Stripes and a two-component interpretation of NMR in cuprates

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Abstract

Based on the experimental fact that the susceptibilities $\chi_i(T)$ and the corresponding Knight shifts $K_i(T)$ $(i = c, ab)$ are linearly related above certain temperature $T^*_\chi(> T_c)$, one normally draws a conclusion that a single Fermi component is operative. We show that this may not be generally valid. As a counter example we propose a two-component system were the susceptibilities are determined by a universal function $f(T)$. The model consist of a Fermi component h^+ and a Bose component B^{++} with triplet spin localized in CuO_5 sites, in chemical equilibrium with respect to reaction $B^{++} \rightleftharpoons 2h^+$, where $f(T)$ gives fraction of bosons and $1 - f(T)$ the fraction fermions. The susceptibilities above T^*_χ are given by adding the fermion and boson contributions in the form $\chi_i(T) = \chi_{i0} + A_i[1 - f(T)] + B_i f(T)$, where χ_{i0}, A_i and B_i are T-independent. Clearly then $\chi_c(T)$ and $\chi_{ab}(T)$ are linearly dependent. If the bosons are localized within the CuO_6 octahedra or CuO_5 pyramids in the ab planes, rows of such tilted sites can explain the occurrence of stripes of localized charge and antiferromagnetic fluctuations in 2D CuO_2 planes.

Key words: superconductivity; NMR; stripes

The main doctrine applied in the analysis of the NMR experiments in that a single Fermi component is responsible for the magnetic properties in the normal state of the cuprates. This is based on the experimental findings that the Knight shift components $K_\alpha(T)$ are linearly dependent [1–3] and the temperature dependence measured with different nuclei ^{17}O, ^{63}Cu, ^{89}Y, etc are determined by a single universal function [1]. Example of linear relationship of susceptibility components $\chi_c(T)$ and $\chi_{ab}(T)$ are recent measurements by Watanabe *et al* on $Bi_2Sr_2CaO_{8+\delta}$[4]. The linear relationship is broken below a temperature $T^*_\chi(> T_c)$.

Based on this one-component approach Mila and Rice [5] developed a hyperfine Hamiltonian method suitable for treatment of CuO_2 plane elements ^{17}O(2) and ^{63}Cu(2) in calculation of the NMR Knight shifts $K_\alpha(T)$ ($\alpha = c, ab$, etc) and the corresponding rates $(^{Q}T_{1\alpha}T)^{-1}$ (Q= ^{17}O, ^{63}Cu). The theory was subsequently generalized by Pines *et al* [6–8] to also include the neutron scattering. The key point in calculation of the rates are the formfactors obtained from Mila-Rice Hamiltonian using nearest neighbour approximation. In order to understand simultaneously the rates for ^{17}O(2) and ^{63}Cu(2) Pines *et al* had to add to the Fermi liquid rates a specific contribution from antiferromagnetic spin fluctuations [AFSF], which in a strict sense is no longer a single component theory. The microscopic origin of AFSF remained unclear. Also the temperature dependencies had to be put in by hand.

The aim of this paper is to show that the observed linear relation between the Knight shift or susceptibility components does not necessarily imply a single Fermi component theory. Our example is a system of triplet bosons B^{++} localized at specific sites and a Fermi system in chemical equilibrium above a temperature T_{BL}. We proceed to show that the model can explain the following four points (1) The linear relationship between $\chi_\alpha(T)$ and $K_\alpha(T)$ above $T_{BL} = T^*_\chi(> T_c)$ (2) The origin of the stripes and AFSF. (3) Relates the temperature dependencies of NMR quantities back to

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the Hall effect. (4) Explain microscopically the pseudogap and spingap and their doping dependencies.

