

## Positron annihilation in the high- $T_c$ superconductors

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A model for positron annihilation in the high- $T_c$  oxides is constructed based on the strongly correlated nature of the electrons in these systems. It is shown that the change in positron lifetime as a function of temperature in superconducting, nearly defect-free  $\text{YBa}_2\text{Cu}_3\text{O}_7$  and  $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$  can be understood on the basis of this model assuming that real hole-pair formation takes place in the superfluid state. The observed positron-lifetime changes in  $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$  as a function of  $x$  is also found to be consistent with this model.

### I. INTRODUCTION

The positron has long been recognized as a very sensitive probe of the electronic structure of solids.<sup>1</sup> It comes as no surprise, therefore, that a large number of positron studies have been conducted in the high- $T_c$  oxides in an effort to elucidate the nature of both the normal and superconducting states of these systems. All of these studies indicate that these superconductors are, at least in some respects, radically different from earlier superconductors. In both powder<sup>2-5</sup> and single-crystal samples<sup>6,7</sup> the positron-annihilation spectra show large changes on going through the superconducting transition. This is in sharp contrast to earlier experiments conducted on Pb and Nb alloys<sup>8,9</sup> which did not indicate any significant difference in the positron response to the normal and superconducting phases. The only change observed was an increased smearing of the Fermi surface in the superconducting state of  $\text{Nb}_3\text{Sn}$  (Ref. 10) consistent with the Bardeen-Cooper-Schrieffer (BCS) picture of superconductivity.<sup>11</sup> The dramatically different behavior of positrons in the oxide superconductors probably does not come as a big surprise since these systems do seem to be different from earlier superconductors in a number of different ways. The sensitivity of the positron to these differences, as indicated by the experiments, makes it a valuable tool for understanding the novel aspects of these new superconductors.

Besides the superconducting transition, the positron also seems to be sensitive to the carrier concentration as indicated by several positron-annihilation-spectroscopy (PAS) studies in  $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ .<sup>12,13</sup> It is also remarkable that the PAS data of sintered powder samples and single crystals are very different. This difference is thought to arise from the sensitivity of the positrons to oxygen vacancies. Therefore, the positron can be used as a probe for understanding both the changes in the electronic structure of these compounds as a function of doping and also the changes accompanying the transition to the superfluid state.

For PAS to be a useful tool of electronic structure, the experiments have to be complemented by theoretical models. The usefulness of combining experimental PAS data with predictions from theoretical models, in elucidating

the nature of the system being probed, has been amply demonstrated in earlier works where the positron had been used as a fingerprinting tool.<sup>1,14</sup> In this work, this philosophy is applied to the high- $T_c$  oxides in an effort to gain as much information as possible about the nature of these very intriguing systems. In order to keep things simple, emphasis will be placed on the experimental positron lifetime data in single crystals since the interpretation of the powder data is expected to be complicated by the presence of defects which can trap the positron.

Experimental observations of positron lifetime in  $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$  and single-crystal  $\text{YBa}_2\text{Cu}_3\text{O}_7$  (Ref. 6) show a single component in the lifetime indicating the lack of defect trapping of the positrons. These systems, in which the positron is not trapped in defects and annihilates from an extended Bloch state, are expected to give information relevant to the nature of the quasiparticles and their condensation into the superfluid state. The experimental results in the two defect-free oxides are very similar, suggesting a common mechanism for superconductivity in the two systems.<sup>6</sup> In both systems, the lifetime increases from a value of  $\sim 176$  ps for  $T \geq T_c$  to a value of  $\sim 182$  ps in  $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$  and a value of  $\sim 187$  ps in  $\text{YBa}_2\text{Cu}_3\text{O}_7$  at  $\sim 5$  K. Signs of saturation are observed in the data in  $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$  at temperatures  $\sim 0.5T_c$ . In comparison, the lifetime in  $\text{YBa}_2\text{Cu}_3\text{O}_7$  seems to be just beginning to saturate at temperatures approximately equal to  $0.2T_c$ .<sup>6</sup>

### II. MODEL

#### A. General features

A common feature of the high- $T_c$  oxides is the presence of fourfold-coordinated Cu atoms arranged in planar structures.<sup>15,16</sup> In the yttrium compounds there are two types of  $\text{CuO}_4$  units; there are  $\text{CuO}_2$  planes just as in the lanthanum compounds, but in addition there are corner-sharing  $\text{CuO}_4$  units arranged in a fence or ribbonlike structure with Cu-O chains running along the center of the ribbons.<sup>15</sup> The oxides are believed to be strongly correlated electron systems. The half-filled-band systems  $\text{La}_2\text{CuO}_4$  and  $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ , in the region  $x \geq 0.7$ , are

insulating and show antiferromagnetism,<sup>17-19</sup> the dominant correlations being in the  $\text{CuO}_2$  planes. There are indications, however, of a moment developing on the Cu atoms in the chains of  $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$  at a temperature lower than the Néel temperature associated with the ordering in the planes.<sup>18</sup> These observations would indicate that the chains and the planes behave similarly in this compound. As the carrier (hole) concentration is increased, the antiferromagnetic order is destroyed and the materials become superconducting.

