an important issue in the high pressure studies.⁵⁻⁷ The $RBa_2Cu_3O_{7-\delta}$ series provides a model system with this attempt. For a single compound such as YBa₂Cu₃O_{7- δ}, the pressure derivative of T_c , dT_c/dP , may vary by changing oxygen content.⁸ Furthermore, across the rare-earth series of RBa₂Cu₃O₇ samples both T_c and dT_c/dP increase modestly with the trivalent rare-earth ion radius.¹ The pressure effect on T_c in PrBa₂Cu₃O_v has drawn particular interest because of the unusual high pressure derivative of T_c , dT_c/dP , of 3.5 K/GPa incompatible with other fully oxygenated series $RBa_2Cu_3O_7$.¹ Moreover, T_c has been observed to exceed 105 K at a pressure of 9.3 GPa and still have a potential increase.⁴ While the pressure effect on T_c in superconducting

 $RBa_2Cu_3O_{7-\delta}$ series seems to yield important insight into superconductivity, at present there is no microscopic theory that can explain it.

Among the various theories proposed so far for the mechanism of high- T_c superconductivity, the t-(t'-t'')-Jmodel is the simplest that describes strongly correlated electrons and has been proposed as the low energy model Hamiltonian that applies to the doped CuO_2 planes.^{9,10} It is suggested that Hall coefficient,¹¹ specific heat,¹² quasiparticle lifetime,¹² high transition temperature,^{12–14} CuO₂ layers effect, T_c among various cuprates¹⁵ might be understood by assuming a presence of the antiferromagnetic van Hove singularities (AVHS) in the quasiparticle density of states. The angle-resolved photoemission spectroscopy (ARPES) measurement on layered cuprates provides a direct test for the t-t'-t''-J model as a model Hamiltonian for the HTSCs. Recent studies show that the t-t'-t''-J model can be used to not only reproduce the ARPES data for the quasiparticle dispersion of Sr₂CuO₂Cl₂ (Refs. 16-18) but also explain the evolution of the quasiparhole-doped ticle dispersion with doping for $Bi_2Sr_2Ca_{1-x}Dy_xCu_2O_{8+\delta}$ as well as electron-doped Nd_{1.85}Ce_{0.15}CuO₄, especially the origin of the AVHS near Fermi surface.^{19,20}

In this paper we explain the pressure effect on T_c in $RBa_2Cu_3O_{7-\delta}$ series in terms of the t-t'-t''-J model with d-wave pairing. The outline of this paper is as follows: In Sec. II we present a theoretical approach for pressure effect on T_c . Section III is devoted to the theoretical results of T_c

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and dT_c/dP as a function of rare-earth ionic size. We also discuss the origin of unusually large T_c enhancement in PrBa₂Cu₃O_y under pressure. A brief summary is given in Sec. IV.

II. THEORETICAL APPROACH

The Hamiltonian considered here is^{9,10}

$$H = J \sum_{\langle ij \rangle_1} \mathbf{S}_i \cdot \mathbf{S}_j - \left(t \sum_{\langle ij \rangle_1, \sigma} + t' \sum_{\langle ij \rangle_2, \sigma} + t'' \sum_{\langle ij \rangle_3, \sigma} \right) \tilde{c}_{i\sigma}^{\dagger} \tilde{c}_{j\sigma},$$
(1)

in the standard notation of the constrained Fermi operators, brackets denoting the first $(\langle ij \rangle_1)$, second $(\langle ij \rangle_2)$, and third $(\langle ij \rangle_3)$ neighbor sites, respectively.

Using the slave fermion-spin wave formalism, one obtains a model describing holons (spinless fermions) strongly coupled to spin-wave excitations¹⁹

$$H = \sum_{q} \omega_{q} b_{q}^{\dagger} b_{q} + \sum_{k} \epsilon_{k} h_{k}^{\dagger} h_{k} + \sum_{kq} (h_{k}^{\dagger} h_{k-q} b_{q} M_{kq} + \text{H.c.}),$$
(2)

where *h* and *b* are spinless fermion and magnon operators, respectively. $\omega_q = 2J\sqrt{1-\gamma_q^2}$ is the linear spin-wave spectrum. The bare hole dispersion has the form

