On self-protecting singlets in cuprate superconductors

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Abstract

The basal area (Cu–Cu grid) of the cuprate superconductors not only tends to shrink on hole doping, as expected from single electron quantum chemistry, but exhibits also an electronically incompressible “hump” around optimum doping \( n_{\text{opt}} \simeq 0.16 \). The hump collapses near critical doping \( n_{\text{opt}} \simeq 0.19 \). We analyze the origin of the hump in terms of a classical liquid of interacting incompressible particles in a container with antiferromagnetic walls. Oxygen holes interacting with the wall form singlets, protect themselves against other holes by an incompressible “spin fence”, and thus interact also with the lattice. Occupation of the CuO\(_2\) lattice with holes must therefore follow a non-double-occupant constraint also for the oxygen cage enclosing the copper hole. Closest packing of self-protecting singlets is found to occur around critical doping; closest packing of \textit{paired} self-protecting singlets around optimum doping. These singlet-states are bosonic, but are not magnetic polarons.
INTRODUCTION

The lattice parameters of the cuprate superconductors are well known strong functions of doping. It is however only poorly understood whether their doping dependence is extrinsically controlled from the complex stereochemistry of the doping blocks outside, or intrinsically by the properties of the strongly correlated electron states residing inside the CuO$_2$ planes. The external chemistry and the embedded metallic layer reside in the same unit cell, and hence both are expected to co-determine the doping induced variations of the cell parameters. How to disentangle the most important intrinsic effects from the extrinsic ones? Detailed inspection of many of the available lattice data [1, 2, 3, 4, 5, 6], displaying doping dependencies in the single- and multi-layer compounds of different families, shows forces of different nature to govern the behaviours of the $a$-, $b$-parameters in the planar directions, and of the $c$- parameter in the perpendicular direction. $a$ and $b$ tend to contract with increasing hole concentration, almost independent on the number of CuO$_2$ layers and the chemistry of the doping block. Uniaxial strain from the dopants may mask or even invert the shortening of one of the basal bondlengths, e.g. in underdoped YBa$_2$Cu$_3$O$_x$ where $a$ contracts as $b$ expands [1]. But the basal area $B$, defined by the square of the basal Cu–Cu distances, turns out almost unaffected by strain from the doping block. Thus $B$ allows better for comparisons between compounds from different families than the individual basal bond lengths. The $c$-parameter however seems to behave arbitrarily: as the basal plane contracts, $c$ may expand, contract, or both [1, 2, 3, 5]. Apparently the problem of entangled intrinsic and extrinsic doping effects on the lattice seems to solve quite naturally: the behaviour of the basal plane is governed by the nearly-2D quantum liquid residing in it, while that of the perpendicular parameter is dominated by the chemistry of the environment. In this article we will focus on the doping dependence of the basal plane $B(x)$, in particular on the origin of the strong hump around optimum doping, see Figs. 1, 2, 3, 4.

EXPERIMENTAL DATA

Figs. 1, 2, 3, 4 display the basal areas $B$ of typical one- and two-layer cuprates as a function of doping. $B$ refers to the grid of $nn$ planar copper atoms as reported from x-ray or neutron diffraction measurements at room-temperature by Radaelli et al. 2 (La$_{2-x}$Sr$_x$CuO$_4$, 
$T_{c_{\text{max}}} = 36 \text{ K}$, Fukuoka et al. [3] (HgBa$_2$CuO$_x$, $T_{c_{\text{max}}} = 96 \text{ K}$; and HgBa$_2$CaCu$_2$O$_x$, $T_{c_{\text{max}}} = 127 \text{ K}$), Böttger et al. [4], and Kaldis [1] (Y$_{1-y}$Ca$_y$Ba$_2$Cu$_3$O$_x$, $T_{c_{\text{max}}} = 92 \text{ K}$). The thick drawn out lines connecting the data points are guides to the eye.