A good starting Hamiltonian for these systems is thought to be the Hubbard-Heisenberg model.<sup>20</sup> Various studies have been conducted to understand the motion of holes in such systems. Studies of hole motion in quantum antiferromagnets suggest that the bandwidth of the hole is much narrower than what would be expected from band-structure calculations, the degree of narrowing depending on the nature of the insulating ground state; e.g., Néel state<sup>21,22</sup> or a disordered state like the resonating-valence-bond state.<sup>23</sup> Other studies of hole motion in Hubbard-like models also indicate a narrow bandwidth and consequently a large effective mass of the hole.<sup>24-26</sup> For the purpose of building a simple model capable of dealing with the essential physics, the dynamics of the hole can therefore be adequately modeled by assigning a large effective mass to the holes.

The single positron introduced into the system as a probe<sup>1</sup> is not subject to any of the constraining effects due to spin ordering and moves about freely in the lattice avoiding the positively charged ion cores.<sup>5</sup> Its effective mass is then expected to be the same as its band mass and much smaller than the hole mass. This positron can annihilate with any of the electrons in the system, and the emitted  $\gamma$  rays are detected for measuring the positron lifetime and angular correlation spectra.<sup>1</sup> Positron densities have been calculated, in both the La and the Y compounds, using different techniques.<sup>5,6,12,13</sup> These calculations indicate that the positron density is peaked around the Cu-O bonds in the lanthanum compound. In the yttrium compound, the positron density is also peaked around the Cu-O bonds, but is concentrated in the region near the chains with very little density in the planes.<sup>5,12,13</sup> These features seem to be insensitive to the details of the calculations, and are consistent with the observation<sup>5,12,13</sup> that the positron is very sensitive to changes in the oxygen content which primarily affects the ordering along the chains, leaving the  $\text{CuO}_2$  planes virtually unaltered.<sup>15</sup> The similarity of the positron lifetime behavior in the two compounds would then suggest that the chains in  $\text{YBa}_2\text{Cu}_3\text{O}_7$  play a role in the superconducting transition.

### B. Model Hamiltonian

The experiments in the oxides indicate that a majority of the annihilations take place with tightly bound corelike electrons.<sup>5,13</sup> These core like electrons are expected to respond very weakly to the positron and one can ignore the effects of enhancement arising from the strong dynamic correlations between electrons and positrons.<sup>1</sup> The important correlations left over are the ones between the

heavy holes and the comparatively light positron. A simple model, describing the holes and the positron, which is expected to capture the essence of the physics of positron annihilation in the high- $T_c$  oxides, can be represented by the Hamiltonian

$$H = \sum_i \frac{p_i^2}{2m^*} + \frac{P^2}{2M} + \sum_n V_{at}(\mathbf{R}_n - \mathbf{R}_0) + \sum_i V_h(\mathbf{r}_i - \mathbf{R}_0). \quad (1)$$

The first term is the kinetic energy of the holes with effective mass  $m^*$ , the second term is the kinetic energy of the single positron, and the third and fourth terms describe the interaction of the positron with the atoms and the holes. The position of the holes are denoted by  $\mathbf{r}_i$ , the position of the atoms by  $\mathbf{R}_n$ , and the position of the positron by  $\mathbf{R}_0$ . In Eq.(1), the electrostatic interaction of the positron with the ions and electrons has been described by taking a superposition of atomic potentials.<sup>27</sup> The correlation potential describing the strong dynamic correlations between the positron and the itinerant electrons<sup>28</sup> has been neglected, the justification for this being the smallness of the overlap with the itinerant electrons. The interaction of the positron with the holes has been similarly approximated as a superposition of the electrostatic potential due to single holes.

In studying the high- $T_c$  oxides, one is interested in that regime of parameters where the effective mass of the hole  $m^*$  is much larger than the positron mass  $M$ . Under these circumstances one can invoke the adiabatic (Born-Oppenheimer) approximation, familiar in the context of the electron-lattice problem. The positron, which is moving on a time scale much shorter than that associated with the hole motion, sees a static distribution of holes and can always be in its ground state. The finiteness of the hole mass could lead to some changes in the effective potential felt by the positron and hence affect its motion. However, as long as the positron mass remains much smaller than the hole effective mass this potential is expected to be very similar to the static potential.<sup>29</sup> The positron wave function can then be calculated as a functional of the hole positions, and the positron-annihilation characteristics would then have to be calculated by taking overlaps of electron and positron states for a given distribution of holes and ensemble averaging over the hole positions. It can be expected then that any change in the nature of the distribution of holes will have a significant effect on the PAS results. It will be argued later that this is precisely what is responsible for the change in the positron lifetime on going through  $T_c$ .