$$\boldsymbol{\epsilon}_{k} = 4C_{1}t\,\boldsymbol{\gamma}_{k} + 4C_{2}t'\,\boldsymbol{\lambda}_{k} + 4C_{3}t''\,\boldsymbol{\eta}_{k}\,, \qquad (3)$$

where C_1, C_2 , and C_3 are the first-order matrix element of the kinetic energy for $\langle ij \rangle_1, \langle ij \rangle_2$, and $\langle ij \rangle_3$, respectively. $\gamma_k = \frac{1}{2}(\cos k_x + \cos k_y), \ \lambda_k = \cos k_x \cos k_y$, and $\eta_k = \frac{1}{2}(\cos 2k_x + \cos 2k_y)$. The holon-spin-wave coupling function is

$$M_{kq} = \frac{4}{\sqrt{N}} [u_q(t \gamma_{k-q} + t' \lambda_{k-q} + t'' \eta_{k-q}) + v_q(t \gamma_k + t' \lambda_k + t'' \eta_k)], \qquad (4)$$

where u_q, v_q are Bogolubov transformation parameters of the linear spin waves.

In building up a model for the cuprates to describe the superconducting phase, the interaction among the hole quasiparticles is necessary. It will be constructed based again on results for the two-dimensional t-J model where it is well known that an effective attractive force exists in an antiferromagnet leading to the bound state of two holes in the d-wave channel. Here we investigate this explicitly, following Dagotto, Nazarenko, and Moreo (DNM),¹² for the case of a static attractive nearest-neighbor interaction $H_{int} =$ $-V_{\text{eff}}\Sigma_{\langle ij\rangle}n_in_j$. Such an interaction is actually provided in the t-J model by the exchange term because of the extra magnetic bond in the system when two polarons are on neighboring sites or, equivalently, by the dominant term of the static approximation to the (actually somewhat longerrange) interaction generated by spin fluctuations.²¹ The binding energy of two holes is $\Delta_B = e_{2h} - 2e_{1h} = J(\langle \mathbf{S}_i \cdot \mathbf{S}_i \rangle)$ -0.25), where e_{nh} is the energy of *n* holes with respect to the antiferromagnetic ground state energy, and i and j are nearest neighbors. It is known¹² that $\langle \mathbf{S}_i \cdot \mathbf{S}_i \rangle \approx -0.3346$, and thus $\Delta_B \approx -0.585J$. To mimic this effect, an effective attractive term is introduced that reduces the energy when two quasiparticles share the same link ($V_{\rm eff} \approx 0.585J$). The effective Hamiltonian considered here for HTSCs is

$$H_{\rm eff} = \sum_{k} \varepsilon_{k} c_{k}^{\dagger} c_{k} - V_{\rm eff} \sum_{\langle ij \rangle} n_{i} n_{j}, \qquad (5)$$

where c_k^{\dagger} is the hole quasiparticle creation operator at momentum k, and $n_i = c_i^{\dagger} c_i$ is the number operator of quasiparticles at site *i*.

Straightforward application of Bardeen-Cooper-Schrieffer pairing theory assuming a *d*-wave order parameter $\Delta_k = \Delta_0(\cos k_x - \cos k_y)$ leads in the familiar way to a selfconsistent equation determining T_c ,

$$\frac{2}{V_{\text{eff}}} = \frac{1}{N} \sum_{k} \frac{\left(\cos k_{x} - \cos k_{y}\right)^{2}}{\varepsilon_{k} - \mu} \tanh\left(\frac{\varepsilon_{k} - \mu}{2T_{c}}\right), \quad (6)$$

where Δ_0 is the parameter to be obtained self-consistently and N is the number of sites. The chemical potential μ satisfies

$$n_H = \frac{1}{2} - \frac{1}{2N} \sum_k \tanh\left(\frac{\varepsilon_k - \mu}{2T_c}\right),\tag{7}$$

where n_H is the quasiparticle hole density. DNM (Ref. 12) obtained the hole dispersion from accurate numerical and analytical studies as $\varepsilon_k \approx 0.16625 \cos k_x \cos k_y + 0.046(\cos 2k_x + \cos 2k_y)$ eV. Recent exact diagonalization results show that this rigidity of quasiparticle dispersion is appropriate over a wide range of doping from underdoped to optimally doped.¹⁹