The overall behavior of $B(x)$ exhibits surprisingly strong similarities in all systems under comparison: i. As expected from the increasing covalency with hole doping the basal areas shrink between the insulator–metal transition and the strongly overdoped regime. The contraction is in the order of 1.5% ii. $B(x)$ exhibits a hump centered around optimum doping. The hump is weakest in La$_{2-x}$Sr$_x$CuO$_4$, and strongest in HgBa$_2$CaCu$_2$O$_x$. Its maximum is centered around optimum doping $x_{opt}$.

Following quantum chemical approximations hole doping will remove electrons from the antibonding $\sigma^*Cu3d_{x^2-y^2}O2p_{x,y}$ band, increase the amount of covalent character in the Cu–O bonds, and will shorten them. The hump indicates a significant deviation from this one electron bandstructure picture. The thin dashed straight lines in Figs. are fitted to the data points at the strongly under- and overdoped ends and, extrapolated towards the underdoped-overdoped phase boundary, turn out to intersect around $x_{opt}$. They may serve as coarse approximations for the quantum chemical “background” $B_0(x)$. Its change of slope around $x_{opt}$ might indicate that the Cu–O bonding changes from semicovalency in the underdoped to covalency in the overdoped regime.

Evidently the hump stems from the strong correlations of the holes in the CuO$_2$ planes. Its location at optimum doping points also to a connection with the superconductivity occurring at much lower temperatures than 300 K. Consider the compressibility of the quantum liquid in the planes is approximated by $\kappa_e \propto -\partial(B - B_0)/\partial n$, where $n$ is the number of holes/Cu/unit area, and $n \propto x$. Then $\kappa_e \simeq 0$ close $x_{opt}$, i.e the quantum liquid is incompressible around the optimum hole concentration $n_{opt} = 0.15 - 0.16$, notably not at quarter filling $n = 0.25$.

In some compounds the collapse of the hump occurs together with subtle structural instabilities in the crystallographic cell, of martensitic type in YBa$_2$Cu$_3$O$_x$ [7, 8], or of order-disorder type in HgBa$_2$Cu$_2$O$_x$ [6]. Evidently these lattice instabilities are connected with the transition into the overdoped regime, but are most likely not at its origin.

Stable long range ordered nano domains might be another source of the hump. La$_{2-x}$Sr$_x$CuO$_4$, due to its octahedral tilts the system most susceptible to stable nano domains, exhibits however the weakest hump. On the other hand the Hg-cuprates with their
almost flat CuO$_2$ lattices, devoid of structural compliance, exhibit the strongest humps.

**THE MODEL**

Consider $B(x)$ reproduces the equation of state of the quantum liquid confined to the CuO$_2$ lattice. Suppose that the temperature is sufficiently high and the density of classical particles sufficiently low, then $B(x)$ exhibits a striking similarity with the van der Waals equation, or related types describing classical real gases. Here we describe the particles by singlets of oxygen hole and copper spins. We address the question, how a quantum liquid, created through singlet formation in a hole doped CuO$_2$ lattice, may be connected with lattice properties such as $B(x)$ and its hump around $x_{opt}$. Further down we will also try to justify why the problem may be phrased in terms of a classical Bose gas scheme.

We consider the antiferromagnetic lattice of the copper spins as the walls of the “container” enclosing the available area for the spin singlets created upon hole doping. The moving holes exert a mean pressure (positive or negative) on the antiferromagnetic lattice given by $p \propto nt$ where $t$ is the average kinetic energy of the hole. Note that a Fermi liquid confined in the volume of its metal exerts its mean pressure only on the atomic lattice.

A doped hole at an oxygen site destroys the antiferromagnetic order in its vicinity and thereby leads to an attractive interaction when it shares the region of depressed antiferromagnetic order with a copper hole. The attractive interaction creating the spin singlet thus tends to keep the oxygen and Cu atoms closer together than it would be the case for noninteracting holes. Böttger and Dichtel [9] find from a three-band Hubbard model an oxygen displacement per hole by -0.04 Å along the Cu–O bond. The creation of singlets has thus the same effect as a slight compression of the basal area complying with an increasing pressure. Thus the oxygen holes interact also strongly with the atomic lattice “eating” spins in the antiferromagnetic wall of its container.