For cuprates we use the following scenario above T_{BL}: Triplet bosons made up of pairs of holes [9,10] with binding energy $E_B = 2k_BT^* = 2\Delta$ exist in the 2D CuO_2 planes in chemical equilibrium with the system holes. The charge balance within each plane is kept if the boson and fermion densities obey the relations [11]

$$n_b(T,x) = n_0(x)f(t)\,,\; n_h(T,x) = 2n_0(x)[1-f(t)], \quad (1)$$

where x is the doping variable and $t = T/T^*(x)$ is scaling temperature. The appearance of scaled temperature variable is characteristic of chemical equilibrium [11]. The equilibrium theory requires $f(t)$ to be a decreasing function with conditions $f(0) = 1$ and $f(\infty) = 0$. The function $f(t)$ is connected with the density of states $D(E)$ by relation [12]

$$1 - f(t) = -2\int_0^\infty D(E)\frac{d}{dE}[1+e^{E/k_BT}]^{-1}dE\,, \quad (2)$$

which means that the fermion part of susceptibility is proportional to $1-f(t)$, i.e. proportional to fermion density $n_h(T,x)$. Using the same argument for bosons we obtain for the susceptibility components ($i = c, ab$)

$$\chi_i(x,T) = A_i(x) + B_i(x)[1-f(T)] + C_i(x)f(T) \quad (3)$$
$$= \chi_i(x,\infty) + D_i(x)f(t)\,. \quad (4)$$

Here $A_i(x)$ is a temperature independent backraund term. Eliminating $f(t)$ one obtains linear relation between χ_{ab} and χ_c. In analogy with the Hall effect [11], we predict the fallowing new scaling law ($t = T/T^*$)

$$A(t) = \frac{\chi_i(x,T) - \chi_i(x,\infty)}{\chi_i(x,T^*) - \chi_i(x,\infty)} = \frac{f(t)}{f(1)}\,. \quad (5)$$

Here $T^*(x)$ is the scaling temperature obtained from Hall coefficient scaling and $A(t)$ is independent of doping x and the magnetic field direction. This gives the possibility to measure $f(t)$ above $T_\chi^* = T_{BL}$. Since the boson density is increased when x is increased from underdoped to overdoped one obtains a maximum of $\chi_i(x,T)$ for higher dopings and the coefficient $D_i(x) > 0$. Since analogous equations (3)-(5) are satisfied also by the Knight shift components $K_i(x,T)$ and we have shown the points (1) and (3) to be true.

If the temperature is lowered more and more bosons get delocalized due to the Coulomb charging effect, since the boson density goes up. This causes the scaling to be broken below T_{BL} both for Hall coefficient and the Knight shift components. It is convenient to write the fraction of singlet (delocalized) bosons in the form $\xi(x,T)f(t)$ and the localized fraction $[1-\xi(x,T)]f(t)$ whereby the fraction of fermions is even below T_{BL} given by $1-f(t)$. Using the same argument as before we obtain for the Knight shifts, by removing the temperature independent orbital parts a way ($i = ab, c$)

$$K_i(x,T) = a_i(x)[1-f(t)] + b_i(x)[1-\xi(x,T)]f(t)\,. (6)$$

Assuming that Korringa type relation is separately valid for fermion and boson parts, we can write for the relaxation rate for a given nucleus

$$({}^Q T_{1i}T)^{-1} = {}^Q c_i(x)[1-f]^2 + {}^Q d_i(x)[1-\xi(x,T)]^2 f^2 + R(x,T)\,, \quad (7)$$

where the correction term $R(x,T)$ is assumed to be small in the temperature range $T < T^*$. Equations (6) and (7) are assumed valid down to $T = 0$. In order to justify this we propose the following scenario: In the normal state the boson localization sites are the CuO_6 octahedra (one plane case) in each CuO_2 plane. The observed tilts [13,14] in these sites are proposed to be caused by the localized boson inside [15]. A row of such tilted sites makes the stripe whose breadht is one unit cell and the distance between the stripes about 2 unit cells [13]. In each CuO_2 plane one obtains antiferromagnetic bosons superlattice, commensurate with the chemical lattice. In this way the points (2) and (4) are understood. Since the boson lattice becomes 3D at T_c, induced antiferromagnetism becomes possible for $T < T_c$ [16]. The breakdown of linear relation between χ_c and χ_{ab} below $T_{BL} = T_\chi^*$ [17] becomes well understood.

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