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Pseudogap and the superconducting energy in hole-doped high-temperature superconductors

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The pseudogap measured by different techniques in the high-temperature superconductors is interpreted as a two-particle screened Zhang-Rice singlet type state. The so-called (neutron) resonance energy measures the energy lowering of the superconducting state relative to the normal one and should be called the superconducting energy or the order parameter. The superconductivity in the high-temperature superconductors is in the crossover regime between a Bose-Einstein condensate and a BCS state, similar in physics to the situation for the fermionic cold atoms. The superconducting transition temperature is given as the product of the pseudogap energy (E_{pg}) and the carrier density, leading to its parabolic dependence on the doping. The formation of the Zhang-Rice singlet and the accompanying creation of the pseudogap are instrumental for the occurrence of the high-temperature superconductivity, as also for the large magnetoresistance in the manganites. The lowest ionization state in transition-metal compounds therefore constitutes a promising tool for the engineering of materials.

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I. INTRODUCTION

The high-temperature superconductors (HTSCs) (Ref. 1) are characterized by two energy scales, namely a pseudogap and a superconducting energy.[2–6] The importance of these two energies and their relevance for the HTSC has not yet been established.[7,8] In this situation a possible approach to get further insight into the problem is to collect data from many experimental techniques in order to recover trends for an analysis. Following earlier studies[2–6] data for the two energy scales were collected[9] within one diagram in order to have a reliable experimental basis.[10–54] The trends that arise from this procedure are given by the straight line and parabola in Fig. 1. The meaning of both curves has not been established at this point. Some authors[2,9] argue that the pseudogap (E_{pg}, straight line) measures the pairing strength of the electrons and the superconducting energy (E_{sc}, parabola, called in the literature frequently as the magnetic-resonance energy) measures the stabilization energy (or the order parameter or the superconducting energy) of the superconducting state. However, it has also been suggested that the pseudogap changes into the superconducting gap in crossing T_c.[23]

The straight line in Fig. 1 is given by the equation $E_{\mathrm{pg}}=[E_{\mathrm{pg}}(x=0.05)/0.22]\cdot(0.27-x)$, with $E_{\mathrm{pg}}(x=0.05)=(152\pm 20)$ meV. One finds this for systems with a $T_c(\max)\approx 95$ K, namely Bi 2212 or Y 123, Tl 2201, and Hg 1201. Similarly the parabola[55] is given by $E_{\mathrm{sc}}=E_{\mathrm{sc}}(\max)[1-82.6\cdot(0.16-x)^2]$, again for systems with $T_c(\max)\approx 95$ K, and $E_{\mathrm{sc}}(\max)=(42\pm 10)$ meV and $E_{\mathrm{sc}}(\max)=(5.1\pm 1)\cdot k_B T_c(\max)$. The values given here are those for the total gaps where, frequently, only half the gap, Δ, is quoted as measured, e.g., in angle-resolved photoemission spectroscopy (ARPES).

The pseudogap energy vanishes as a function of temperature around T^*, where T^* does not seem to be a phase-transition temperature. The nature of T^* is not yet settled. Some experiments[53,56,57] find a small magnetic signal in the pseudogap phase where the line connecting the temperatures of the occurrence of this signal meets the superconducting dome near optimal doping ($x=0.16$). A similar diagram has been derived by Tallon and Loram.[58] It is not clear at this point whether this "magnetic line" is indeed identical to the "pseudogap line" in Fig. 1.

In finding that, in the HTSC, the pairing energy (pseudogap) is larger than the superconducting energy puts the HTSC in the Bose-Einstein condensate (BEC) regime,