On the other hand short-range repulsive forces between the singlets keep them sufficiently apart to prevent them from occupying the same places at the same time. The area occupied by a singlet themself must be thus subtracted from the area available to any other singlet in the container. For sufficiently high doping the repulsive interaction between singlets will start to outweigh the contraction of lattice driven by singlet creation. Long range attractive interactions between the singlets will pack them more closely in the container and thus may
act as an additional pressure.

The potential energy $U$ of the interaction between the singlets may be expressed only by their relative separation $R$, in its simplest form as

$$U(R) = \begin{cases} 
\infty & : R < R_0 \\
-U_0(R_0/R)^s & : R > R_0
\end{cases}$$

(1)

$R_0$ is the minimum possible separation between incompressible singlets. The exponent $s$ is e.g. $\simeq 6$ in typical van der Waals gases.

Long range interactive forces may create also paired singlets excluding a larger area than two unpaired singlets. Then the area available to other singlets will be even more reduced than by closely packed unpaired singlets. As a result formation of paired singlets will render the CuO$_2$ lattice even less compressible than most closely packed unpaired singlets. It is therefore suggesting to assume that the optimum doped incompressible CuO$_2$ lattice accommodates its holes ($n_{opt} = 0.16$) in closest packed paired singlets.

The self-protecting singlet (SPS)

How large will be the incompressible areas covered by a paired singlet, and a unpaired singlet, respectively? Paired singlets in the most closely packed conformation have to match the maximum of the hump at $n_{opt} \simeq 0.16$. Unpaired singlets in the most closely packed conformation are expected to match a critical hole concentration $n_{crit}$, slightly larger than $n_{opt}$. For $n > n_{opt}$ paired singlets will start to overlap with each other and thus will be broken, and the hump will collapse. We locate the collapse of the hump around $n_{crit} \simeq 0.19$. For $n > n_{crit}$ even unpaired singlets will be broken, but may create a new type of singlet state excluding a smaller area than the singlets at $n < n_{crit}$.

We consider a perfect antiferromagnetic CuO$_2$ lattice. The non-double-occupant constraint for the Cu$3d^9$ sites requires that doping must create additional holes on the oxygen sites. Hirsch [10] showed that without flipping Cu spins a doped oxygen hole can only move within a “cage” of four oxygen atoms surrounding the nearest Cu atom. This is due to the phase coherence in the symmetric combination of the four oxygen states. Zhang and Rice [11] worked out that the binding energy of the resulting spin-singlet state of the symmetric oxygen hole and the Cu hole is 4 times higher compared to that of a spin-singlet state.
of an oxygen hole sitting at a fixed site, and the Cu hole. Thus the so-called Zhang-Rice (ZR) singlet distinguishes itself from other possible singlet states by its extraordinarily high stability. The cage determines the area covered by a ZR singlet and is given by $d_{O-O}^2 = a^2/2$. Here $d_{O-O}$ is the $nn$ oxygen-oxygen distance, and $a$ the Cu–Cu distance. The ZR singlet has no magnetic interactions with all other copper holes. But two neighbored holes trying to share their oxygen cages with each other will feel a strong repulsion. Thus formation of $nn$ singlets in connected cages will be very unlikely. Rather the ZR singlets will strongly repel each other, and thus will create an excluded area around their cages.