There has been a great deal of interest in recent years to extract the intrinsic pressure dependence of T_c in cuprates. It has been postulated that the application of pressure leads to a change of hole carrier concentration n_H , which has been supported by measurements of Hall effect,²² thermopower,²³ and neutron powder diffraction²⁴ under high pressure. It is expected that the pressure-induced change of n_H is an important factor responsible for the pressure dependence of T_c . Meanwhile, Raman scattering experiments and model analysis^{25–27} suggest that the in-plane superexchange interaction J is a pressure-sensitive parameter which is directly related to the effective pairing interaction $V_{\rm eff}$. Therefore, it is reasonable to assume that pressure-induced change of $V_{\rm eff}$ is the second variable that would best describe the pressure dependence of T_c . In order to generalize Eqs. (6) and (7) to include the effect of pressure, we assume that the pressure dependence of the T_c is related to the pressure dependences of n_H and $V_{\rm eff}$. That is,

$$n_H(P) = n_H + \frac{dn_H}{dP}P \tag{8}$$

and

$$V_{\rm eff}(P) = V_{\rm eff} \left(1 + \frac{d \ln V_{\rm eff}}{dP} P \right). \tag{9}$$

This approximation is reasonable for low values of *P*, but is likely to breakdown for large *P* since one expects $V_{\text{eff}}(P)$ and $n_H(P)$ to saturate at large pressures.

Therefore, the pressure dependence of T_c can be simply written as

$$T_c(P) = T_c[n_H(P), V_{\text{eff}}(P)].$$

$$(10)$$

The initial pressure derivative of T_c is then calculated from Eqs. (6) and (7) as

$$\frac{dT_c}{dP} = \left[\frac{F_4}{I} - \frac{F_5}{2T_c I}\right] \frac{dn_H}{dP} + \frac{F_1}{2T_c I V_{\text{eff}}} \frac{d\ln V_{\text{eff}}}{dP}, \quad (11)$$

with

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$$\begin{split} I &= \frac{1}{4T_c^3} [F_1 F_3 + 2T_c F_2 F_4 - F_2 F_5], \\ F_1 &= \frac{1}{2N} \sum_k \operatorname{sec} h^2 \left(\frac{\varepsilon_k - \mu}{2T_c}\right), \\ F_2 &= \frac{1}{2N} \sum_k (\varepsilon_k - \mu) \operatorname{sec} h^2 \left(\frac{\varepsilon_k - \mu}{2T_c}\right), \\ F_3 &= \frac{1}{2N} \sum_k (\cos k_x - \cos k_y)^2 \operatorname{sec} h^2 \left(\frac{\varepsilon_k - \mu}{2T_c}\right), \\ F_4 &= \frac{1}{2N} \sum_k \frac{(\cos k_x - \cos k_y)^2}{(\varepsilon_k - \mu)^2} \operatorname{tanh} \left(\frac{\varepsilon_k - \mu}{2T_c}\right), \\ F_5 &= \frac{1}{2N} \sum_k \frac{(\cos k_x - \cos k_y)^2}{\varepsilon_k - \mu} \operatorname{sec} h^2 \left(\frac{\varepsilon_k - \mu}{2T_c}\right). \end{split}$$

From Eqs. (10) and (11), one notices that in order to study the pressure dependence of $T_c(P)$ and dT_c/dP , one must have a knowledge of the values of dn_H/dP and $d \ln V_{\rm eff}/dP$. Hall effect and thermoelectric power experiments under pressure can provide results for dn_H/dP . Meanwhile, $d \ln V_{\rm eff}/dP$ can be estimated from the Raman scattering measurements of the in-plane superexchange J under pressure. In general, J is a function of the in-plane lattice parameter a^{25} It is reasonable to assume the pressure-induced relative change of $V_{\rm eff}$, $d \ln V_{\rm eff}/dP$, as

$$\frac{d\ln V_{\rm eff}}{dP} = 3\,\kappa_a\,,\tag{12}$$

where $\kappa_a = -d \ln a/dP$ is the lattice compressibility along the *a* axis. The pressure-induced change of n_H can be obtained from the bond valence sum (BVS) analysis^{28,29}

$$\frac{dn_H}{dP} = \eta \left[\frac{dr_0}{dP} V_{\rm Cu} + \sum_i r_{ij} \kappa_i \exp\left(\frac{r_0 - r_{ij}}{0.37}\right) \right].$$
(13)