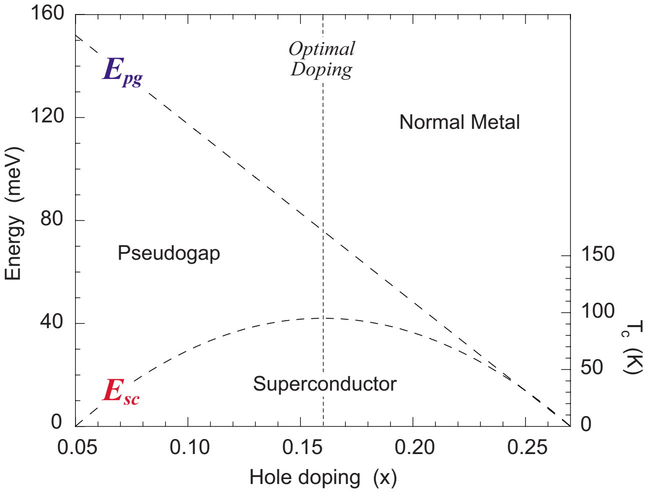

FIG. 1. (Color online) Pseudogap energy $E_{\mathrm{pg}}=2\Delta_{\mathrm{pg}}$ and resonance energy $E_r=\Omega_r=2\Delta_{\mathrm{sc}}$ for Bi 2212, Tl 2201, and Y 123, as measured by ARPES, tunneling [superconductor/insulator/superconductor (SIS) and superconductor/insulator/normal (SIN) metals, STM, and AR-Andreev–Saint-James reflection), Raman scattering (RS), and neutron scattering (INS), as well as heat conductivity (HC) as a function of hole doping x. The data fall on two universal curves with $E_{\mathrm{pg}}=152\ \mathrm{meV}/0.22\cdot(0.27-x)$ and $E_{\mathrm{sc}}=E_{\mathrm{sc}}(x=0.16)\cdot[1-82.6\cdot(0.16-x)^2]$ with $E_{\mathrm{sc}}(x=0.16)=42$ meV and $E_{\mathrm{sc}}=(5.1\pm 1)\cdot k_B T_c$. pg stands for pseudogap state; the other area designations are self explanatory (see Ref. 9).

but quite close to the BCS regime, for which the pairing and the condensation energies coincide.[2,3,6,15]

It will be argued here that the pseudogap is produced by the doping of the Mott Hubbard parent system of the HTSC. The pseudogap is the remnant of the lowest hole state in the parent system. In addition it will be shown that the doping dependence of T_c can be rationalized by assuming it to be the product of the pairing strength, as measured by the pseudogap and the carrier density. This means that the HTSC can be described in the framework suggested first by Anderson[59] and further developed by many authors,[60–63] where it is impossible to quote even a fair fraction of the theoretical work in this field. This means that the HTSC are in the intermediate regime between BCS and BEC.[2,3,15,64–66]

II. MEASUREMENTS OF THE PSEUDOGAP AND THE SUPERCONDUCTING GAP

In this section a brief discussion, going beyond what has been given in Ref. 9, of the data from which Fig. 1 is derived will be presented in order to make the following sections more readable.

ARPES (Ref. 12) and scanning tunneling microscopy (STM) (Ref. 23) are one-electron spectroscopies. They measure one-electron states such as band structure. If they measure a two-particle energy, as in the measurement of the superconducting gap in a conventional superconductor, they do it by breaking up the pair and measuring the energy of the electron left behind. The measurement of the pseudogap in a HTSC is, in this sense, the measurement of Δ_{pg} or $E_{\mathrm{pg}}/2$. In a BEC the coupling energy between two particles is larger than the condensation (gap) energy. Therefore a measurement of the excitation energy by a one-electron spectroscopy in a HTSC results in the determination of the pairing energy (pseudogap).

The measurement of the condensation energy in a HTSC is a measurement of a two-electron energy, which ARPES cannot measure directly. ARPES is able to measure the superconducting gap energy in a conventional BCS superconductor only because, in this case, the pairing and the condensation energies coincide. Because of this coincidence, the BCS state can be considered a special one. The Bose-Einstein (BE) state is a much more general one because there is no fixed relation between the condensation and the pairing energies. The latter one only has to be larger than the former one.

Experiments that measure two-electron energies can measure the superconducting energy directly. This has been done most transparently by Andreev–Saint-James reflection.[2,3] The superconducting gap can also be measured in one-electron experiments via the sidebands ("dips") (Refs. 4, 27, 39, and 40) in the same way as the phonon generated $a^2F(w)$ is seen in tunneling spectra of conventional superconductors.

Another way of measuring the pseudogap or the superconducting energy is by measuring the renormalization of the one-electron energies, produced through them ("kinks"), in the nodal[36] and antinodal directions,[36,37] respectively.

Forming a picture out of the trends presented in Fig. 1 will now be tried. The starting point is the observation that the pseudogap is a two-electron state und thus measures the pairing energy of two electrons.

The pseudogap couples to the dispersive electrons in the system, giving rise, e.g., to the kink in the nodal direction,[12,36] which has approximately the energy of the pseudogap and disappears at T^*. The coupling leads to an admixture of a two-electron (bosonic) wave function to the electrons in the system. Below T_c, these preformed pairs form a BEC state, exhibiting a condensation energy that follows T_c. This condensation energy of the bosons can be measured directly by a two-particle experiment such as Raman and neutron scatterings, or Andreev–Saint-James reflection, and is indeed seen in these experiments.

