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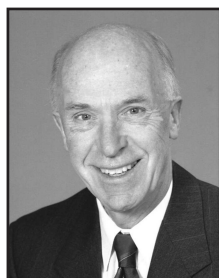
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EMERGENT SPIN TOPOLOGY IN CUPRATE SUPERCONDUCTORS SEEN WITH NEUTRONS

BY ZAHRA YAMANI AND WILLIAM J.L. BUYERS



Since the discovery of high-temperature superconductivity in cuprates, neutron scattering has been instrumental in revealing their magnetic properties. The parent compounds are ordered antiferromagnets whose spin excitations travel freely in copper oxide planes as spin waves arising from the exchange coupling of copper spins. As carriers are doped into the material, magnetic order is destroyed, but strong spin correlations persist and coexist with a relatively low density of carriers. These form pairs that produce a phase of coherent superconductivity remarkably close to the magnetic phase. Since the neutron has a magnetic moment, scientists have been able to see with neutron beams how the magnetic correlations evolve as superconducting pairs increase.

By now a generic phase diagram as a function of doping for the cuprates has been generated by neutron scattering. Such a phase diagram is shown in Fig. 1 for $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ (YBCO_{6+x}) based on refs. [1 to 4]. Different experimental probes give a similar diagram.

The magnetic moment of the neutron allows scientists to see that the background that charges move through consists of spin fluctuations from which they can likely acquire a sufficiently strong pairing to account for the large T_c . In part this is because the energies of the spin waves of the doped antiferromagnet, while damped, extend to large energies of order 400 meV, much higher than the phonons. It is also because the magnetic spectrum is strongly changed by the onset of superconducting order at energies of the order of the superconducting transition temperature. However present theory is unable to make a realistic prediction of the transition temperature from the measured spin fluctuations.

The carriers may be introduced into the insulator either as electrons, or as holes, on which we focus. In single-layer $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ (LSCO) a hole is added to the CuO_2 plane.

SUMMARY

Neutron scattering has shown that magnetism is intimately related to the unconventional superconductivity in cuprate superconductors.

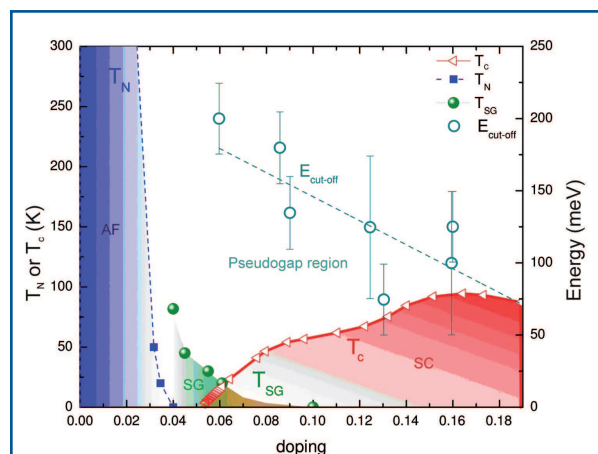


Fig. 1 Phase diagram of YBCO_{6+x} . The plotted Néel temperature is from neutron diffraction^[1] and T_c from magnetization^[2]. Spin correlation lengths grow rapidly as doping is reduced but there is no break to this trend as doping descends below a critical doping, $p_c = 0.052$, that takes the system out of its superconducting phase. Concomitantly a spin-glass (SG) structure grows and the temperature where its elastic moment squared has grown to half its low temperature value, indicated by T_{SG} , shows that static magnetism is inimical to superconductivity (Ref. [3] and Yamani *et al.* unpublished). At high energies inelastic neutron scattering on YBCO and several other cuprate families has recently shown that the spin spectral weight is suppressed above a pseudogap energy $E_{\text{cut-off}}$; this pseudogap cut-off declines with doping as T_c rises. See ref. [4-11] and references therein for details.

Carriers can also be introduced by doping with oxygen. For example, in YBCO_{6+x} , with two CuO_2 planes in its unit cell, the extra oxygen is chemically located in a chain outside the magnetic CuO_2 plane. It then attracts a valence electron to itself by creating a hole in the magnetic layer. The hole is on the planar oxygen sublattice. Thus the chemical change upon doping in a separate chain produces a much smaller charge perturbation in the 2D layers than does the hole doping by a nearby charge impurity in the single-layer materials.

Adding a few holes destroys the antiferromagnetic order, at a doping, p , that is surprisingly low, below 4%.