A rough picture of the nature of the positron ground state, in the presence of a static distribution of holes, can be envisaged without doing any detailed calculations. The holes are expected to be localized around the Cu or O atoms and, to the positron, these sites then look like "impurity" atoms with one extra positive charge. The hole could possibly be smeared out over a few lattice sites in which case the effective extra positive charge per impurity site will be less than one. Compared to the "host" atoms the "impurity" atoms appear more repulsive to the positron due to the latter's extra positive charge. As a result

the positron redistributes; the positron density gets depleted in the region near the impurity atoms and its overlap with the tightly bound electrons of the impurity sites decreases. The effect does not have to be very large in order to cause a significant change in the positron lifetime as the impurity distribution is varied.

### C. Nature of the condensate

The Hamiltonian describing the nature of the positron dynamics has to be complemented with a description of the nature of the superfluid state before one can answer any questions regarding the change in PAS results from the normal to the superfluid state. There have been quite a few suggestions in the literature regarding the nature of the condensation in strongly correlated systems like the oxides.<sup>11,24,30-32</sup> These theories can be roughly divided into two broad categories; the ones involving Cooper pairs and the ones involving real (local) pair formation of the holes. This leaves out theories which do not involve any pairing. In the spirit of trying to build a model with unique features, the real-pair formation model will be adopted here. However, the consequences of taking a condensate of Cooper pairs will also be discussed.

In the present model of the superfluid state, where the holes form real pairs, the ground-state ( $T=0$ ) wave function can be written as a product of pair wave functions,  $\phi(\mathbf{r})$ , with the same wave function for all pairs.<sup>11</sup> Real pairing would also imply that  $\phi(\mathbf{r})$  be strongly peaked around small values of the pair separation and not have the long tail characteristic of Cooper pairs.<sup>11</sup> In the superconducting state, the positron would then see a strongly correlated distribution of impurities (cf. Fig. 1) since the fluctuations in the pair amplitude would be negligible in the condensed state and a classical picture of impurity

pairs can be applied. Above  $T_c$ , thermal fluctuations in the pairing amplitude would wash out any effects of pairing on the positron lifetime. This implies that ensemble averaging in the normal and superconducting states would involve very different impurity distribution functions. The effect of this can be simulated by taking a random distribution of isolated impurities above  $T_c$ , and a random distribution of impurity pairs (of varying sizes) and isolated impurities below  $T_c$ . The overlap of the positron with the bound pairs is expected to be different from that with two isolated impurities, and this could then be the source for the difference in positron lifetime between the normal and the superconducting states.

This completely defines the model system for which the positron annihilation spectra are to be calculated. Comparison of these results with experimental observations would then serve to show how good the model is in describing the high- $T_c$  oxides.

## III. POSITRON LIFETIME

### A. Normal and superconducting states

The positron lifetime is given by the inverse of the overlap of the electron and positron densities, if the enhancement of the electron density at the positron site can be neglected.<sup>1,28</sup> This is usually a good approximation for the overlap with tightly-bound electrons.<sup>27,28</sup> In the high- $T_c$  oxides, the majority of the annihilations takes place with tightly-bound electrons,<sup>5,13</sup> and the total lifetime can therefore be well approximated by the inverse of the overlap of the positron density with the density of core like electrons which is strongly peaked near the atomic sites. In the rest of the paper, the term overlap will refer to the overlap with *the tightly bound corelike electrons*. The correlation between the positron and the heavy holes has, however, to be taken into account in calculating this overlap. Within the adiabatic approximation, this is taken care of by considering a system of host atoms with a dilute concentration of impurities which have extra positive charge. The overlap, for a given distribution of holes, can then be written as

$$\Lambda(\{\mathbf{r}_i\}) = \sum_i \Lambda(\{\mathbf{r}_i\}) + \sum_n \Lambda_n^{\delta}(\{\mathbf{r}_i\}). \quad (2)$$

Here, the first term on the right represents the overlap with the impurity sites, and the second term the overlap with the host sites. The lifetime would be obtained by taking the inverse of this overlap, averaged over impurity sites with a given impurity distribution.

