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The origin of the 60 K plateau in $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$

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Abstract

A model for the charge transfer mechanism in $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ high- T_c cuprate based on the critical chain length concept is proposed to account for the 60 and 90 K plateaus in the $T_c(x)$ dependence. It has been shown that, when the statistics of CuO chain formation was described in terms of the two-dimensional asymmetric next-to-nearest neighbor Ising (ASYNNNI) model, at any constant temperature below the top of ortho-II phase there exists a uniquely defined value of critical chain length $l_{cr}(T)$ that yields a constant doping $p(x) \approx \text{const}$ over the regime of ortho-II phase (related to the 60 K plateau of $T_c(x)$), while the 90 K plateau coincides with the monotonically increasing $p(x)$ over the optimal doping level $p = 0.16$ in the regime of the ortho-I phase. Short length chains ($l < l_{cr}(T)$), together with the first $l_{cr}(T) - 2$ holes in longer chains ($l \geq l_{cr}(T)$), are taken as not capable of attracting electrons from CuO_2 planes. It is shown that only a part ($\approx 41\%$) of the remaining $l - l_{cr}(T) + 1$ holes in the long chains can capture electrons. The results obtained indicate that the ASYNNNI model and two-plateau-like behavior of $T_c(x)$ in $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ are closely connected.

CuO_2 layers are key ingredients in all high- T_c cuprates given the fact that superconductivity occurs in these materials when a part of 3d copper electrons, usually between 5% and 27%, is taken away from the layers. The missing electrons are commonly referred to as 'holes' which can move throughout the layers and make the material superconducting if the temperature is low enough. The electrons are conventionally subtracted from the layers either by chemical substitution of interlayer metal atoms, as for example, with the substitution of La^{2+} by Sr^{3+} in $\text{La}_{1-x}(\text{Sr})_x\text{Cu}_2\text{O}_4$ and Y^{2+} by Ca^{3+} in $\text{Y}_{1-b}(\text{Ca})_b\text{Ba}_2\text{Cu}_3\text{O}_{6+x}$, or by pumping oxygen into the material. Oxygen is introduced into separate layers in which it orders to form CuO chains, and it is these chains that are known to act as efficient attractors of electrons from the CuO_2 layers. The number of created holes per Cu atom is typically denoted as the 'doping', p , and the notion that CuO_2 layers have an unavoidable role in the onset of superconductivity is further corroborated by the fact that a number of important physical characteristics, such as, for example, the pseudogap energy E_g and critical transition temperature T_c , are coupled to p by universal relations that are common to practically all high- T_c cuprates. Thus, it has

been obtained empirically that the T_c is scaled with $T_{c,\max}$ (the maximal transition temperature) through the following, approximately parabolic, function of the hole concentration [1, 2]:

$$T_c(p) = T_{c,\max}[1 - 82.6(p - 0.16)^2], \quad (1)$$

which has its onset, maximum and termination at $p = 0.05$, 0.16 (optimal doping) and 0.27 , respectively.

$\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ superconductor has probably been the most thoroughly studied compound of all high- T_c cuprates, because it has a relatively simple synthesis route, and it was the first superconductor discovered with T_c above the liquid nitrogen temperature. The value of T_c changes in a nonlinear manner with oxygen composition, revealing two well-known plateaus at 60 and 90 K. These features are clearly associated with the ortho-II and ortho-I phases, respectively [3]. While the 90 K plateau is in fact a broad maximum at $x \approx 0.92$ that is associated with transition from underdoped to overdoped regime, the origin of 60 K plateau at $0.5 < x < 0.7$ is not yet well understood [3–5] (although, in fact, some advance has recently been made along this line [6]). One popular explanation is that when the oxygen content is increased over $x = 0.5$, where the ortho-II phase emerges in the form of alternating columns of fully occupied and empty oxygen sites (directed along the b -axis), additional oxygen fills the empty columns, making a relatively small contribution to hole doping, inasmuch as they are far apart from each other and only a small fraction of them are able to form CuO chains that are long enough to initiate the charge transfer process. It has often been guessed that there might be a certain minimal (critical) chain length l_{cr} defined so that only chains of length that is equal to, or greater than, l_{cr} can effectively attract electrons from CuO_2 layers [3–6]. However, even though the existence of the ortho-II phase was resolved long ago in terms of the classical two-dimensional asymmetric next-nearest-neighbor Ising (ASYNNNI) model [7], no convincing explanation has been provided over the last 20 years as to why exactly the concentration $p(x)$ of holes induced in CuO_2 sheets would remain constant when x changes within the ortho-II phase regime, nor, if the critical chain length concept is presupposed, what the value of l_{cr} would be equal to and how it can be determined.