To protect the symmetric oxygen hole in the cage from other holes, the excluded area has to extend at least over the four neighbored cages containing the 4 $nn$ Cu spins. The 4 $nn$ Cu spins are exempted from the formation of own singlet states but act as a “fence” enclosing the ZR singlet. We label this as “self-protection” of the ZR singlet for a safe life, at least within its spin fence. Hence a Cu$_5$O$_{16}$ cluster occupied by one oxygen hole in the central cage appears to be the minimum conformation for a stable singlet, that is a self protecting singlet (SPS). It covers nine $nn$ oxygen-oxygen squares with an area $3d_{O-O}^2 = 9/2a^2$. Fig. 5 displays a SPS in the antiferromagnetic CuO$_2$ lattice. The circle enclosing the central cage indicates the ZR singlet, the hatched cages the excluded area with the spin fence.

The Cu$_5$O$_{16}$ cluster comprising a self protecting singlet (SPS) looks alike a polaron, but is not a conventional spin polaron polarizing the Cu lattice ferromagnetically. Here holes and spins are in the same band unlike the situation in the magnetic polarons.

Upon propagation of the SPS from a given site to a neighbored site the oxygen hole has to flip its spin, and will thus be able to create a singlet with the $nn$ Cu hole. The Cu spin of the abandoned site will recover and hence a possible “loop-hole” in the spin fence will be closed. Thus the spin fence moves together with the propagating hole while the antiferromagnetic lattice remains intact. This scenario has appealing similarities with the “spin-bag” mechanism proposed by Schrieffer et al. [12] in that both, the spin-bag and the self protecting singlet, are both polaron-like, but are not conventional spin-polarons with heavy masses. We understand however that a fundamental difference occurs in that in the spin-bag mechanism the propagating hole and its surrounding bag act as fermionic quasiparticle, whereas a hole propagating in a self-protecting singlet has to be considered as a bosonic particle.

We may phrase the description of the SPS in terms of another non-double-occupant
constraint for the doped holes: the grid of the 5 oxygen corner linked oxygen cages in a Cu$_5$O$_{16}$ cluster may be only singly occupied. Or alternatively expressed: the spin fences of self-protecting singlets are not allowed to overlap.

Respecting both non-double-occupant constraints, that for the Cu sites and that for the oxygen cages, it is apparent that the maximum number of singlet states in a doubly constrained CuO$_2$ lattice will be much smaller than in the only singly constrained case. We will show further below that the doubly constrained doping of holes in a CuO$_2$ lattice will be generically inhomogenous for sufficiently high concentrations. Ignoring the non-double-occupant constraint for the oxygen cage will however allow for homogenous hole distributions at optimum doping, as e.g. in the RVB models [13].

Using the information from the experimental B(x) we will estimate the minimal size of the particles occupying the CuO$_2$ lattice in the different regimes of doping.

The paired self-protecting singlet (PSPS)

Fig. 6 displays two self-protecting singlets sharing a common oxygen site along the direction of the Cu–O bond. This conformation may lead to an exchange of holes between two intact ZR singlets (closed circles) through opened spin fences as indicated by the dashed circles. The thus connected SPS are fully antisymmetric in respect to the connecting oxygen and may form in principle a paired ZR singlet state as proposed by Müller [14]. Self-protection of the “paired” singlet will be achieved by an enlarged spin fence as indicated by the cross-hatched squares in Fig. 6. The area, covered by the spin fence of the PSPS, is nominally 12a$^2$, significantly larger than 9a$^2$, the area protected by the spin fences of two nonbonding SPS. Thus formation of a PSPS will reduce the area available to other singlets much more than most closely packed SPS. Notably the PSPS extends over 4a $\approx$ 15 Å (a chain of four corner-linked oxygen cages), nearly coinciding with the experimentally established planar superconducting coherence length $\xi_{ab}$.