Where $\eta = 2.7(n_H^{\text{opt}} - n_H^{\text{min}})/(V_{\text{Cu}}^{\text{opt}} - V_{\text{Cu}}^{\text{min}}), n_H^{\text{opt}}(V_{\text{Cu}}^{\text{opt}})$ denotes the optimum n_H (Cu valence) corresponding to the T_c^{max} and $n_H^{\min}(V_{Cu}^{\min})$ is the minimum n_H (Cu valence) resulting in superconductivity, r_{ii} is the distance of Cu-O(i) bond, r_0 is the constant that depends upon the atoms constituting the bond,³⁰ and $\kappa_i = -d \ln r_i/dP$ is the Cu-O(i) bond compressibility. The compressibility of HTSCs can be estimated by using the anisotropic bond model proposed by Cornelius, Klotz, and Schilling (CKS).^{31,32}

It is worth noting that the present t-t'-t''-J model is based on the assumption of *d*-wave pairing which is generally supported in experiments.^{21,33,34} Recent investigations on the t-Jmodel exhibits discrepant results. Exact numerical studies³⁵ for small clusters within the t-J model show a d-wave superconducting instability. Shih et al.³⁶ found that this model does not have long-range d-wave superconducting correlation in the interesting parameter range. While Yokoyama and Ogata argued³⁷ that near the half filling where the high- T_c superconductivity is expected, the $d_{x^2-y^2}$ -wave pairing state is always the most stable among various symmetries. Interestingly, Newns et al.³⁸ found that the van Hove singularity scenario with s-wave pairing renders similar results to d-wave symmetry. Considering that the two intrinsic factors responsible for the value of T_c under pressure are the same with different symmetries, the t-t'-t''-J model with the $d_{x^2-y^2}$ -wave pairing would not make much difference compared with the case of the s wave for the pressure effect on T_c , at least qualitatively.

III. RESULTS AND DISCUSSION

A. Anisotropic compressibility and pressure-induced charge transfer

The crystal structure of the $RBa_2Cu_3O_{7-\delta}$ system is made up of three distinct layers. The first consists of the $Cu(1)O_6$ and BaO₁₂ polyhedra. The second is a perovskite layer containing the $Cu(2)O_5$ and BaO_{12} polyhedra. The third contains the single RO₈ polyhedron. The compressibility of the individual layers κ_L can be obtained by using the compressibilities of the component polyhedron. The linear compress-

TABLE I. Results of the model calculation for the anisotropic and volume compressibilities and the bulk modulus for rare earth series $RBa_2Cu_3O_7$. Ionic radii (coordination number eight) for R^{3+} ions are taken from Ref. 42.

$\overline{R^{3+}}$	Yb	Tm	Er	Но	Y	Dy	Gd	Eu	Sm	Nd
r(Angstrom)	0.985	0.994	1.004	1.015	1.019	1.027	1.053	1.066	1.079	1.109
$\kappa_a(\times 10^{-3} \text{ GPa}^{-1})$	2.36	2.37	2.38	2.39	2.39	2.41	2.38	2.41	2.44	2.44
$\kappa_h(\times 10^{-3} \text{ GPa}^{-1})$	2.42	2.42	2.43	2.44	2.44	2.46	2.43	2.46	2.48	2.49
$\kappa_c(\times 10^{-3} \text{ GPa}^{-1})$	2.88	2.86	2.87	2.86	2.87	2.86	2.86	2.86	2.86	2.85
$\kappa_V (\times 10^{-3} \text{ GPa}^{-1})$	7.65	7.66	7.68	7.69	7.70	7.72	7.68	7.73	7.78	7.78
B(GPa)	130.6	130.5	130.2	130.0	129.8	129.5	130.2	129.3	128.5	128.6