Although it is well known that high- T_c cuprates are complex quantum many-body systems with the pairing mechanism still remaining controversial, here we unambiguously provide grounds that it is the classical ASYNNNI model combined with the concept of minimal chain length (needed for charge transfer to take place) that accounts for constant doping at $p \approx 0.094$ in the region of the 60 K plateau, as well as for the broad maximum of T_c at optimal doping ($p = 0.16$) at $x \approx 0.92$.

There is a general agreement that copper in the chain (basal) plane can be either Cu^{1+} , which is the case when it is not coupled to the in-plane oxygen (but connected only to two apical O(4) ions and therefore two-fold coordinated), or Cu^{2+} , when it is inserted within a CuO chain (four-fold coordinated), or at the chain end (three-fold coordinated). If isolated oxygen is introduced into the basal plane it then takes away two electrons from the two nearest-neighbor Cu^{1+} , transferring them into the Cu^{2+} state. Thus, isolated oxygen does not have a tendency to attract an additional electron from the other parts of the system. When another oxygen is added to make a chain with two O atoms (chain of length $l = 2$) there is only one electron available from its nearest-neighbor copper coordination, and the absence of another electron, needed for oxygen to become O^{2-} , is usually referred to as a ‘hole’. In this way, a chain of length l is seen as to have created $l - 1$ chain-holes, which in principle can attract electrons from the other parts of the system, presumably from CuO_2 layers.

Since the state of a quasi-one-dimensional electronic subsystem of a chain of a given length (say, l), which reflects the charge transfer effectiveness of the chain, is not expected to depend upon the history of chain formation, one is free to assume that the chain has been formed by

adding oxygen atoms one by one as that would allow one to shadow the evolution of charge transfer process as a function of l . Within the concept of critical chain length no charge transfer is supposed to occur unless $l = l_{\text{cr}}$, so the first $l_{\text{cr}} - 2$ initially created holes will stay inactive in attracting electrons from the planes. As l further increases beyond l_{cr} , the transfer of charge begins, during which process the remaining $l - l_{\text{cr}} + 1$ holes are created. Therefore, our strategy for counting doping is, first of all, to discard the contribution not only of all holes in short chains ($l < l_{\text{cr}}$), but also of the first $l_{\text{cr}} - 2$ holes in long chains ($l \geq l_{\text{cr}}$), for they have been created before any charge transfer takes place (we denote these holes as *passive* holes). It then naturally evolves that the number of attracted electrons (transferred holes) from a chain of length $l \geq l_{\text{cr}}$ should become greater as more holes are created after the charge transfer process has been triggered (at $l = l_{\text{cr}}$), i.e. it should be proportional to $l - l_{\text{cr}} + 1$ (we call these holes *the active* holes since their occurrence coincides with the development of charge transfer). In the case of the ortho-II phase, the concentration of active holes h (the number of active holes per Cu) is given by

$$h = \frac{1}{4} \left[n_{\alpha 1} \sum_{l=l_{\text{cr}}}^{\infty} (l - l_{\text{cr}} + 1) f_{\alpha 1}(l) + n_{\alpha 2} \sum_{l=l_{\text{cr}}}^{\infty} (l - l_{\text{cr}} + 1) f_{\alpha 2}(l) \right], \quad (2)$$

where $n_{\alpha 1}$ and $n_{\alpha 2}$ denote the fractions of three-fold coordinated Cu ions on two different sublattices of oxygen sites (usually denoted as α_1 and α_2), and $f_{\alpha 1}(l)$ and $f_{\alpha 2}(l)$ are corresponding fractions of CuO chains of the same length l .