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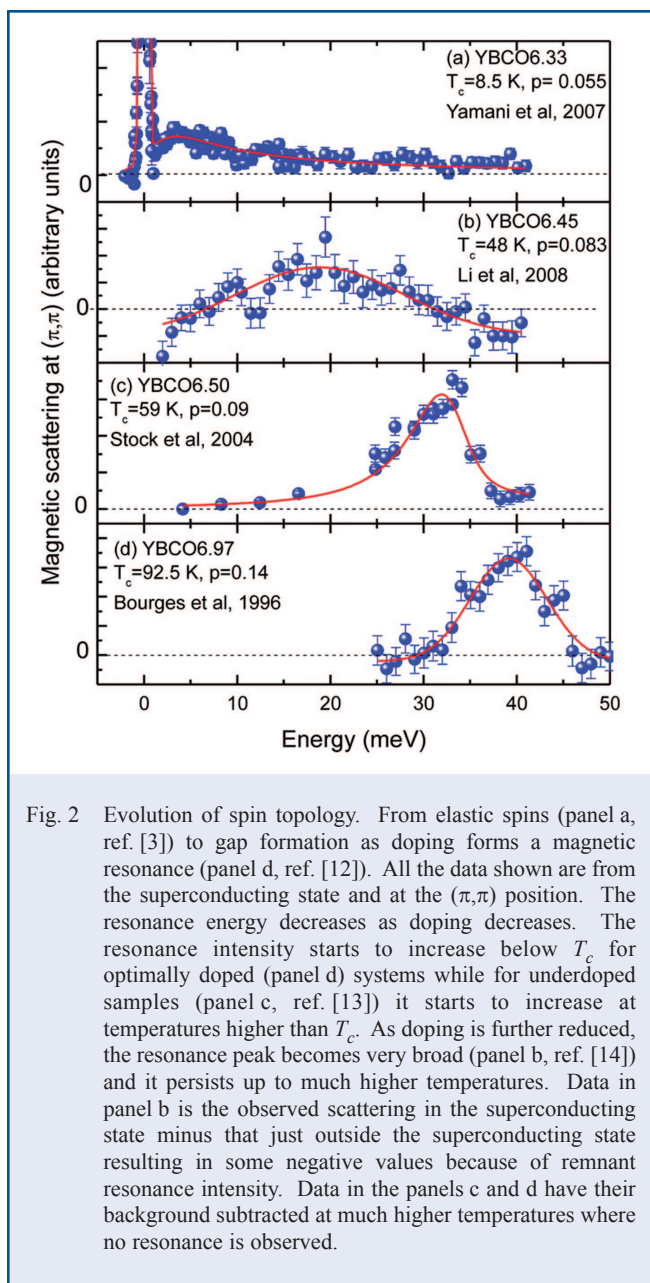


Fig. 2 Evolution of spin topology. From elastic spins (panel a, ref. [3]) to gap formation as doping forms a magnetic resonance (panel d, ref. [12]). All the data shown are from the superconducting state and at the (π, π) position. The resonance energy decreases as doping decreases. The resonance intensity starts to increase below T_c for optimally doped (panel d) systems while for underdoped samples (panel c, ref. [13]) it starts to increase at temperatures higher than T_c . As doping is further reduced, the resonance peak becomes very broad (panel b, ref. [14]) and it persists up to much higher temperatures. Data in panel b is the observed scattering in the superconducting state minus that just outside the superconducting state resulting in some negative values because of remnant resonance intensity. Data in the panels c and d have their background subtracted at much higher temperatures where no resonance is observed.

Conduction ensues but the material remains resistive. More holes allow the carriers to pair for a critical planar hole doping as little as $p \sim 5\%$ and gain entrance to the superconducting phase. The hole dopant in cuprates thus plays a dramatically stronger role than a magnetic vacancy in insulators, where loss of magnetic order requires a critical doping exceeding $\sim 50\% \sim 2/z$, the percolation limit for the $z=4$ bonds of the two-dimensional square lattice. A hole doped into cuprates affects many sites rather than one. In the plane an oxygen spin-one-half hole can form a singlet with the spin one-half of the Cu^{2+} atom and change the state of all four of its oxygen neighbours. Moreover the hole singlet can move and disorder a larger region of spins. The weakening of spin order is particularly

effective because each oxygen hole changes the sign of the exchange coupling between its two neighbouring Cu^{2+} spins from the usual antiferromagnetic superexchange of the insulator to ferromagnetic parallel-spin coupling.