The pseudogap and the superconducting states interact, meaning that the wave functions of the two systems mix. This mixing gives rise to the coherence peak observed at the pseudogap position in the superconducting state and explains why, in going from the pseudogap state into the superconducting state, one-electron spectroscopies[12,23] seem to see an evolvement of the superconducting gap out of the pseudogap. The so-called superconducting gap measured by ARPES or STM measures the superconducting fraction of the bosonic wave function in the pseudogap state.

It seems that the most important spectroscopic data for the understanding of the physics of the HTSC are those that show the mixing of different states, much in the same way as the electron phonon features were important for the understanding of the conventional superconductors. In the case of the HTSC, these are the kinks and the dips seen in various spectroscopies. Unfortunately these features are, at present, not very well defined experimentally. Although the experimental situation is not completely settled, it seems to be possible to state that, for systems with approximately optimal doping, the kinks at the nodal point (disappearing at T^*) measure the pseudogap energy and the kinks at the antinodal point measure the superconducting energy (disappearing at T_c).

One can elaborate somewhat on the direct measurement of E_{sc} by Andreev–Saint-James reflection,[2] and Raman[18] and neutron[5] scatterings. The most transparent experiment is Andreev–Saint-James reflection, which injects an electron pair at the Fermi energy into the superconducting system and thus measures directly the binding energy of that pair, yielding the superconducting energy following T_c as a function of doping.

Raman and neutron scatterings are the reverse experiments of Andreev–Saint-James reflection in that they excite an electron pair out of the condensate to the Fermi energy, thus also measuring the superconducting energy. In Raman scattering this is done in the B_{2g} mode, which has its intensity maxima at the nodes. These are the points on the Fermi surface to which the pairs have to be excited because there the gap vanishes. This excitation is performed with zero added momentum, as must be in the optical transition. Neutron scattering also excites a pair of electrons to the nodal position, which is why the experiment uses a momentum transfer in the nodal (antiferromagnetic) direction. However, in this case an antiferromagnetic wave vector is added to the pair.

Finally, a fact that shows up in some ARPES measurement should be commented upon, namely the so-called twocomponent gap,[45,52] seen perhaps most clearly in the work by Kondo *et al.*[45] on Bi 2201. This means that if one plots the ARPES measured gap as a function of angle going from the antinodal to the nodal direction, the dependence of the gap magnitude on the angle can best be described by assuming two gaps. This effect is large near the nodal point and it vanishes in going toward the antinodal point. In the interpretation given here, this behavior comes from the fact that, at the antinodal point, the superconducting gap and the pseudogap are well separated, and ARPES only measures the pseudogap. Near the nodal point, the two gaps are of similar magnitude (they coincide directly at the nodal point) and therefore they mix strongly. Therefore near the node, ARPES measures an average of the two gaps, which is smaller than the pseudogap.

In this context the interesting ARPES data by Lee *et al.*[46] have to be mentioned. They find the closing of a gap in ARPES (one-electron) spectra near the node below T_c and attribute it to the signature of a BCS superconductor. This closing vanishes if one moves along the Fermi surface toward the antinodal point. Similar data on the closing of a gap near the node have been obtained by Kanigel *et al.*[47] and these authors gave a different interpretation of their results. One can suggest that Lee *et al.*[46] saw the closing of the pseudogap in an area of k space where the pseudogap is smaller than the superconducting gap at the antinode. In this region of k space the thermodynamics of the pseudogap, which is observed to go to zero as T_c is approached, is governed by that of the superconducting gap. This is in line with the experimental finding that the Fermi arc extends from the node to a point on the Fermi surface where the antinodal superconducting gap equals $E_{\mathrm{pg}} \cdot \cos(2\varphi)$.

III. MODEL ELECTRONIC STRUCTURE FOR THE HIGH-TEMPERATURE SEMICONDUCTOR

In this section a picture for the development of the pseudogap is outlined. It was found early in the investigation of the HTSC (Ref. 11) that, with respect to their low doping behavior, they can be treated in some aspects approximately like conventional semiconductors. In lightly doped $La_{2-x}Sr_xCuO_4$ (LSCO), Kastner *et al.*[11] found a position of the acceptor level with respect to the Fermi level to be at 19 meV. The HTSC are (doped) highly correlated materials. This means that in the parent insulating compound, the lowest ionization state is a singlet hole state with a binding energy[12] of about 0.5 eV [Zhang-Rice singlet (ZRS)].[67,68] Chemical hole doping can be viewed as introducing (many) ZRS states into the parent insulating compound. These holes are not bound by 0.5 eV, as in undoped LSCO but with a smaller energy, due to screening by the electron in the acceptor state and, once the system has become metallic, by the conduction electrons.