If N_{Cu} and $n = (n_{\alpha 1} + n_{\alpha 2})/2$ are the total number and the fraction of three-fold coordinated Cu in the basal plane, then $(n/2)N_{\text{Cu}}$ is the total number of CuO chains, and the number of passive holes per Cu is surely not greater than $(n/2)(l_{\text{cr}} - 2)$, given the fact that none of the chains with $l < l_{\text{cr}}$ has more than $l_{\text{cr}} - 2$ holes. At $x = 1$ (OI stoichiometry) the chains are very long, virtually infinite, and there are just a few chain ends in the system. This means that n tends to zero as x approaches 1, so the concentration of passive holes becomes negligible whatever the value of l_{cr} . This in turn implies that practically each chain ordered oxygen has created one active hole, i.e. $h \approx 1$ at $x \approx 1$. Since, in the $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ system, one chain plane supplies holes to two CuO_2 layers, the doping would have been equal to $p = 0.5$ if each active hole had succeeded in capturing one electron. Experimental findings, however, clearly contradict such a scenario, for it was found that $p(x \approx 1)$ only slightly overshoots 19% [2]. Thus, at least at $x \approx 1$, it can be stated that $p = (\chi/2)h$ where $\chi (\approx 40\%)$, as defined by the number of effectively attracted electrons (transferred holes) per active hole, reflects the capability of an active hole to capture an electron. On the other hand, long (infinite) chains also prevail at $x = 0.5$ (OII stoichiometry) on every even column of oxygen sites. The concentrations of passive holes is also negligible here, but h cannot be greater than 0.5; in fact, h can be only less than 0.5 due to thermally activated chain fragmentation (for example, one might expect that $h \approx 0.48$, as at $x \approx 0.5$, so in the region of the 60 K plateau). Given the fact that the 60 K plateau of T_c , according to (1), corresponds to the doping level $p \approx 0.094$ it appears that it is the same fraction (nearly 40%) of active holes that is transferred to the layers not only at $x \approx 1$, but also at $x \approx 0.5$. The charge transfer model that we propose here assumes that the same percentage of active holes is transferred, not only at stoichiometries $x = 0.5$ and 1, at which long CuO chains are known to dominate, but also at off-stoichiometry $0.5 < x < 1$ (and also at $x < 0.5$) where chain fragmentation is more intense. We therefore propose that doping is connected to the active hole concentration h , as given by (2), by $p = (\chi/2)h$ ($\chi \approx 40\%$) throughout the whole range of oxygen concentration $0 < x < 1$. The quantity χ introduced in this way should be perceived as the average capability of an active hole to capture an electron from the CuO_2 planes that lie above, or below, the basal plane (averaging is done over all chains in the system, or equivalently, over the whole volume of the material).