ibility along α th axis in the component polyhedron is written as $\kappa_{l(\alpha)}^p = 0.44 \times 10^{-3} \times r_{ij}^3 / V_j$ GPa⁻¹, where V_j denotes the valence of central cation in polyhedron which can be determined in terms of BVS method.³⁹ Knowing the fraction of the total volume (f_i) that each layer occupies in a unit cell, the anisotropic compressibility of HTSCs is given by $1/\kappa_a$ $= \sum_{i} f_{i} / \kappa_{a(i)}, 1 / \kappa_{b} = \sum_{i} f_{i} / \kappa_{b(i)}, \text{ and } \kappa_{c} = \sum_{i} f_{i} \kappa_{c(i)}.$ From this, the volume compressibility of material, $\kappa_{V} = \kappa_{a} + \kappa_{b}$ $+\kappa_c$, and its bulk modulus, $B \equiv 1/\kappa_V$ can be calculated.^{31,32,40} Based on the consistent set of structural parameters at temperature T=10 K for the series $RBa_2Cu_3O_{7-\delta}$ ($R = Y, Yb-Nd; \delta = 0.00 \pm 0.02$) determined by neutron diffraction,⁴¹ one can evaluate the anisotropic compressibilities of the compound on the basis of the anisotropic bond model of CKS. The calculated results as well as trivalent rare-earth ion radii (coordination number 8)42 are summarized in Table I. As can be seen, the compressibility along the c axis is always higher than that either along the a axis or the b axis. Furthermore, the volume compressibility κ_V increases gradually with increasing the trivalent rareearth ion radius. It is well established that the κ_V decreases with increasing n_H .^{24,43,44} This implies that the n_H in RBa₂Cu₃O₇ decreases with increasing the trivalent rare-earth ion radius. The model calculation of charge distribution demonstrates that the $RBa_2Cu_3O_7$ phases with R = La, Nd, are underdoped and those with R = Y, Sm-Lu are overdoped.⁴⁵ It is therefore indicated that the κ_V is a valid probe of the n_H in HTSCs.

The pressure-induced change of n_H , dn_H/dP , can be calculated by using the Eq. (13) according to the neutron diffraction data.⁴¹ The Cu-O(i) bond compressibility can be estimated by using the anisotropic bond model.³¹ In the holedoped HTSCs, the superconductivity occurs for a $n_H \sim 0.06$ holes and the maximum T_c is attained at a value of $n_H^{\text{opt}} \sim 0.25$ holes.^{8,45–47} The $V_{\text{Cu}}^{\text{min}}=2.082$ and $V_{\text{Cu}}^{\text{opt}}=2.135$ are obtained by using the structural data for YBa₂Cu₃O_{7- δ} compounds⁴⁸ in terms of the BVS analysis.^{28,39} Following *et al.*, 24 Jorgensen we assume $dr_0/dP = -2.9$ $\times 10^{-3}$ Å/GPa (Ref. 29) which can reproduce a reasonable dn_H/dP for the fully oxygenated RBa₂Cu₃O₇. Figure 1 shows both the n_H and the dn_H/dP versus the trivalent rareearth ion radius in $RBa_2Cu_3O_7$ family. The values of n_H are taken from the work of Samoylenkov, Gorbenko, and Kaul (SGK).⁴⁵ It was found that n_H decreases smoothly with the increase of trivalent rare-earth ion radius. While the dn_H/dP increases with the increase of the trivalent rare-earth ionic radius.

The hole concentration can be written as $n_H = Q/V$, where Q is the number of carriers and V the volume of the sample.



FIG. 1. Ionic radius of trivalent rare earths dependences of hole concentration n_H (a) and pressure-induced changes of hole concentration dn_H/dP (b) for the fully oxygenated $RBa_2Cu_3O_7$ series. The hole concentration data are taken from SGK in Ref. 45.

Taking the partial derivative of n_H with respect to pressure P, one can obtain the relative change of pressure-induced carrier number

$$\frac{d\ln Q}{dP} = \frac{1}{n_H} \frac{dn_H}{dP} - \kappa_V. \tag{14}$$

With the calculated dn_H/dP , volume compressibilities, and n_H , one can evaluate the values of $d \ln V_{\rm eff}/dP$ and $d \ln Q/dP$ from Eqs. (12) and (14), respectively. The results of the model calculations for the $RBa_2Cu_3O_7$ series are displayed in Table II. As can be seen from Table II, $d \ln Q/dP$ increases significantly with the trivalent rare-earth ion radius. We note that $d \ln V_{\rm eff}/dP$ increases modestly with increasing ionic radius of R^{3+} , with an almost constant value of $\sim 7.0 \times 10^{-3}$ GPa⁻¹.