In the normal state there is a dilute concentration of holes, and the impurities can be taken to be randomly distributed; no correlation is expected between the positions of two holes. The overlap  $\Lambda_h^i$  can then be taken to be independent of the site index  $i$ . The overlap with the host sites can also be assumed to be independent of the site index, and the ensemble-averaged overlap written as

$$\Lambda^N = \Lambda_h n_h + \Lambda_0 (1 - n_h). \quad (3)$$

Here  $\Lambda^N$  denotes the total overlap with the tightly bound electrons,  $\Lambda_h$  denotes the overlap with the electrons bound

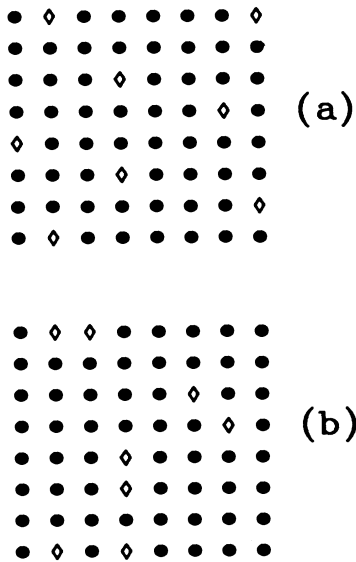


FIG. 1. Schematic plot of a square lattice with (a) isolated holes (diamonds), above  $T_c$  and (b) correlated pairs, below  $T_c$ .

to the impurity sites, and  $\Lambda_0$  denotes the overlap with the host sites. The number density of impurity sites, which is the same as the number density of holes, is given by  $n_h$ . The individual overlaps  $\Lambda_h$  and  $\Lambda_0$  depend on the specifics of the model and can be calculated, and, as discussed earlier, the former is expected to be smaller than the latter. The difference between  $\Lambda_h$  and  $\Lambda_0$  is, however, not very important in determining the trend in the temperature dependence of the lifetime in the superconducting compounds. What is important is the change in the total overlap upon pairing of the holes. The changes in lifetime as a function of doping, on the other hand, depends on the magnitude of this difference. This aspect will be briefly discussed later. The main aim of this work, however, is to understand the response of the positron to the superconducting transition.

In the superconducting state, there is a condensate of hole pairs and this implies a short-ranged correlation between the impurities. Allowing for the presence of impurity pairs in the impurity distribution, and making the same approximation about the site independence of the overlap with pairs, the ensemble averaged overlap in the superconducting state can be written as

$$\Lambda^s(T) = \Lambda_p \frac{n_s(T)}{2} + \Lambda_h [n_h - n_s(T)] + \Lambda_0 (1 - n_h) \quad (4)$$

$$= n_s(T) (\Lambda_p/2 - \Lambda_h) + \Lambda^N. \quad (5)$$

Here  $n_s(T)$  denotes the number density of correlated impurities, the condensate density. The average overlap with the pairs,  $\Lambda_p$ , is given by

$$\Lambda_p = \int \Lambda_p(\mathbf{r}) \phi(\mathbf{r}) d\mathbf{r}, \quad (6)$$

where the function  $\Lambda_p(\mathbf{r})$  is the overlap of the positron with the electrons in the region of an impurity pair, as a function of the pair separation. If the average overlap with the pair,  $\Lambda_p$ , is less than the overlap with two isolated impurities then  $\Lambda^s(T)$  will be less than  $\Lambda^N$ , i.e., the lifetime below  $T_c$  will be larger than that above  $T_c$ . The average overlap with the pair is expected to have this behavior if the pair wave function favors pair separations small enough for the impurity potentials to overlap. For Cooper pairs the long tail of the pair wave function would dominate the integral and no significant difference would exist between  $\Lambda_p/2$  and  $\Lambda_h$ .

At  $T=0$ , the condensate density reaches its maximum value as does the lifetime. At temperatures above  $T=0$  but below the transition temperature, a finite fraction of the holes are excited out of the condensate due to pair breaking. These holes then appear to the positron as isolated impurities. If it is assumed that the nature of the pair wave function does not change with temperature,<sup>33</sup> then the only temperature-dependent factor entering the positron lifetime would be the condensate density. This implies that the temperature dependence observed in the experiments is that of the condensate density  $n_s(T)$ . By fitting the experimental lifetime data to the inverse of the overlap given by Eq. (4), the temperature dependence of  $n_s(T)$  could therefore be extracted.

Muon-spin-relaxation ( $\mu$ SR) experiments give a measure of the superfluid density,<sup>34</sup> and a comparison of the

two types of experiments does indicate similar trends in the positron lifetime and the relaxation rate in  $\mu$ SR. It is not absolutely clear that the same physical quantity is measured in the two experiments. In  $\mu$ SR, the penetration depth is measured and related to the superfluid density which is defined in terms of the long-wavelength response of superconducting electrons to a transverse vector potential. According to the present model, the positron lifetime measures the condensate density, and there is no real justification for identifying this with the superfluid density.<sup>35</sup> The condensate density, measured by the positron, seems to show a linear temperature dependence over a larger temperature region<sup>6</sup> than the superfluid density as measured by muons.<sup>34</sup> The superfluid density and the condensate density are both expected to saturate at low enough temperatures. However, the characteristic temperature could be different in the two cases and is expected to be model specific.