To calculate the hole concentration h (equation (2)) and doping $p = \chi h/2$, at a given point of (x, T) space, it is necessary to determine the fractions of the three-fold coordinated Cu and length distributions of CuO chains $f_{\alpha_1}(l)$ and $f_{\alpha_2}(l)$. We used the Monte Carlo (MC) method applied to the ASYNNNI model to calculate these quantities, for it is known that the model stabilizes both structures ortho-II and ortho-I that are responsible for the 60 K and 90 K plateaus [9]. Although the ASYNNNI model cannot stabilize other structures with longer periodicities along the a axis, like ortho-III, ortho-IV and ortho-V, their superstructure reflections have already been reported to be much weaker than those of the main phases [8, 9], so they are thought to appear only as small patches embedded in large domains of the main phases [10]. Besides, since these structures were mainly observed at oxygen compositions that correspond to the transition region between the two plateaus it implies that the ASYNNNI model alone should account for both plateaus of $T_c(x)$, especially given the fact that none of these structures, except ortho-II, was reported at $x < 0.62$ [9]. The chain length distributions $f_{\alpha_1}(l)$ and $f_{\alpha_2}(l)$ were determined in the following way: in each MC step we counted the total numbers of chains, N_{α_1} and N_{α_2} , on sublattices α_1 and α_2 , respectively (N_{α_1} and N_{α_2} are in fact equal to one half of the unlike V_2 bonds on the corresponding α sublattices), as well as the numbers of chains of the same length, $N_{\alpha_1}(l)$ and $N_{\alpha_2}(l)$, for lengths ranging from $l = 1$ to 300. The ratios $N_{\alpha_1}(l)/N_{\alpha_1}$ and $N_{\alpha_2}(l)/N_{\alpha_2}$ were then equilibrated through the MC process and the values thus obtained were finally assigned to $f_{\alpha_1}(l)$ and $f_{\alpha_2}(l)$. The MC calculations were performed using single-spin-flip Glauber dynamics, where the oxygen concentration x is a function of temperature T and chemical potential μ . We have studied lattices with periodic boundary conditions that consisted of 400×400 oxygen chain sites (O(1) sites, that split into two nonequivalent sublattices α_1 and α_2 , in the OII phase), and as many sites on the β sublattice (O(5) sites). One MC step included flipping of all $2 \times (400 \times 400)$ lattice spins and one MC run (at a particular point (x, T)) typically consisted of 3×10^4 to 5×10^4 MC steps, where only every tenth was used to calculate the chain length distributions $f_{\alpha_1}(l)$ and $f_{\alpha_2}(l)$, $l = 1, 2, \dots, 300$, and other relevant quantities (oxygen sublattice occupancies x_1 and x_2 , three-fold Cu fractions n_1 and n_2 , etc). At a certain number of points we have even used a really large number of MC steps, ranging from 10^5 to 3×10^5 .

At all calculated points of (x, τ) space (τ is a quantity that scales with T according to $\tau = k_B T/V_1$, where k_B is Boltzman constant and V_1 the nearest-neighbor O–O interaction of the ASYNNNI model) it was obtained [11] that

$$f_{\alpha_i}(l) = \frac{1}{l_{av,\alpha_i}} \left(1 - \frac{1}{l_{av,\alpha_i}} \right)^{l-1}, \quad i = 1, 2, \quad (3)$$

where l_{av,α_i} ($i = 1, 2$) denotes the average chain length on the corresponding sublattice (α_1 or α_2). Such a behavior of length distributions $f_{\alpha_1}(l)$ and $f_{\alpha_2}(l)$ was subsequently explained theoretically by analyzing microscopic features of the ASYNNNI model lattice configurations [12]. In brief terms, the l dependence of probability of a chain to have particular length l can be derived in the following way. Consider a sequence of N_y oxygen chain sites that are aligned along the b -axis (N_y is a large number, and the sites are connected by copper-mediated $V_2 < 0$ bonds). Let xN_y denote the number of oxygen atoms on this column of α sites and let nN_y stand for the number of unlike V_2 bonds (n is therefore the fraction of three-fold coordinated Cu along the column, and, consequently, $2x/n$ equals the corresponding average chain length, l_{av}). These xN_y oxygen atoms are generally divided into $(n/2)N_y$ groups (chains) that can have various lengths $l = 1, 2, \dots$. It is useful to recall that an each chain has two ends: one that is oriented towards the positive side of the b -axis (the ‘positive’ end) and the other one, oriented towards negative b -axis (the ‘negative’ end). Among these xN_y oxygen atoms there are $(n/2)N_y$ of them that are located at the positive chain end, and thus the

probability for an oxygen to be lying at the positive chain end is equal to $\omega = n/2x = (l_{\text{av}})^{-1}$. Consequently, $1 - \omega$ is the probability for oxygen to be located either within the interior of the chain, or at the negative chain end. Assuming that chains are created by adding oxygen one by one, starting from the negative end, one arrives at the conclusion that the probability for obtaining a chain of length l is equal to $f(l) = \omega(1 - \omega)^{l-1}$ [11, 12] (such a form of $f(l)$ dependence is known in the theory of probability as a ‘geometric’ probability distribution [13]). It should be noted, however, that a deeper analysis shows that the above reasoning applies only if the fluctuations of energy of the ASYNNNI model are not too large [12]. Indeed, a certain deviation from linear behavior of $\ln[f(l)]$ versus l dependence has been found in the vicinity of the second-order ortho-I-to-ortho-II phase transition curve (at $x > 0.5$) [12] but, fortunately, such departures were observed only in a relatively narrow interval $\Delta x \approx 0.07$ around critical points. Furthermore, our extended analysis (not shown here) shows that in the critical regime these deviations of calculated $f_{\alpha 1}(l)$ and $f_{\alpha 2}(l)$ dependences from the expected behavior were in a certain way compensated by summations in (2), so the calculated $h(x)$ dependences were obtained to vary smoothly over the transition region at all $\tau = \text{const}$.