Their binding energy can be estimated from a simplistic one-dimensional model. Let us assume for the matter of the argument that one is dealing with CuO chains. Then the ionized valence-band state can be formally written as $-Cu^{2+}-O^{2-}-Cu^{2+}-O^{-}-Cu^{2+}-O^{2-}$. This is equivalent to the final state in a photoemission experiment (PES). Conversely the state with an ionized acceptor Na (for the sake of argument) can be written as $-Cu^{2+}-O^{2-}-Na^{+}-O^{2-}-Cu^{2+}-O^{2-}$, which is the final state in an inverse photoemission experiment (IPES). These states are approximately mirror images of each other. Thus if the latter state has an energy E_A above the Fermi energy, the former state has an energy $-E_A$ below the Fermi energy. These considerations have been verified by data on NiO and Li doped NiO (Ref. 69): the Li acceptor state is at 1.2 eV above E_F and the NiO photoemission final state (hole state) at 1.4 eV below E_F.

In lightly doped LSCO, Kastner *et al.*[11] found E_A at 19 meV above E_F, which would suggest that the valence hole state is at approximately the same energy below E_F. An extrapolation [Fig. 67(c) in Ref. 12] of the doping dependence of the pseudogap energy Δ_{pg} in LSCO leads to (16 ± 5) meV for very low doping levels, in surprising agreement with the above estimate, rendering support for the model presented here.

These considerations lead to the conjecture that the pseudogap in the HTSC is a ZRS-type state. It is screened by the charge carriers in the material but perhaps even more by the electron on the acceptor ion. The energy of the ZRS is given by atomic multiplet and crystal-field interactions, and these are the interactions that determine the hole binding energy. In simple terms one can state that the binding energy of the ZRS is magnetic in origin. One can thus argue that it is the large antiferromagnetic coupling[67,68] between the oxygen hole and the Cu hole that produces the ZRS. With increasing doping, the screening of the ZRS increases; it moves nearer to E_F and reaches it at a doping level of 0.27. At this doping level the HTSCs become normal metals. The pairs (ZRS) with binding energy E_{pg} no longer exist.

At this point in the discussion, one has to introduce the anisotropy provided by the CuO_2 plaquettes. There is no gapping of the density of states around $(\pi/2,\pi/2)$, meaning also that charge transport is dominant along the zone diagonal.[70] On the other hand along the bond direction $(\pi,0)$, the bonding leads to a strong oxygen copper interaction, leading to the formation of a ZRS in this direction, if an electron is removed (a hole injected).

The excitation connected with the superconductivity [the so-called resonance energy $(E_r = \Omega_r)$, which we would rather call the superconducting energy] disappears above T_c. On the other hand, the excitations at $(\pi,0)$ above T_c but below T^* reflect the ZRS binding energy and these excitations only gradually disappear with temperature[13] because the pseudogap state is not a state with long-range order.

These considerations are in line with the finding of Steeneken *et al.*[71] who observed that the charge carrier in the hole (and electron) doped HTSC have a singlet nature.

These considerations are visualized schematically in Fig. 2. Panel (a) shows the photoemission valence band of CuO with the p^5d^9 final state. The zero of the energy is the top of the valence band. Panel (b) gives the spectral function of a slightly doped HTSC-like LSCO, where the Sr acceptor has produced a localized p^5d^9 hole state. Again the zero of the energy is the top of the valence band. In the metallic state, the spectral function around $(\pi/2,\pi/2)$ [panel (c)] is different from that around $(\pi,0)$ [panel (d)]. In the former case we have a metal while in the latter case the pseudogapped state

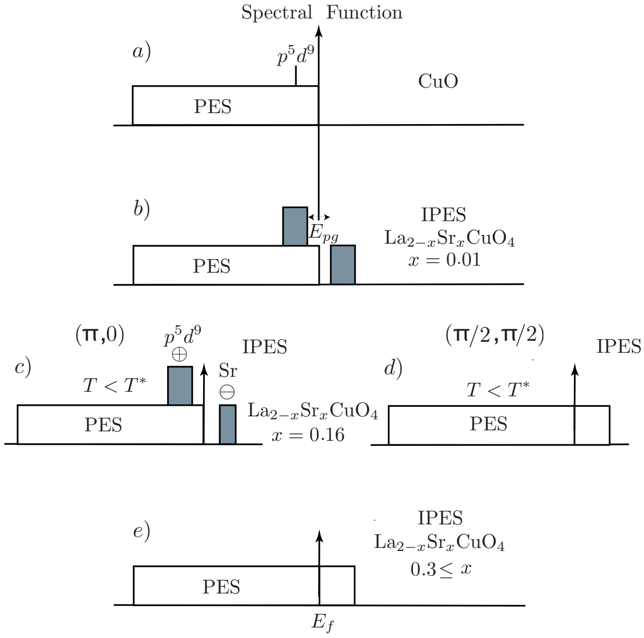

FIG. 2. (Color online) (a) Schematic spectral function of CuO and of $La_{2-x}Sr_xCuO_4$ as an example of a hole-doped HTSC for $T_c < T < T^*$. (b) Low doping insulating state. (c) Optimal doping at the antinode $(\pi,0)$, showing the pseudogap below T^*. (d) Same as panel (c) at the node, showing no gap. (e) Situation for doping above 0.3, showing the normal metallic state.