The  $\mu$ SR experiments indicate a nearly linear relationship between  $n_s(T=0)$  and  $T_c$ .<sup>34</sup> A comparison of the positron lifetime data in  $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$  and  $\text{YBa}_2\text{Cu}_3\text{O}_7$  (Ref. 6) shows that the difference between the lifetime at  $T=0$ ,  $\tau^S(T=0)$ , and the normal-state lifetime,  $\tau^N$ , is smaller in the former than in the latter compound. According to Eq. (4), the relative difference in the lifetimes is given by

$$\frac{\tau^S(T=0) - \tau^N}{\tau^S(T=0)} = n_s(T=0) \left( \Lambda_h - \frac{\Lambda_p}{2} \right) \tau^N. \quad (7)$$

There can, therefore, be two sources of the observed difference; the value of the condensate density at  $T=0$  or the difference in the overlaps,  $\Lambda_p$  and  $\Lambda_h$ . Assuming that the overlaps are the same, the ratio of the condensate densities can be calculated from the experimental data<sup>6</sup> and is found to have a value close to 2. This is similar to the ratio of the superfluid densities deduced from the  $\mu$ SR data. In making any detailed numerical comparison between experimental positron lifetime data and the present model, it should be remembered that the valence-electron contribution to the positron lifetime has been completely neglected in the model.

According to the present description of PAS in the oxides, any model of superfluidity which involves real-space pairing would lead to a Bloch-state lifetime increasing with temperature below  $T_c$ . More specific information can be obtained by comparing in detail the experimental values with predictions of  $\Lambda_p$  and  $\Lambda_h$  obtained from realistic calculations. The experimental observations can be used as a guide in choosing specific models.

## B. Calculation of overlap

The experimentally observed difference in lifetime between the lowest observed temperature and  $T_c$  for both compounds is of the order of 10–15 ps, i.e., less than 10% of the value above  $T_c$ . This would imply [cf. Eq. (7)] that  $(\Lambda_p/2 - \Lambda_h)/\Lambda^N$  is of the order of 10%. To check if the present model would predict anything in this range, a simple calculation of holes in a jellium background was carried out.

It was assumed that in the absence of the holes the positron saw a uniform neutral background. A pair of holes was then introduced into this system and the hole potentials were taken to be the muffin-tin versions of the Coulomb potential due to two positive point charges (cf. Fig. 2). The separation between the holes was then varied, and the positron wave function calculated by the Wigner-Seitz method.<sup>36</sup> The boundary condition imposed was that the positron wave function be a constant in the region where the potential remains constant, the radial derivative of the wave function going to zero at this boundary.

An important aspect of positron annihilation in the high- $T_c$  oxides is the predominance of the overlap of the positron with tightly bound corelike electrons, indicating that the density of delocalized electron is very small in

these systems. It was for this reason that the analysis in this paper has been restricted to the overlap of the positron with *only the tightly bound electrons*. To simulate this effect in the jellium, where the electron density is a constant, the electron-positron overlap was calculated by restricting the integrals to within the volume of the muffin-tin sphere around each hole: this gives an effective "core" overlap. If instead, the total overlap had been calculated, with a constant electron density throughout the volume of the system, there would be no effect due to the pairing, or the presence, of the holes since the positron wave function is normalized. Normalization implies that a decrease in the positron wave function in the region of the holes has to be accompanied by an increase elsewhere in the system. In the context of the oxides, this implies that if the electron density in the core and the interstitial regions were comparable then there would be a near cancellation between the decrease in the core-electron overlap and the accompanying increase in the valence-electron overlap. It is therefore worth stressing again the importance of the observation that the overlap with corelike electrons is much larger than the overlap with the delocalized electrons. Admittedly, the overlap with the valence electrons will increase as the core overlap decreases. However, this will be a much smaller effect and is not expected to change the trend in the positron lifetime. A quantity that measures *only* the overlap with the tightly bound electrons is the Doppler-broadening parameter  $(1-S)$  and this is seen to decrease with temperature below  $T_c$ .<sup>6</sup>

Results of the jellium calculation of the "core" overlap are shown in Fig. 2. It can be seen clearly that this overlap is much smaller than the isolated hole value for pair separations of the order of the hole radius. Even when the holes are as far apart as five times this value, the difference in the overlap with that of an isolated hole is large enough to give the difference observed in experiment. Admittedly, this simple model is very far removed from the real system of Cu and O atoms. However, it does serve to show the effect of the pairing of holes on the positron.