The so-obtained values of length distributions $f_{\alpha 1}(l)$ and $f_{\alpha 2}(l)$ for $l = 1, \dots, 300$ were inserted into (2) to calculate the concentration h of active holes at different points (x, T) . The geometric-like behavior of $f(l)$ dependences ensures rather fast convergence of the sums in (2). It should be mentioned, however, that the specific form of length distributions (3) makes it possible, instead of evaluating the summations in (2) by the first 300 terms, to transform each of the sums into a closed analytical form, so that h would be connected through analytical expression with average oxygen occupancies, x_1 and x_2 , the three-fold Cu fractions n_1 and n_2 , and the parameter l_{cr} . Whatever the approach we used the calculated values of h were obtained to be practically indistinguishable from each other (even in the critical region of the ortho-I/ortho-II transition), but we nevertheless gave credence to calculation of the first 300 terms in estimating sums in (2), as we wanted to keep under control the possible departures of length distributions from (3) that are known to particularly occur in the critical regime [12]. In addition, at each point of (x, T) space h was calculated for the whole range of values of cutoff parameter l_{cr} spanning from $l_{\text{cr}} = 1$ to 50, so that h can be regarded as a function of three variables, i.e. $h = h(x, \tau, l_{\text{cr}})$ (aside from the fact that it also depends upon input parameters that define the ASYNNNI model, i.e. on O–O interactions $V_1 > 0$ (nearest neighbor) and $V_2 < 0, V_3 > 0$ (next-nearest neighbor)). There is one remarkable feature of the hole concentration $h = h(x, \tau, l_{\text{cr}})$, as defined by (2), that we have found while thoroughly analyzing its behavior: whatever the magnitudes of interactions V_1, V_2 , and V_3 , when h is considered as a function of l_{cr} at different points (x_i, τ) that correspond to the same $\tau = \text{const}$ and oxygen concentrations $x_i, i = 1, 2, \dots$ spanning over the region of ortho-II phase, all of these $h_{x_i}(l_{\text{cr}})$, $i = 1, 2, \dots$ functions intersect at a single, well-defined value of l_{cr} . This is shown in figure 1 for interactions obtained by the linear-muffin-tin orbital (LMTO) method [14] and at three different temperatures $\tau = 0.45, 0.38$ and 0.30 , but we have also obtained a similar behavior (not shown here) for the so-called ‘canonical’ interactions $V_2 = -0.5V_1, V_3 = 0.5V_1$. From figure 1 it can be clearly seen that at a given $\tau = \text{const}$, the value of l_{cr} at which all $h_{x_i}(l_{\text{cr}})$ curves intersect depends on temperature in the way that it increases with the temperature decrease. Thus, at the three temperatures $\tau = 0.45, 0.38, 0.30$, the intersection values were found to be $l_{\text{cr}} = 4(5), 6(7), 11(12)$, respectively. At a given temperature, we name the so-obtained intersection value of l_{cr} ‘the optimal minimal (critical) length’ (denoted by $l_{\text{cr,opt}}(\tau)$) for it is the value at which $h(x)$ stays constant over the regime of the ortho-II phase. Such behavior of $h(x)$ at $\tau = \text{const}$, for the corresponding $l_{\text{cr,opt}}(\tau)$, is shown in figure 2 at two temperatures: $\tau = 0.45$ (figures 2(a) and (b), for $l_{\text{cr,opt}}(\tau) = 4$ and 5 , respectively) and $\tau = 0.30$ (figure 2(c), for $l_{\text{cr,opt}}(\tau) = 12$). From these results it can be seen that indeed