has developed. At high doping $(0.3 < x)$, the pseudogap has disappeared and the system is a normal metal [panel (e)].

This picture of the electronic structure of HTSC, which comes essentially out of spectroscopic data is fully supported by the electrodynamics of these compounds.[25,39,41] The c-axis conductivity shows the pseudogap as it develops below T^*. This means that the resistivity in the c direction increases with decreasing temperature in a similar way as a semiconductor would show it. On the other hand the resistivity in the $(a$-$b)$ plane decreases with decreasing temperature because of the development of coherence. Thus the in-plane conductivity can be called coherent because it shows the peak at zero frequency (Drude-like peak). On the other hand the conductivity in the c axis can be called incoherent because it shows no peak at zero frequency.

This can be viewed also in a different way using local language. In the antiferromagnetic state, the spins point in ferromagnetic rows along the diagonal of the CuO_2 plaquette. Thus, along a row, a moving charge does not have to flip a spin, making its movement easy. On the other hand, along the O-Cu-O bond direction, the spins have an antiferromagnetic order and thus a moving charge has to flip a spin, making this difficult by an energy of order J.

In terms of the diagram in Fig. 2, this means that at $(\pi/2,\pi/2)$, one is dealing with a normal metal. The hole and the acceptor bands have merged at the Fermi level, forming a band that crosses the Fermi level. At $(\pi,0)$ the acceptor level is still above the Fermi level and the hole it produces by accepting electrons are distanced from the Fermi level by the screened exchange energy that determines the binding energy of the ZRS, thus forming the pseudogap. One thus have a very anisotropic electron liquid in the HTSC with coherent conductivity along the diagonal of the plane and incoherent conductivity along the c axis.

IV. SUPERCONDUCTING STATE

In the BCS theory, the Cooper pairs are created by an attractive coupling between electrons, mediated by a boson. In conventional superconductors this coupling is the electron phonon coupling and the boson is a phonon. Phonons also have been considered as the coupling bosons for the HTSC but the consensus is that while they may contribute to the interaction, they cannot be its single source.[12]

A much dealt with candidate in the HTSC for the coupling boson is the so-called magnetic-resonance mode detected by neutron scattering around 40 meV for $T_c = 95$ K systems.[5,12] While this looks as a very likely candidate, so far no formal theory of superconductivity on the basis of the magnetic resonance has appeared. There is one argument against the (neutron) magnetic resonance being the superconducting coupling boson: the temperature dependence of this resonance follows that of T_c, meaning that the coupling mechanism would act in a kind of a bootstrap, creating the coupling boson and the resulting coherent superconducting state simultaneously, a quite unlikely scenario. Finally, Fig. 1 demonstrates that the (neutron) magnetic resonance is rather the superconducting gap or the superconducting order parameter.

Besides the neutron magnetic resonance, which can be excluded as the coupling boson for the HTSC, and besides the phonon, which probably does not play the decisive role for the coupling, there is another boson that has to be considered for the superconducting pairs, namely the $(\pi,0)$ ZRS derived pseudogap. However it would be driving the analogy to BCS too far to call this the coupling boson or even the glue. The pairing in the HTSC is magnetic and is given by the pseudogap state (if one wants to talk in terms of glue, which we think is misleading, this glue is J, which couples the electrons in the pseudogap state together). However, it seems much more appropriate to abandon BCS language and talk of pairs (coupled by J) that condense into the superconducting state.

Dordevic *et al.*[39] and Zasadzinski *et al.*[40] have extracted the electron boson coupling function $a^2F(w)$ from infrared and photoemission data for optimally doped Bi 2212. For the ARPES data, experiments along the nodal direction were used. The $a^2F(w)$, derived from the two different experiments, agree approximately and lead to a peak in that quantity around 70 meV. This is the pseudogap energy at optimal doping, as can be seen from Fig. 1. Thus the suggestion that the pseudogap represents the boson condensing into the superconducting state below T_c is supported by the experimentally derived coupling function $a^2F(w)$. This is, in principle, only a different analysis of the kink as measured by ARPES.