More realistic calculations can be carried out with the actual lattice structure and electronic configuration of the atoms taken into account. The conclusions regarding the lifetime are, however, not expected to change very much since the most important ingredient of the calculation is that the positron sees a more repulsive potential due to, say a  $(\text{Cu}^{1+}, \text{Cu}^{1+})$  pair as compared to a  $(\text{Cu}^{0+}, \text{Cu}^{1+})$  pair; a fact evident from results of atomic calculations.<sup>37</sup> Detailed calculations are expected to be very useful in trying to sort out differences between different hole sites (Cu or O) and also in obtaining the angular correlation spectra. An important question which can be addressed there would be the symmetry of the pair wave function, since this will be reflected in the symmetry of the impurity pair, taken to be spherically symmetric in the jellium calculation. The anisotropy of the pair wave function can be expected to determine the anisotropy of the calculated angular correlation spectra. Realistic calculations can also sort out questions about the relative importance of core and valence overlaps.

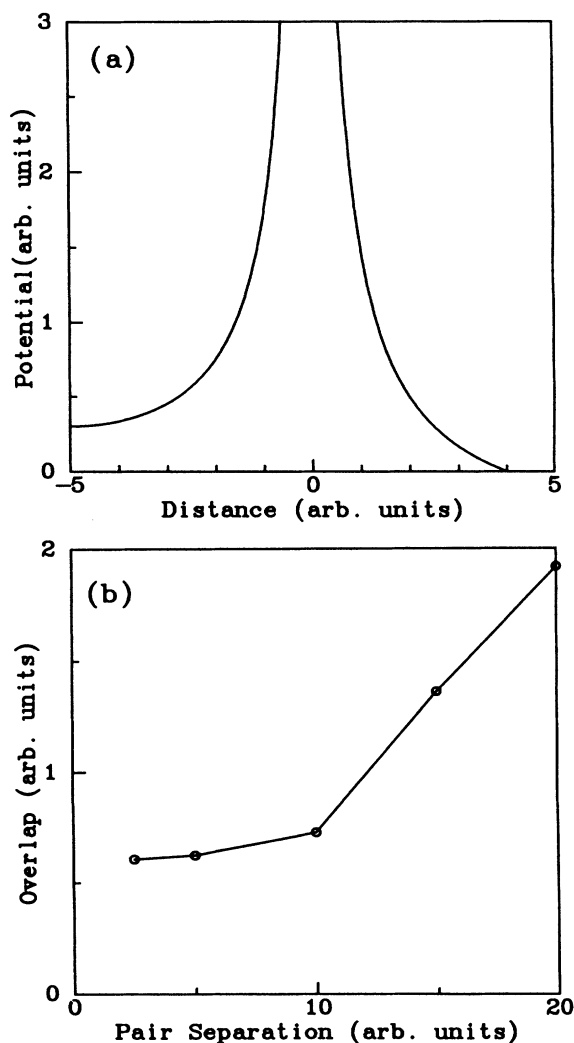


FIG. 2. Muffin-tin potential due to a hole pair in a uniform background; the holes are situated at 0.0 and  $-10.0$  and the hole radius (muffin-tin radius) is 4.0. (b) The overlap  $\Lambda_p(r)/2$  as a function of the pair separation. The value of  $\Lambda_h$  in these units is 2.0. The pair separation is measured in the same units as the distance in (a).

It should be noted that in the actual systems, the positron sees a random potential due to the static holes and will therefore not be in a truly extended state. The envelope of the positron wave function would be peaked in regions away from the holes and depending on the degree of disorder introduced by the holes it could undergo something akin to Anderson localization.<sup>38</sup> In particular, clustering of holes could lead to an increase in the degree of disorder and to a decrease in the localization length. This seems to be an attractive way of understanding the change in the nature of positrons on going from the normal to the superconducting state and would be worth pursuing. However, the effects of the finite mass of the holes would probably have to be taken into account.

### C. Effects of doping

As mentioned before, the positron lifetime depends on doping. This is consistent with the model for  $\Lambda^N$  given by Eq.(3). According to this model, the lifetime should increase (the core overlap decrease) with increasing hole concentration. This could provide an explanation for the observed trend in the Bloch-state lifetime in  $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$  between  $x=0.2$ ,  $\tau^N=165$  ps and  $x=0.0$ ,  $\tau^N=176$  ps. The application of the model would require that the Bloch states be similar as the hole concentration is varied. This is not the case for  $x \geq 0.5$  and, therefore, a straightforward application of the model is not possible. It would be interesting to study in detail the behavior of the Bloch-state lifetime in the region  $0.0 \leq x \leq 0.2$  and correlate it with the hole concentration in the chains and the planes.<sup>39</sup>

### D. Trapped state lifetime

The polycrystalline data show a *decrease* in the trapped state lifetime as a function of temperature below  $T_c$ . A possible explanation for this in light of the present model is a change in the binding energy and, therefore, the trapped state of the positron. Hole pairing can increase the probability of finding a vacancy with two holes close to it. Such a vacancy has fewer electrons leaking into it, and, hence, a less attractive potential than a vacancy with only one hole close to it. Below  $T_c$ , the positron can therefore annihilate from two types of traps, one with a lower binding energy than the other, and the concentration of the trap with the lower binding energy increases as the temperature is decreased. The positron lifetime in the shall-

lower trap is expected to be smaller than that in the deeper trap since it can leak out more into the core regions of atoms when the binding energy is lower. Since the vacancies are thought to be at the oxygen sites, holes on the Cu sites would have a larger effect on the vacancy potential, since they are closer to the vacancy, than holes on the O atoms, which are farther away. Detailed calculations could therefore be used to distinguish between the two types of hole sites.