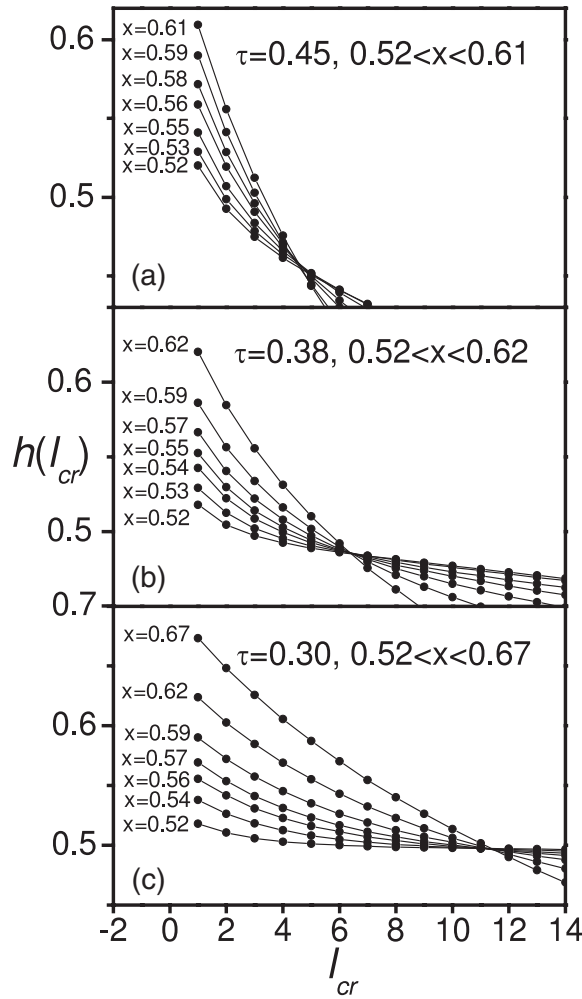


Figure 1. Calculated $h(l_{cr})$ dependences at $\tau = \text{const}$ for several values of oxygen composition x that span the range of the OII phase: (a) $\tau = 0.45 = \text{const}$; $0.52 < x < 0.61$ (shown at the top), (b) $\tau = 0.38 = \text{const}$; $0.52 < x < 0.62$ (shown in the middle section), and (c) $\tau = 0.30 = \text{const}$; $0.52 < x < 0.67$ (shown at the bottom).

$h(x)$ demonstrates a constant section at $x > 0.5$ that is even more pronounced at lower temperatures.

Calculated $h(x)$ dependences were used to obtain doping versus x dependences, $p(x) = \chi h(x)/2$, that were then inserted into (1) to yield the corresponding $T_c(x)$ s (figures 3(a)–(c)). The parameter χ was varied slightly around its expected value $\approx 40\%$ [2] to achieve a better correlation between the so-obtained $T_c(x)$ s and those from experiments [15] (shown by a solid line). We have indeed obtained h in the plateau regime to be slightly lower than 0.5: $h = \text{const} = 0.467$ (0.450) at $\tau = 0.45$ for $l_{cr} = 4$ ($l_{cr} = 5$), $h = \text{const} = 0.483$ at $\tau = 0.38$ for $l_{cr} = 7$, and $h = \text{const} = 0.495$ at $\tau = 0.30$ for $l_{cr} = 12$. This gives $\chi = 40.33\%$, 41.84% , 38.98% , 38.04% for $h = 0.467$, 0.450 , 0.483 , 0.495 , respectively. Thus, not only experimental data on doping at $x \approx 1$ [2], but also the analysis at $x \approx 0.5$ (that falls into the regime of 60 K plateau) both infer that χ lies at some point between $\approx 38\%$ and $\approx 42\%$. It should be noted that