The resulting exchange frustration leads to a highly-correlated spin-glass static structure whose short-range order reflects a memory of the ordered antiferromagnet and for which the low-energy spin fluctuations are damped^[3,15]. This behaviour coexists with strengthening superconductivity up to a planar doping as large as 8% ($x \sim 0.4$). When the doping reaches $\sim 9\%$ a dramatic change in the spin spectrum then takes place as shown in Fig. 2 based on refs. [3,12-14]. The quasielastic spectrum of the spin-glass regime is raised upward to form an intense, well-defined, commensurate “resonance” peak at larger energies. Its energy scales as $E_{\text{res}} \approx 5 k_B T_c$ for T_c around the optimal doping. Intermediate doping ($x=0.45$) gives an intermediate but more broadened resonance^[14]. The dramatic spectrum change suggests a phase change occurs close to this doping. The removal by doping of elastic spin scattering leads to better metallic transport and formation of a Fermi surface as revealed through quantum oscillations in $\text{YBCO}_{6.5}$ ^[16].

Below the resonance the lowest excitations are split from the antiferromagnetic zone centre by an incommensurate wave vector. Here the charge carriers have formed enough ferromagnetic bonds to create antiphase spin domains where the phase of the underlying antiferromagnetic correlations is reversed across a row of hole bonds – a conducting stripe (for a review see [17]). This destroys scattering right at the wave vector (π, π) but allows constructive interference displaced by a wave vector that grows with doping as the domain length declines. At energies higher than the resonance energy an upward dispersion is observed resulting in an overall “hourglass”-type dispersion in the energy-momentum diagram with the resonance at the “neck” of the hourglass. The excitations at very high energies disperse away from the antiferromagnetic wave vector (π, π) similarly to the high-velocity spin waves of the undoped systems. However their lifetimes are extremely short. To access these high energies requires a pulsed spallation neutron instead of a reactor-based source. See references [4-11] for an illustration of the hourglass dispersion and the cut-off of high energy excitations.

Neutron scattering has shown that cuprates may be superconducting independently of whether incommensurate spin correlations (stripes) are observed. Stripes may arise in a Fermi-liquid picture but may be hidden by strong magnetic correlations such as the elastic spin glass structure of Fig. 1 whose presence destroys Fermi-liquid oscillations^[18]. Stripes are seen in YBCO_{6+x} for large doping, $x > 0.45$, but not for $x < 0.35$. Neither are stripes present in electron doped systems like PLCCO^[19], yet all systems are superconducting. Neutron scattering then shows, despite the large body of theoretical work, that stripes may accompany high temperature superconductivity but are not necessarily an essential requirement, e.g. a result not a cause of superconductivity.

Likewise the neutron resonance is well formed only for strongly doped superconductors, but is not an essential requirement for all superconductors. It occurs when superconductivity is strong, but again may be a result, not a cause of superconductivity, especially as its spectral weight is so low (~2%) relative to the substantial density of high-energy spin fluctuations.

In the pseudogap phase the NMR spin susceptibility shows suppression below temperatures well above T_c , similar to the temperatures where neutron scattering shows an incipient resonance. In the superconducting phase the resonance is known to behave like a lower bound to the spin wave spectrum, but only for large doping where a resonance exists. In recent years it has been found that the pseudogap energy sets an upper bound above which defined spin fluctuations do not exist^[4-11].

We think the antiferromagnetic interactions provide the glue for pairing. At zero doping, the pairing coupling is the strongest but there are too few carriers to create superconductivity. As carrier density increases with doping the superconducting phase at first onsets and its critical temperature, T_c , should then increase. However we now know

from very high energy neutron scattering^[4] that, above the pseudogap energy, doping destroys the high-energy spin correlations that drive pairing, so there are fewer high frequency spin fluctuations and thus a lower superconducting coupling constant. For this reason the transition temperature reaches a maximum at about 15% doping before declining, despite the increasing carrier concentration. Beyond that doping the decline of the transition temperature is not from lack of carriers but from the great weakening of the pairing coupling. At such high doping, antiferromagnetic interactions are too weak for the pair formation. A decrease with doping in the local pair formation temperature is also occurring for doping from 5% to the optimum 15%, but the phase coherence temperature shows a net increase because the weakening of the pairing mechanism is overwhelmed by the increase in carrier density.

Regardless of whether the unusual magnetic correlations are responsible for the Cooper pairing or just a consequence of unconventional superconductivity, any successful microscopic theory of superconductivity in cuprates should be capable of explaining the doping and temperature dependence of the energy-momentum map drawn by neutron scattering.

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