## IV. CONCLUSION

In conclusion, a very simple model has been presented for understanding the trends in the PAS of the high- $T_c$  oxides. The major prediction of the model is that the overlap of a delocalized positron with the core electrons decreases with temperature below  $T_c$ , the decrease being proportional to the *condensate density*. This implies an increasing positron lifetime below  $T_c$ , which is in qualitative agreement with experiment. A comparison of the experimental lifetime data with the present model indicates a correlation between  $T_c$  and the condensate density at  $T=0$  which is similar to the correlation observed in  $\mu\text{SR}$  experiments. The model can also provide an explanation for the trend in lifetime as a function of doping and the change in the trapped state lifetime from the normal to the superconducting state.

A simple jellium calculation has been carried out to demonstrate the effect of pairing on the positrons. More realistic calculations, based on the present model, should be extremely useful in gaining detailed knowledge about the nature of the holes and their pairing.

The generally good agreement between the predictions of the model and the experimental observations would suggest a mechanism for superfluidity which involves real pairing of the holes. The model is built on the basic premise of the holes having a narrow bandwidth and its success would then imply that the holes do indeed have a much narrower bandwidth than would be expected from band theory.

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<sup>1</sup>R. N. West, Adv. Phys. **22**, 263 (1974).

<sup>2</sup>C. S. Sundar, A. K. Sood, A. Bharathi, and Y. Hariharan, Pragma **30**, L161 (1988).

<sup>3</sup>Y. C. Jean, S. J. Wang, H. Nakanishi, W. N. Hardy, M. E. Hayden, R. F. Kiefl, R. L. Meng, H. P. Hor, J. Z. Huang, and C. W. Chu, Phys. Rev. B **36**, 3994 (1987).

<sup>4</sup>S. G. Usmar, P. Sferlazzo, K. G. Lynn, and A. R. Moodenbaugh, Phys. Rev. B **37**, 8854 (1988).

<sup>5</sup>E. C. Von Stetten, S. Berko, X. S. Li, R. R. Lee, J. Brynstad, D. Singh, H. Krakauer, W. E. Pickett, and R. E. Cohen, Phys.

Rev. Lett **60**, 2198 (1988).

<sup>6</sup>Y. C. Jean, J. Kyle, H. Nakanishi, P. E. A. Turchi, R. H. Howell, A. L. Wachs, M. J. Fluss, R. L. Meng, H. P. Hor, J. Z. Huang, and C. W. Chu, Phys. Rev. Lett. **60**, 1069 (1988).

<sup>7</sup>D. R. Harshman, L. F. Schneemeyer, J. V. Waszczak, Y. C. Jean, M. J. Fluss, R. H. Howell, and A. L. Wachs, Phys. Rev. B **38**, 848 (1988).

<sup>8</sup>B. Green and L. Madansky, Phys. Rev. **102**, 1014 (1956).

<sup>9</sup>C. V. Briscoe, J. Beardsley, and A. T. Stewart, Phys. Rev. **141**, 379 (1966).