B. Rare-earth ionic size effect on dT_c/dP in $RBa_2Cu_3O_7$

In Fig. 2 we plot the transition temperature as a function of the hole concentration n_H with different values of V_{eff} using the dispersion relation of DNM. It is clearly seen that the magnitude of T_c depends strongly on the doping level and reaches its maximum at $n_H \approx 0.246$ holes, which is very close to the prediction of 0.25 holes of several groups.^{8,45,46} On the other hand, the transition temperature increases with V_{eff} and rises rapidly at the optimal doping. In fact, the varia-

TABLE II. Predicted values of the pressure-induced changes of hole concentration, the pressure-induced relative changes of the number of hole carriers, and the effective interaction as well as hole concentration in the CuO_2 planes taken from Ref. 45 for rare-earth series $RBa_2Cu_3O_7$.

R^{3+}	Yb	Tm	Er	Но	Y	Dy	Gd	Eu	Sm	Nd
n_H (holes)	0.303	0.298	0.296	0.292	0.287	0.284	0.273	0.265	0.262	0.233
$dn_H/dP(\times 10^{-3} \text{ holes/GPa})$	2.90	3.68	3.89	4.37	4.70	5.03	6.47	6.59	6.92	8.44
$d \ln Q/dP(\times 10^{-3} \text{ 1/GPa})$	1.92	4.69	5.46	7.27	8.68	9.99	16.02	17.14	18.63	28.44
$d \ln V_{\rm eff}/dP(\times 10^{-3} \ 1/{\rm GPa})$	7.06	7.11	7.13	7.16	7.17	7.22	7.16	7.23	7.32	7.32



FIG. 2. Variation of T_c with hole concentration n_H as a function of effective interaction V_{eff} =0.0393, 0.0403, and 0.0413 eV.

tion in maximum T_c among various cuprate superconductors seems to indicate that T_c should be correlated with V_{eff} .¹⁵ These results demonstrate that both n_H and V_{eff} significantly affect the values of T_c .

In Fig. 3 we plot the T_c as a function of the trivalence rare earth ionic radius with the n_H of SGK as well as V_{eff} = 0.0396 eV using the dispersion relation of DNM. It is clearly seen that T_c depends on the ionic radius of R^{3+} for the fully oxygenated $RBa_2Cu_3O_7$. T_c increases modestly from T_c =92.4 K for R=Yb to T_c =94.8 K for R=Nd with increasing trivalent rare-earth ionic radius. For comparison, experimental data from Lin *et al.*¹ and William and Tallon² are also displayed. It is clear that our theoretical predictions are in qualitative agreement with experiments. Noting that the T_c is an increasing function of the trivalent rare-earth ion radius in $RBa_2Cu_3O_7$ series, we suggest that the maximum T_c in optimally doped PrBa_2Cu_3O_y should be near to 95 K. This implies that the PrBa_2Cu_3O_y crystal grown by Zou *et al.*⁴ may be underdoped.

Lin *et al.*¹ measured systematically the rare-earth ion size effect on dT_c/dP for fully oxygenated $RBa_2Cu_3O_7$ (R = Yb, Tm, Ho, Dy, Gd, Sm, and Nd). They found that dT_c/dP increases with the ionic radius of R^{3+} . With the



Ionic radius of R³⁺ (Angstrom)

FIG. 3. Ionic radius of trivalent rare earths dependence of T_c for the $RBa_2Cu_3O_7$ superconductors with $V_{eff}=0.0396$ eV. The experimental data are those from Refs. 1,2.



lonic radius of R³⁺ (Angstrom)

FIG. 4. Predicted pressure derivative dT_c/dP as a function of ionic radius of trivalent rare earths for $RBa_2Cu_3O_7$ series. The experimental data points are taken from Lin *et al.* in Ref. 1.

calculated n_H and dn_H/dP , and $d \ln V_{\rm eff}/dP$ shown in Table II, one can obtain dT_c/dP from Eq. (11). In Fig. 4 we plot dT_c/dP against the ionic radius of R^{3+} for the $RBa_2Cu_3O_7$ series. The dT_c/dP is an increasing function of the radius of R^{3+} ions, which agrees qualitatively with the experiments.¹ The predicted dT_c/dP is in good agreement with the measurements in the fully oxygenated RBa₂Cu₃O₇ compound with small radius of rare-earth ion except Yb. For the larger rare-earth ion NdBa₂Cu₃O₇ material, the calculated dT_c/dP of 0.97 K/GPa is comparable with the experimental result of 1.21 K/GPa.¹ Interestingly, the predicted value of dT_c/dP of 0.50 K/GPa in YBa₂Cu₃O₇ is very near the the experimental result of 0.4 K/GPa.⁸ Considering that the pressure-induced relative change of $V_{\rm eff}$ does not depend significantly upon the trivalent rare earth ionic radius, the increase of dT_c/dP with the trivalent rare earth ionic radius is mainly due to the increase of dn_H/dP . It is therefore indicated that the origin of the ionic size effect on dT_c/dP observed in the fully oxygenated RBa₂Cu₃O₇ series is the pressure-induced charge transfer from the charge reservoir Cu(1)-O chain to the conducting CuO₂ planes.