The 70 meV kink[38] in the nodal self energy of Bi 2212 [which measures the electron boson interaction from which $a^2F(w)$ has been derived] disappears at T^*, which is the pseudogap temperature, lending support to the conjecture that this kink is produced by a coupling to the pseudogap.

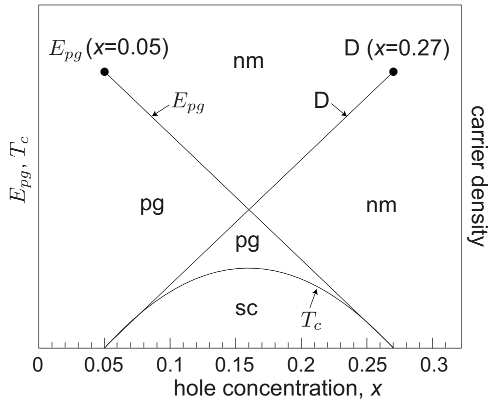

FIG. 3. Schematic showing the pseudogap energy $E_{\mathrm{pg}}E_{\mathrm{pg}}(x=0.05)/0.22\cdot(0.27-x)$, the carrier density $D=D(x=0.27)/0.22\cdot(x-0.05)$, and the superconducting transition temperature $T_c\sim E_{\mathrm{pg}}\cdot D\sim[1-82.6\cdot(0.16-x)^2]$. sc=superconducting phase, pg=pseudogap phase, and nm=normal metal phase.

In contrast the kink at $(\pi,0)$ disappears around T_c and can therefore be produced by a coupling to the superconducting gap.

This picture of the superconductivity in the HTSC is one of a BEC (Refs. 15, 64, 65, and 72) that is produced by preformed pairs that condense into a coherent state rather than of a BCS state, where the coupling of the electrons also measures the stabilization of the superconducting state. The amount of the BEC is measured, e.g., by the strength of the coherent ARPES peak as it appears below T_c.[12,32,37]

One can drive this argument somewhat further by using the calculations of Nozieres and Schmitt-Rink,[66] which show that, in the BEC/ BCS crossover regime, the stability of the superconducting state, as measured by T_c, is given by the magnitude of the boson energy (E_{pg}) multiplied by the number of charge carriers in the system.[6,32,33,73] By looking at various different experiments, one can assume[32,33] that the number of charge carriers D increases approximately linearly from about $x=0.05$ to $x=0.27$, meaning that $D=D(x=0.27)/0.22\cdot(x-0.05)$. The superconducting transition temperature T_c (or the superconducting gap energy) is therefore given by $T_c\sim E_{\mathrm{pg}}\cdot D$, leading to $T_c=T_c(x=0.16)\cdot[1-82.6\cdot(0.16-x)^2]$ if one uses $E_{\mathrm{pg}}=E_{\mathrm{pg}}(x=0.05)/0.22\cdot(0.27-x)$ from Fig. 1, which is the commonly used empirical relation connecting the doping x with the superconducting transition temperature T_c (Ref. 55) (see Fig. 3). This simple picture will only hold near optimal doping, and has to be modified for very low and very high dopings.

These considerations lead to the phase diagram for the HTSC given in Fig. 3, showing the superconducting state below the dome, the pseudogap phase below the pseudogap line, and the "normal" metal phase beyond the pseudogap line.[74]

It is interesting that the phase diagram of Fig. 3, if taken at face value, leads to a useful relation between E_{pg} and E_{sc}. Due to the construction used in Fig. 3, the E_{pg} line represents the tangent to the E_{sc} parabola at $x=0.27$. This leads to the relation $E_{\mathrm{pg}}(x=0.05)=4\cdot E_{\mathrm{sc}}(x=0.16)$. Thus the two parameters E_{pg} and E_{sc} are not independent but coupled by the given relation. The E_{pg} line in Fig. 1 obtained from a fit of many experimental data leads to $E_{\mathrm{pg}}(x=0.05)=(152\pm20)$ meV, while the arguments just presented yield $E_{\mathrm{pg}}(x=0.05)=(168\pm40)$ meV, using $E_{\mathrm{sc}}(x=0.16)=(42\pm10)$ meV as an average from many experiments.[9] Thus the relation between E_{pg} and E_{sc} suggested here is fulfilled within the experimental error margin.