Because of the contraction of the Cu–O bonds upon singlet formation both, the SPS and the PSPS, are expected to exhibit important vibrational properties. Notably the oxygen holes are expected to breathe within the rigid 2a cell of the spin fence as observed in e.g. optimum doped La$_{1.85}$Sr$_{0.15}$CuO$_4$ by McQueeney et al. [15].
Characteristic distributions of SPS and PSPS

Consider the CuO\textsubscript{2} lattice as an array of corner linked oxygen cages each enclosing one Cu atom (Figs. 7-10). One SPS covers five of these cages and thus forms a 3 × 3 supercell. The 3 × 3 supercells will create a checkerboard lattice of black (dark/red) fields with “crosses” of 5 cages, and white (grey) fields with “squares” of 4 cages. Doping will distribute the holes as SPS over this checkerboard lattice. At sufficiently high concentrations the SPS will touch each other, form clusters, or most likely PSPSs. A full occupation of the lattice may be realized by many different distributions leading to a remarkable sequence of characteristic hole concentrations. Figs. 7-10 sketch four possible distributions relevant for the understanding of the phase diagram of the cuprates. The SPS are indicated by objects with a circular cage (the singlet hole) enclosed by a square (the spin fence).

*Stripy long range ordering: n = 0.11 \simeq n_s*

In Fig. 7 each “cross” (dark/red) is occupied with one SPS. Hence the “squares” (grey) will not be available for the SPS. The SPS will thus align in crossing chains along \(a\). One hole rich chain alternates with two empty chains creating therewith a 3\(a\) superstructure. Presumably pairing of neighbored SPS to PSPSs will be suppressed by long range ordering. Only 0.11 holes/Cu are accommodated by this “stripy” distribution.

*Critical Doping: n = 0.20 \simeq n_{crit}*

To achieve closer packing of holes the SPS have to be distributed over the crosses and the squares of the checkerboard lattice. Fig. 8 displays a possible distribution for a high density of holes. Cells excluded by the spin fences are cross-hatched. The distribution for the maximum number of SPS will be realized by most closely packing at \(n_{crit}\). For \(n > n_{crit}\) the spin fences will overlap and destroy the self-protection of the singlets. Interestingly this leads generically to an inhomogeneous hole distribution, apparently because the “crosses” and “squares” in the checkerboard lattice are not equivalent for the cross-shaped SPS. The inhomogenous hole distribution favors the formation of PSPSs as it is indicated by the cigar-shaped spin fences enclosing the two neighbored SPS connected along \(a\). The SPS may only disappear for dopings exceeding \(n_{crit}\). Boundary effects destroying the self-protection of the
singlets will result from the finite size of the crystal. SPS damaged by boundary effects are indicated by filled circles with dashed spin fences. About $\simeq 0.18$ holes/Cu may be accomodated in this distribution. Closest packing of SPS accomodates $1/5 = 0.2$ holes/Cu.

*Optimum Doping:* $n \simeq 0.16 \simeq n_{opt}$

Fig. 9 displays as an example a distribution of nearly closest packed paired self protected singlets. About 0.15 holes/Cu may be accomodated by this distribution. The boundary effects are even more serious for the PSPSs than for the SPS: PSPSs will be destroyed within $3a$ from the edges of the crystal. Closest packing of PSPSs accomodates $1/6 = 0.166$ holes/Cu.

*"Destructive" doping:* $n_{des} > 0.2$

For $n_{des} = 0.22$ each SPS must overlap its spin fence with that of the $nn$ SPS (see Fig. 10). At such high hole concentrations the singlets will be unable to protect against other holes, break apart or possibly localize. Phrased in terms of the classical theory of gases: for $n_{des}$ the antiferromagnetic lattice may no longer serve as the walls of the container enclosing the liquid.

**SUMMARY AND CONCLUDING REMARKS**

The ubiquitous observation of a hump in $B(x)$ of cuprate superconductors has led us to an attempt analyzing the quantum liquid confined to doped CuO$_2$ lattices in terms of the theory of classical real gases or liquids. Most importantly here the walls of the container enclosing the quantum liquid are formed by the antiferromagnetic lattice which couples to the atomic lattice by creation of self-protecting spin singlets. It is basically internal magnetostriction, although of a novel type, that allows for insights into the structure of strongly correlated electrons from an analysis of the lattice parameters.