C. Origin of unusually large T_c enhancement in PrBa₂Cu₃O_y under pressure

Although the mechanism of the superconductivity in $PrBa_2Cu_3O_{\nu}$ is still needed to clarify, a remarkable T_c enhancement in a PrBa₂Cu₃O_v crystal has drawn much attention. There are at present no available experiment values of $d \ln V_{\rm eff}/dP$ and dn_H/dP for PrBa₂Cu₃O_y. From Table II, we know that the values of $d \ln V_{\rm eff}/dP$ and dn_H/dP for fully oxygenated $PrBa_2Cu_3O_7$ should be larger than those for NdBa₂Cu₃O₇ with small radius of rare-earth ion. Neglecting the possible change of dn_H/dP with hole concentration, we adopt $dn_H/dP = 1.37 \times 10^{-2}$ holes/GPa in PrBa₂Cu₃O_y as that in the underdoped YBa₂Cu₃O_{6.78} compound.⁴⁹ For concreteness in discussion, we take $d \ln V_{\rm eff}/dP = 1.0$ $\times 10^{-2}~{\rm GPa^{-1}}$ for ${\rm PrBa_2Cu_3O_y}$ in the present study. Figure 5 shows the transition temperature dependence of pressure derivatives of T_c of PrBa₂Cu₃O_y. The solid line is our theoretical prediction based on Eq. (11). It can be seen that the



FIG. 5. Calculated dT_c/dP as a function of transition temperature T_c in PrBa₂Cu₃O_y along with the experiment data from Zou *et al.* in Ref. 4 and Ye *et al.* in Ref. 50.

 $T_c \sim dT_c/dP$ curve displays a familiar behavior which is well known for other HTSCs.⁵⁻⁷ With increasing transition temperature, the magnitude of dT_c/dP decreases modestly. The theoretical results coincide well with the experimental data of Zou et al.⁴ and Ye et al.⁵⁰ The calculated value of the maximum pressure derivative dT_c^{max}/dP is 1.13 K/GPa, which just falls in the consistent tendency of other optimally doped $RBa_2Cu_3O_{7-\delta}$ series.¹ Even though the pressure derivative of T_c for PrBa₂Cu₃O_y with $T_c = 85 \text{ K}(dT_c/dP)$ = 3.5 K/GPa) is almost an order of magnitude higher than that of optimally doped YBa₂Cu₃O_{7- δ}, this value is comparable to 4.0 K/GPa in the underdoped YBa2Cu3O6.78 with $T_c \approx 87.6$ K.⁸ Interestingly, the underdoped SmBa₂Cu₃O_{7- δ} sample with $T_c = 78$ K possesses the same dT_c/dP = 3.5 K/GPa.⁵¹ These results strongly indicate that the *un*usual large value of dT_c/dP in superconducting $PrBa_2Cu_3O_{y}$ possibly comes from the underdoped nature.

With the parameters given above, we calculated T_c in PrBa₂Cu₃O_y compound with $T_c=85$ K as a function of pressure *P* in the range of $0 \le P \le 20$ GPa by using Eq. (10) with $V_{\text{eff}}=0.0396$ eV($T_c^{\text{max}}=95$ K). The numerical results are presented in Fig. 6. For comparison, the experimental



FIG. 6. Calculated values of $T_c(P)$ with pressure P in the underdoped PrBa₂Cu₃O_y compound with T_c =85 K up to 20 GPa. The solid circles are the experiment data from Zou *et al.* in Ref. 4.