- <sup>10</sup>G. Faraci and M. Spadoni, Phys. Rev. Lett **22**, 928 (1969).
- <sup>11</sup>J. R. Schrieffer, *Theory of Superconductivity* (Benjamin, Reading, Massachusetts, 1964).
- <sup>12</sup>A. Bharathi, Y. Hariharan, A. K. Sood, V. Sankara Sastry, M. P. Janawadkar, and C. S. Sundar, in *Proceeding of the International Conference on High  $T_c$  Superconductors, Interlaken, Switzerland, 1988*, edited by J. Müller and J. L. Olsen [Physica C **153–155**, 111 (1988)].
- <sup>13</sup>M. J. Fluss, A. L. Wachs, P. E. A. Turchi, R. H. Howell, Y. C. Jean, J. Kyle, H. Nakanishi, C. W. Chu, R. L. Meng, H. P. Hor, and J. Z. Huang, in *Proceedings of the World Congress on Superconductivity, Houston, Texas, 1988*, edited by C. G. Burnham and R. D. Kane, Progress in High Temperature Superconductivity (World Scientific, Singapore, 1988), Vol. 8, p. 357.
- <sup>14</sup>Michael J. Fluss, S. Berko, Bulbul Chakraborty, K. R. Hoffmann, P. Lippel, and R. W. Siegel, J. Phys. F **14**, 2831 (1984).
- <sup>15</sup>J. D. Jorgensen, M. A. Beno, D. G. Hinks, L. Soderholm, K. J. Volin, R. L. Hitterman, J. D. Grace, Ivan K. Schuller, C. U. Segre, K. Zhang, and M. S. Kleefisch, Phys. Rev. B **36**, 3608 (1987).
- <sup>16</sup>J. D. Jorgensen, H. B. Schuttler, D. G. Hinks, D. W. Capone II, K. Zhang, M. B. Brodsky, and D. J. Scalapino, Phys. Rev. Lett. **58**, 1024 (1987).
- <sup>17</sup>J. M. Tranquada, D. E. Cox, W. Kunnann, H. Moudden, G. Shirane, M. Suenga, P. Zolliker, D. Vaknin, S. K. Sinha, M. S. Alvarez, A. L. Jacobson, and D. C. Johnston, Phys. Rev. Lett. **60**, 156 (1988).
- <sup>18</sup>J. W. Lynn, W. H. Li, H. A. Mook, B. C. Sales, and Z. Fisk, Phys. Rev. Lett **60**, 2781 (1988); H. Kadowaki, M. Nishi, Y. Yamada, H. Takeya, H. Takei, S. Shapiro, and G. Shirane, Phys. Rev. B **37**, 7932 (1988).
- <sup>19</sup>T. Freltoft, J. E. Fischer, and G. Shirane, D. E. Moncton, S. K. Sinha, D. Vaknin, J. P. Remeika, A. S. Cooper, and D. Harshman, Phys. Rev. B **36**, 826 (1987); S. Mitsuda, G. Shirane, S. K. Sinha, D. C. Johnston, M. S. Alvarez, D. Vaknin, and D. E. Moncton, *ibid.* **36**, 822 (1987).
- <sup>20</sup>P. W. Anderson, Science **235**, 1196 (1987).
- <sup>21</sup>S. Schmitt-Rink, C. M. Varma, and A. E. Ruckenstein, Phys. Rev. Lett. **60**, 2793 (1988), and references therein.
- <sup>22</sup>S. Sachdev, Phys. Rev. B **38**, 826 (1988).
- <sup>23</sup>C. L. Kane, P. A. Lee, and N. Read (unpublished).
- <sup>24</sup>V. J. Emery, Phys. Rev. Lett. **58**, 2794 (1988).
- <sup>25</sup>J. R. Schrieffer, X. G. Wen, and S. C. Zhang, Phys. Rev. Lett. **60**, 944 (1988).
- <sup>26</sup>E. Kaxiras and E. Manousakis, Phys. Rev. B **38**, 866 (1988).
- <sup>27</sup>M. J. Puska and R. M. Nieminen, J. Phys. F **13**, 333 (1983).
- <sup>28</sup>Bulbul Chakraborty and R. W. Siegel, Phys. Rev. B **27**, 4535 (1983).
- <sup>29</sup>Bulbul Chakraborty, Mats Nylén, and P. Hedegård, J. Phys. C **21**, 3437 (1988).
- <sup>30</sup>M. J. Rice and Y. R. Wang, Phys. Rev. B **37**, 5893 (1988).
- <sup>31</sup>E. J. Mele (unpublished).
- <sup>32</sup>J. M. Wheatley, T. C. Hsu, and P. W. Anderson, Phys. Rev. B **37**, 5897 (1988).
- <sup>33</sup>In BCS theory this would amount to the approximation that the  $k$  dependence of the gap function  $\Delta_k$  did not vary with temperature (cf. Ref. 11).
- <sup>34</sup>Y. J. Uemura, V. J. Emery, A. R. Moodenbaugh, M. Suenaga, D. C. Johnston, A. J. Jacobsen, J. T. Lewandowski, J. H. Brewer, R. F. Kiefl, S. R. Kreitzman, G. M. Luke, T. Rise-man, C. E. Stronach, W. J. Kossler, J. R. Kempton, X. H. Yu, D. Opie, and H. E. Schone, Phys. Rev. B **38**, 909 (1988).
- <sup>35</sup>L. D. Landau and E. M. Lifshitz, *Statistical Physics*, Pt. II (Pergamon, Oxford, 1980), Chap. V.
- <sup>36</sup>M. J. Stott and P. Kubica, Phys. Rev. B **11**, 1 (1975).
- <sup>37</sup>F. Herman and S. Skillman, *Atomic Structure Calculations* (Prentice Hall, Englewood Cliffs, New Jersey, 1963).
- <sup>38</sup>P. W. Anderson, Phys. Rev. **109**, 1492 (1958).
- <sup>39</sup>J. Zaanen, A. T. Paxton, O. Jepsen, and O. K. Andersen, Phys. Rev. Lett. **60**, 2685 (1988).