We have shown that the hump is strong evidence for the existence of relatively large incompressible particles interacting with each other. The area of the particles can be estimated from the location of the hump around $x_{opt} = 0.16$, and from its collapse around
$x_{\text{crit}} > x_{\text{opt}}$, respectively. At a microscopic level neither simple (nn) singlets, nor the ZR-singlet will match the area of $6.25a^2$ to be covered for hard core repulsion at $n_{\text{opt}} = 0.16$. The area of pairs of PSPS however is close to this requirement. On the other hand the area $9/2a^2$ covered by an unpaired SPS leads to close packing at $n_{\text{crit}} \simeq 0.20$, and seems to match even the number of destructive doping $n_{\text{des}} \simeq 0.22$ where in IR experiments the bosonic excitations disappear [16].

The SPSs are most likely bosonic, and not fermionic. Clearly this and other issues of the SPS and the PSPS will raise a bunch of challenging questions, which certainly cannot be answered from our so far almost only phenomenological approach which lead us via a geometrical construction to these particles. It is clear however that displacive lattice degrees of freedom must be involved in the formation of the singlet states. Otherwise the hump would not occur.

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FIG. 1: Basal area of one-layer La$_{2-x}$Sr$_x$CuO$_4$ as a function of doping using neutron diffraction data of Radaelli et al. [2].

FIG. 2: Basal area of one-layer HgBa$_2$CuO$_x$ as a function of doping using x-ray diffraction data of Fukuoka et al. [3].
FIG. 3: Basal area of two-layer $Y_{1-y}Ca_yBa_2Cu_3O_x$ using x-ray diffraction data of Böttger et al. (overdoped by Ca, $y \simeq 0.96 = const.$), and Kaldis and collaborators (underdoped).

FIG. 4: Basal area of two-layer HgBa$_2$CaCu$_2$O$_x$ as a function of doping using x-ray diffraction data of Fukuoka et al.
FIG. 5: Self-protecting singlet (SPS) in an antiferromagnetic CuO$_2$ lattice. The open circle in the center of the hatched supercell of $3 \times 3$ nn oxygen–oxygen cells indicates the symmetric oxygen cage accommodating a ZR singlet of the copper and the oxygen hole. The cross-hatched squares protect the ZR singlet against other holes with their intact spins (“spin fence”). The SPS covers an area of $9/2a^2$ in the CuO$_2$ lattice.

FIG. 6: Two self-protecting singlets sharing a common oxygen site along the Cu–O bond direction create one paired self-protecting singlet (PSPS). The spin fence in the cross-hatched squares protects the exchange between the two SPS against other holes and the loss of symmetry. The PSPS covers an area of $6a^2$ in the CuO$_2$ lattice. The PSPS extends over four oxygen cages along $a$. 
FIG. 7: “Stripy” doping: Perfectly ordered distribution of oxygen holes over the antiferromagnetic CuO\textsubscript{2} lattice by self-protecting singlets indicated by the open circle and the squared spin fence. Note the checkerboard lattice of “crosses” (dark/red) and “squares” (grey). Only 0.11 holes/Cu are accommodated.
FIG. 8: Critical doping: Possible high density packing of oxygen holes in the antiferromagnetic \( \text{CuO}_2 \) lattice by SPS and PSPSs over the “crosses” and “squares”. Cross-hatched cells indicate protecting areas. Note that the distribution must is inhomogeneous favoring the formation of paired singlets (large cigar-shaped spin fences). Boundary effects are indicated by filled circles and dotted broken spin fences. In this example about 0.18 holes/Cu are accomodated.
FIG. 9: Optimum doping: Nearly closest packing of oxygen holes in the antiferromagnetic CuO$_2$ lattice by PSPSs. Note that closest packing of PSPSs will pair all available SPS. In this example about 0.15 holes/Cu are accommodated. Boundary effects are indicated by dashed spin fences.
FIG. 10: Destructive doping: In this example 0.22 holes/Cu are accommodated. All spin fences are broken.