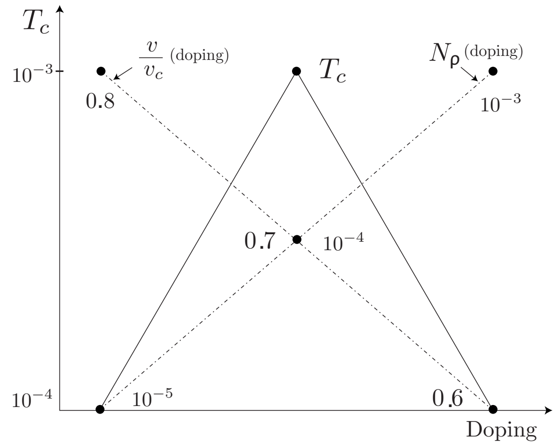

FIG. 4. Schematic phase diagram for the HTSC as derived from Ref. 66. The charge-carrier density and the potential between the electrons were given as parameters. The diagram shows the same structure as that in Fig. 3.

The phase diagram shown in Figs. 3 and 4 (the derivation of Fig. 4 will be discussed below) comes also out of calculations[60,61] based on the concept of Anderson.[59] In these calculations, a doping dependence of the pairing energy is found, which is approximately linear with decreasing doping. The superconducting order parameter is then given by the product of the pairing energy and the doping. The order parameter can be identified with the superconducting energy.

The phase diagram in Fig. 3 shows that for all doping levels, one has $E_{\mathrm{pg}}/E_{\mathrm{sc}}>1$, meaning that one is in the BEC/BCS crossover regime.[2,24,64,66] In principle, although the parameter values are very different, the HTSC are systems similar to the fermionic cold atom condensates.[75,76] In these systems the transition temperature is determined by the attractive potential between the atoms and the density of the paired atoms. The schematic phase diagram in Fig. 3 also shows that the canonical BEC state is reached asymptotically at $x=0.05$ with $E_{\mathrm{pg}}/E_{\mathrm{sc}}=\infty$ and the canonical BCS state is reached asymptotically at $x=0.27$ with $E_{\mathrm{pg}}/E_{\mathrm{sc}}=1$ in the HTSC.

One can generate the structure of this phase diagram also from the results of the calculations of Nozieres and Schmitt-Rink.[66] They have obtained, for the complete range from the BCS to the BEC situation, the dependence of T_c on the attractive potential of the electrons and the charge-carrier density. If one makes the sensible assumption that the charge-carrier density is proportional to the doping and that the potential is inversely proportional to the doping, one can construct the schematic phase diagram given in Fig. 4 from their work. Here V_c is a critical potential. If, in the system under investigation, the potential is larger than V_c, the transition temperature depends no longer on V and one has reached the BEC regime where T_c is independent of the internal structure of the boson. Note that for the construction of Fig. 4, only three points where taken from Ref. 66 in order to make the structure of the plot as simple as possible.

In the BCS theory[77] one has $T_c = w_D \cdot \exp[-1/(N_0 V_0)]$, where w_D is the Debye frequency, V_0 the electron phonon coupling strength, and N_0 the density of states at the Fermi energy. The convenient thing in the HTSC is the fact that the whole process of BEC formation occurs within the electron system and is not a phonon or another boson mediated pairing such as in classical BCS. Thus, the existence of the so-called superconducting dome, namely the quadratic dependence of T_c (or the superconducting energy or the order parameter), as a function of doping argues against the HTSC being BCS superconductors but argues for them being a BEC.

V. SUMMARY

It has been shown that the pseudogap in the HTSC originates from screened Zhang-Rice singlet derived states.[67,68] This is in line with what Anderson[59] suggested very early in the study of the HTSC. Recent forms of that theory can be found, e.g., in the studies by Paramekanti *et al.*[60] and Eddeger *et al.*[61] to name only two representative examples.

The magnitude of the pseudogap decreases (linearly) with increasing doping x because the doping increases the number of charge carriers[6] that leads to an increased screening. The density of charge carriers, on the other hand, increases linearly with doping. If the superconducting transition temperature is calculated as the product of these two quantities, this leads to the parabolic shape of the doping dependence of T_c for all HTSC. This is only approximately correct and will break down near $x=0.05$ and $x=0.27$.

In order to support the reasoning given in this paper, it is interesting to point to two qualitative arguments given by Paramekanti *et al.*[60]

If one assumes that the magnetic pairing of the electrons is the driving mechanism for the superconducting state, one realizes that the exchange interaction between two spins gets smaller with increasing doping x, namely one has $J_{\text{eff}} = J \cdot (1-4 \cdot x)$, where the factor of four is the coordination number in the two-dimensional (2D) square lattice, which applies to the CuO_2 superconducting planes. This leads to $x=0.25$, which is in good agreement with experiment.