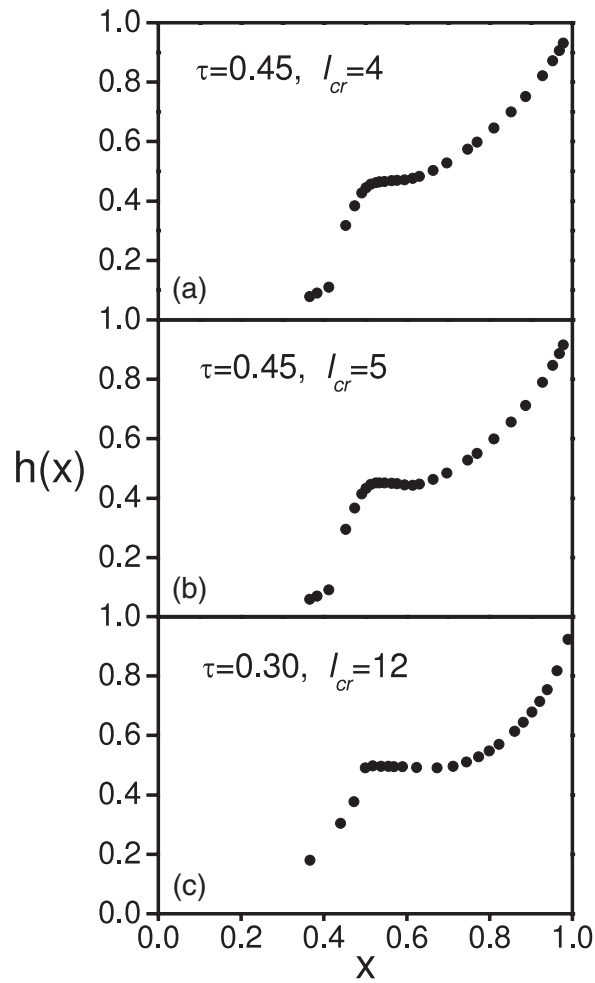


Figure 2. Calculated values of h as a function of x at $\tau = \text{const}$: (a) $\tau = 0.45 = \text{const}$, for $l_{cr} = 4$ (shown at the top), (b) $\tau = 0.45 = \text{const}$, for $l_{cr} = 5$ (shown in the middle section), and (c) $\tau = 0.30 = \text{const}$, for $l_{cr} = 12$ (shown at the bottom).

this result disagrees with the estimations of Gawiec *et al* [16, 17] that long chains release up to 70% of their holes.

Although we used here the ASYNNNI model interactions V_1 , V_2 , and V_3 as obtained by Sterne and Wille [14] the issue of magnitudes of these interactions is still open, so new values were subsequently suggested [10]. Regardless of that, it seems very well established that the nearest-neighbor interaction V_1 should be ranking around 6.9 mRyd [10, 14], which fixes the scaling between T and τ to $\Delta\tau \approx 0.1 \Leftrightarrow \Delta T \approx 100$ K. On the other hand, as one of the most important features of the $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ phase diagram is the location of the top of ortho-II phase along the τ -axis (at $x \approx 0.5$) and that it may well be affected by the magnitudes of V_2 and V_3 (which in fact are not known precisely), perhaps the best strategy to estimate the reduced temperature τ corresponding to room temperature is to determine the ‘distance’ (in units of τ) between room temperature and the top of ortho-II phase. According to experimental data the top of ortho-II phase corresponds to $\approx 125\text{--}140$ °C [5, 9], while the theoretically obtained phase