FIG. 7. Predicted $T_c(P)$ as a function of pressure for the optimally doped PrBa₂Cu₃O_y superconductor with $T_c = 95$ K up to 10 GPa.

data from Zou *et al.*⁴ are also displayed. It can obviously that there is a parabolic-shaped curve which is extended along the pressure axis. Remarkably, our prediction agrees well with experiments. The value of T_c already reaches 95 K at 3.2 GPa, the predicted maximum value of T_c at ambient pressure. For a pressure of 9.7 GPa, T_c is calculated to be 105.6 K, in good agreement with the work of Zou *et al.* The maximum T_c of 106.5 K on the $T_c(P)$ curve is exhibited at 12.2 GPa. Note that this maximum is very close to 109 K in the YBa₂Cu₄O₈ at P = 12 GPa.⁵²

Now that the PrBa₂Cu₃O_v crystal of Zou et al. is underdoped, let us evaluate $T_c(P)$ for the optimally doped $PrBa_2Cu_3O_v$ with $T_c = 95$ K. We integrate Eq. (10) utilizing the parameters $dn_H/dP = 1.37 \times 10^{-2}$ holes/GPa and $d \ln V_{\rm eff}/dP = 1.0 \times 10^{-2}$ GPa⁻¹. The results are plotted in Fig. 7. As seen, $T_c(P)$ passes through a maximum of 97.2 K at 4.0 GPa followed by a sizable decrease. In the ac susceptibility measurements on the nearly optimally doped YBa₂Cu₃O_{7- δ} crystals Tissen *et al.*⁵³ and Klotz *et al.*⁵⁴ indeed observed the existence of a maximum in $T_c(P)$ near 4 GPa. Interestingly, the increase of T_c under pressure is not over 3 K in the optimally doped PrBa₂Cu₃O_v material. It appears that the optimally doped $PrBa_2Cu_3O_{\nu}$ compound has a common intrinsic property of other optimally doped $RBa_2Cu_3O_{7-\delta}$ materials. In this respect it is desirable to investigate experimentally the pressure effect on T_c of an optimally doped $PrBa_2Cu_3O_{\nu}$ sample.

Finally, we propose experiments to enhance T_c in PrBa₂Cu₃O_y compounds at ambient pressure. The comparison of pressure effect on T_c in the electron- and hole-doped superconductors⁵⁵ suggests that a change in the bondlength between copper and apical oxygen in the pyramids may play a major part in determining the change of T_c under pressure. One can conjecture that the pressure-induced charge transfer is the result of a shift of the apical oxygen toward the CuO₂ plane with the application of pressure. This has been confirmed in YBa₂Cu₃O_{7- δ} and other cuprates.⁵⁻⁷ However, in the substitution of Y by the small size Gd ion (chemical pressure), Fernandes *et al.*⁵⁶ found that the apical Cu-O distance presents opposite trends. Thus, the substitution of Pr by the large size La would result in the enhancement of T_c in the PrBa₂Cu₃O_y system due to the possible shortening of the

apical Cu-O distances. Another possible way is to reduce the in-plane distances, which could induce the increase of superexchange J. Consequently, T_c should increase at ambient condition. Therefore, higher T_c is expected for a sample with higher compressive stress in the *a-b* plane. In fact, a higher $T_c = 49.1$ K was recently reported for a thin film of La_{1.9}Sr_{0.1}CuO₄ with large compression of the *a-b* plane by the epitaxial strain.⁵⁷

IV. CONCLUSIONS

We have investigated systematically the pressure effect on T_c in $RBa_2Cu_3O_{7-\delta}$ series in terms of the t-t'-t''-J model with d-wave pairing. Assuming the two effects of pressure application on HTSCs being a change of the effective interaction and a redistribution of the hole concentration, our simple model is able to give a good qualitative account of the experimentally observed pressure dependence of T_c as a

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function of ionic radius of the rare-earth elements. We found that the pressure derivative dT_c/dP increases with the ionic radius of R^{3+} in fully oxygenated $RBa_2Cu_3O_7$ system. We suggest that this ionic size effect orginates from the pressure-induced charge transfer from the charge reservoir Cu(1)-O chain to the conducting CuO₂ planes. The experimental observations of the unusually large T_c enhancement in superconducting PrBa₂Cu₃O_y under pressure are reproduced in terms of our simple model. Further experiments are proposed to increase T_c at ambient pressure.

ACKNOWLEDGMENTS

We acknowledge useful discussion with H. Q. Lin, W. G. Yin, and F. X. Han. The work was supported by the Hong Kong Research Grants Council under account number C001 2160089/2160108 and in part by the China Postdoctoral Science Foundation.

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