If the pseudogap measures the pairing strength, the order parameter E_{sc} should be proportional to E_{pg}. Now one has, in addition, the square of the order parameter (E_{sc}^2) that it is proportional to F if F is the probability of moving a pair of electrons from adjacent sites to a distant pair of adjacent empty sites. Since the number of empty sites is proportional to x, the number of adjacent empty sites is proportional to x^2, making also F proportional to x^2. This makes the order parameter E_{sc} proportional to x and if one takes the already mentioned additional proportionality to E_{pg}, one gets that the order parameter (or T_c) is the product of the doping and the pseudogap energy.

In the picture developed here, the pseudogap is a necessary essential ingredient in the high-temperature superconductivity. The superconducting gap occurs when the system gains additional energy by forming a coherent state.

The pseudogap can be considered to provide the bosons, which condense to a coherent state below T_c. In this context the discussion about a possible glue that holds the superconducting pairs together seems somewhat unfortunate. The pairs in the pseudogap are coupled by the antiferromagnetic coupling J, which one should rather not call a glue.

The superconducting gap is only visible below T_c, in contrast to the pseudogap, (magnetic in origin) which disappears gradually if the temperature reaches the pseudogap energy (which is of the order of T^*).

The mechanism described here for the formation of the pseudogap applies also to other highly correlated doped materials such as, e.g., the manganites,[78,79] showing the colossal magnetoresistance. In this case the lowest hole state (which forms the pseudogap upon doping) is magnetic and therefore the manganites are not superconducting metals but have a metallic ferromagnetic ground state. In addition, the recent experiments[34] on $La_{2-x}Ba_xCuO_4$ ($x=0.125$) can be rationalized at least qualitatively by the present model. Around $x=0.125$ the charge-carrier density and the superconducting transition temperature decrease, which is in accord with $T_c \sim E_{\text{pg}} \cdot D$. In addition, at $x=0.125$ a slight increase in E_{pg} is found compared to the value at a lower doping, which agrees with the suggestion that screening (charge-carrier density) regulates the pseudogap energy.

It is evident that doped transition-metal compounds with localized d states can be used to create interesting magnetic or superconducting systems. Using semiconductor language, this statement is made with the restriction that the pseudogap energy, which is the energy of the first ionization state, is not too far below the Fermi energy, meaning that it must be accessible to thermal excitation, placing an upper limit of this energy to about five times the room temperature, meaning 150 meV.

Finally, one has to mention recent measurements of the polar Kerr effect.[53] These experiments found a transition to a magnetic state in the pseudogap phase where the line connecting the transition temperature as a function of doping meets the T_c curve around optimal doping. These experiments support earlier μ-SR experiments[56] and neutron-scattering experiments.[57] However, while the Kerr data are compatible with a ferromagnetic state, the neutron data rule out a ferromagnetic state.

These experiments do not detect necessarily a long-rang magnetic state. They are compatible with a fluctuating state as noted by Fauqué *et al.*[57] Also this magnetic state reaches into the superconducting dome,[58] which would also argue for a fluctuating state. With the limited information available at this point, one can only suggest that broken pseudogap pairs couple to each other for a short period of time. This is in accordance with the suggestions by Fauqué *et al.*[57] that the spins are on the oxygen sites and would, in addition, argue for a ferromagnetically ordered state. Since the pseudogap reaches into the superconducting state, as demonstrated by STM experiments,[23] this can also explain the coexistence of the superconducting state and the fluctuating magnetic state.

VI. CONCLUSIONS

The main conclusions from this work are as follows: (1) There are two excitation energies in the hole-doped HTSC, namely a pairing gap (pseudogap, vanishing at T^{*}) and a superconducting energy (vanishing at T_c), as early suggested by Deutscher.[2,3] The phase diagram for the HTSC is given in Fig. 1.[80] (2) The two excitation energies have different doping dependence but over the whole doping range, $E_{\mathrm{pg}}/E_{\mathrm{sc}} > 1$ hold. This puts the HTSC in the BEC-BCS crossover regime.[2,3,6] (3) The magnitude of the superconducting energy E_{sc}, exhibiting a quadratic doping dependence x, is given by the product of the pseudogap energy and the charge-carrier density, which are both linear functions of the doping x.[73] (4) The pseudogap is a ZRS derived state (created by doping) while the superconducting energy gives the energy needed to stabilize the superconducting state.[67,68] (5) The mechanism described here for the creation of superconductivity in the HTSCs does also apply to the manganites exhibiting the high magnetoresistance. In principle this mechanism can be used to tailor new compounds with interesting properties. (6) It would be a very good test for the ideas explored in this communication to perform a STM experiment going from the tunneling into the Andreev–Saint-James regime by just changing the tip sample distance.

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