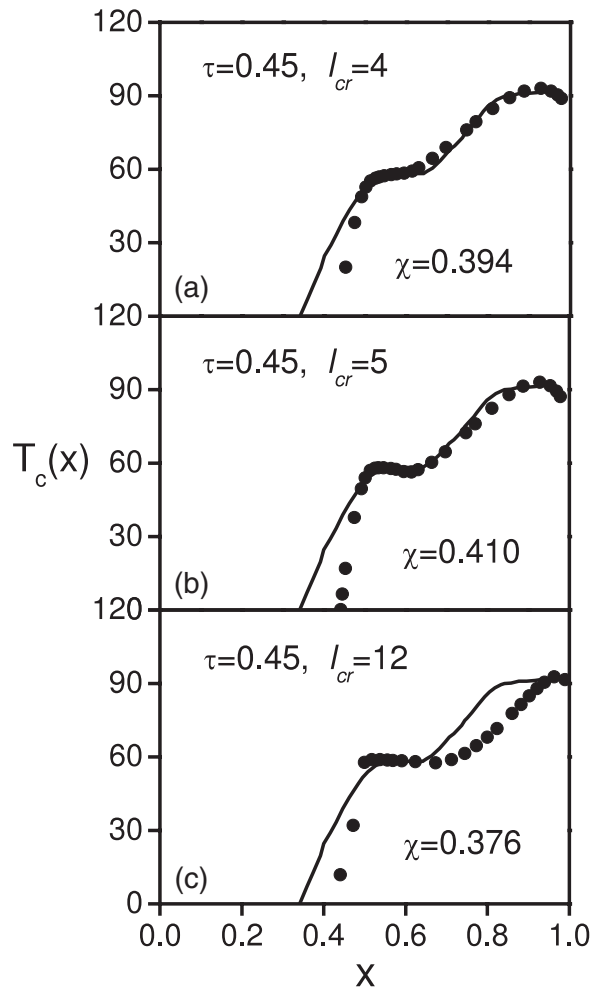


Figure 3. Calculated $T_c(x)$ dependences, using $h(x)$ dependences from the figure 2 and thereafter obtained $p(x) = \chi h(x)/2$ dependences, that were then inserted into (1): (a) $\tau = 0.45 = \text{const}$, for $l_{cr} = 4$ and $\chi = 39.4\%$ (shown at the top), (b) $\tau = 0.45 = \text{const}$, for $l_{cr} = 5$ and $\chi = 41\%$ (shown in the middle section), and (c) $\tau = 0.30 = \text{const}$, for $l_{cr} = 12$ and $\chi = 37.6\%$ (shown at the bottom).

diagram for the LMTO interactions [18] points to the top of the ortho-II phase lying at $\tau \approx 0.58$, thus making $\tau \approx 0.45$ a fairly reliable estimation of room temperature.

The established correlation between room temperature and $\tau = 0.45$ renders $l_{cr, \text{opt}}(\tau)$ (that plays the role of l_{cr} in (2)) 4, or 5 (figure 1(a)). A better estimation seems to be 5, for it yields a somewhat more pronounced 60 K plateau than $l_{cr} = 4$ (figures 3(a) and (b)), despite the fact that $l_{cr} = 4$ would be closer to $l_{cr} = 3$ that was proposed in some theoretical studies [16, 17, 19]. Besides, $l_{cr} = 5$ appears to be well correlated with $\chi \approx 2/5$ and with the basic idea lying in the background of the minimal (critical) chain length concept, suggesting that one isolated hole cannot efficiently attract an electron, but only a combined effect of several holes can achieve this goal. Both $l_{cr} = 5$ and $\chi \approx 2/5$ imply that three chain-holes are still not enough to effectuate charge transfer, but that the joint impact of five holes suffices to attract two electrons (one per CuO_2 layer).

In summary, despite the well-known fact that in such highly correlated electron systems, as are the high- T_c cuprates, the nature of the controversial pairing mechanism is genuinely quantum mechanical, we have shown here that certain aspects of their behavior can be explained in terms of classical models. Such is the classical ASYNNNI model, that successfully accounts for the unusual two-plateau-like behavior of $T_c(x)$ in $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$. The obtained $T_c(x)$ dependence is in a remarkable correlation with experiment [15] for both $l_{\text{cr}} = 4$ and 5, although we believe the later value is more realistic. It should be also pointed out that the presented results on the $T_c(x)$ dependence are in a qualitative agreement with some previous results on the same topic [20, 21]. Generally, it can be expected that the capability of an active hole to attract an unpaired 3d electron, as expressed by the value of χ , should depend upon the density ρ_e of available electrons immediately above (below) the chain (aside from the fact that χ should also depend on a certain coupling between chains and planes). Our recently obtained results on $T_c(x)$ in the $\text{Y}_{1-b}(\text{Ca})_b\text{Ba}_2\text{Cu}_3\text{O}_{6+x}$ ($b = 0.2$) system [22] seem to be in correlation with this kind of reasoning, since the obtained $\chi \approx 33\%$ can be understood in the light of the fact that the introduction of $\approx 20\%$ of Ca has additionally increased the doping, and therefore reduced ρ_e , so that χ attained a lesser value than in the parent $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ compound.

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