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Magnetic susceptibility of itinerant electrons and Knight shift of Li in YBCO

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Abstract

The Knight shift ΔK of the ${}^7\text{Li}$ RMN line in Li doped YBaCuO has been measured recently by Sauv et al. [Physica C 223 (1994) 145; Physica C 235–240 (1994) 1731]. The authors find that the variation of ΔK with temperature follows a logarithmic law, $\Delta K \sim \ln(1/T)$ in the normal state and is independent of the Li concentration x , for $x < 0.02$. Such a law has been predicted theoretically by Bok and Labbé [C.R. Acad. Sci. 305 (1987) 555] assuming that the Fermi level lies at a van Hove logarithmic singularity characteristic of a two-dimensional metal. This calculation has been extended to small variations of the doping level of Li. The experimental results [Physica C 235–240 (1994) 1731] agree with our calculation. We think that this pure 2D behavior is due to the fact that the Li atoms are located in the CuO_2 planes and thus have an ideal location to test the behavior of the free carriers in the CuO_2 planes. This is different from the other nuclei studied in NMR measurements, such as ${}^{17}\text{O}$, ${}^{63}\text{Cu}$ or ${}^{89}\text{Y}$.

The origin of the high T_c in the superconducting cuprates is still controversial. One of the proposed models [4] is based on the existence of a van Hove [5] singularity in the density of states. Such a singularity exists in the normal state and the properties of the cuprates above T_c should also be explained in the framework of this model. The existence of singularities in the electron density of states in a normal metal has been predicted by van Hove [5]. It is a general topological theorem for itinerant electrons in a periodic potential and does not depend on the details of the band-structure calculation. In two dimensions the constant energy surfaces $E(k_x, k_y)$ must have saddle points. Near a saddle point the density of state is

$$n(E) = \frac{N}{\pi^2 D} \ln \frac{D}{|E - E_s|}, \quad (1)$$

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where D is the width and E_s the position of the van Hove singularity. We assume that this model applies to electrons (or holes) in the CuO_2 planes of the cuprates; in that case $N = 8$ per Cu atom in YBCO. These singularities have also been observed experimentally in angular-resolved photoemission spectroscopy (ARPES) in YBaCuO [6] and bismuth compounds [7].

We have computed the Pauli susceptibility $\chi(T)$ for YBaCuO, assumed to behave like a 2D normal metal, for various doping levels in Li, i.e. when the Fermi level is displaced from E_s . We use the general formula for the susceptibility:

$$\chi(T) = \mu_0 \frac{M(T)}{B},$$

with

$$M(T) = \mu_0(N_+ - N_-),$$

and

$$(N_+ - N_-) = \frac{1}{2} \int_{-\infty}^{+\infty} n(E) [f_{\text{FD}}(E_F + \mu_B B) - f_{\text{FD}}(E_F - \mu_B B)] dE,$$

where $M(T)$ is the magnetization of the sample, B the applied magnetic field, here $B = 8.5$ T, cf. Refs. [1] and [2], $n(E)$ is the density of state given by the formula (1), E_F the Fermi level energy, and f_{FD} is the Fermi–Dirac distribution:

$$f_{\text{FD}}(E - E_F \pm \mu_B B) = \frac{1}{\exp\left(\frac{E - E_F \pm \mu_B B}{k_B T}\right)}.$$

We obtain the following formula for the susceptibility $\chi(T)$ per Cu atom and per unit volume:

$$\chi(T) = \frac{1}{2} \frac{\mu_0 \mu_B}{B} k_B T \sinh u \frac{8}{\pi^2 D} \left(I_1 \ln \frac{D}{k_B T} + I_2 \right), \quad (2)$$

where

$$I_1 = \int_{-\infty}^{+\infty} \frac{1}{\cosh y' + \cosh u} dy,$$

$$I_2 = - \int_{-\infty}^{+\infty} \frac{\ln |y|}{\cosh y' + \cosh u} dy,$$

$$u = \frac{\mu_B B}{k_B T} \ll 1, \quad y = \frac{E}{k_B T}, \quad y' = y - \delta,$$

$$\delta = \frac{E_F - E_s}{k_B T};$$

k_B is the Boltzmann constant, $\mu_0 = 4\pi \times 10^{-7}$ in SI units, μ_B the Bohr magneton.

We can see that δ represents the relative shift of the Fermi level from the singularity. For the Fermi level E_F lying exactly at E_s , i.e. $\delta = 0$, we find the result already published by Bok and Labbé [3]:

$$\chi(T) = \frac{8\mu_0 \mu_B^2}{\pi^2 D} \left(\ln \frac{D}{2k_B T} + \frac{\pi^2}{12} \right). \quad (3)$$

For comparison with the experimental results we have to take into account the other contributions to the

magnetic susceptibility which are temperature independent (core electrons, diamagnetic contributions, etc).

We write

$$\chi_{\text{total}}(T) = \chi_{\text{i.e.}}(T) + \chi_0,$$

where $\chi_{\text{i.e.}}$ is the itinerant-electron contribution given by Eq. (2).

The magnetic fluctuations which could lead to a deviation from the linear law $\ln(1/T)$ [8,9] are negligible for an $\text{YBa}_2\text{Cu}_3\text{O}_7$ compound with a low, non-magnetic, Li doping.

Sauv et al. [1,2] have measured the Knight shift ΔK of the ^7Li NMR line in disoriented ceramics $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}\text{Li}_x$. The Li ion is supposed to go into the CuO_2 planes and so can play the role of a local probe for the 2D itinerant electrons in these planes. The experimental results fit very well a linear behavior in $\ln(1/T)$ of the form

$$\Delta K = a \ln \frac{1}{T} + b. \quad (4)$$

These results are well explained with our calculations using formula (2) and the fact that

$$\Delta K = \alpha \chi_{\text{i.e.}}(T) + \beta \chi_0, \quad (5)$$

where α and β are given by

$$\alpha = \frac{1}{\mu_B} H_{\text{eff}}^{(0)} \quad \text{and} \quad \beta = \frac{1}{\mu_B} H_{\text{eff}}^{(1)},$$

where $H_{\text{eff}}^{(0,1)}$ is a hyperfine field experienced by the Li nucleus. We also may write

$$\alpha = \frac{B_f}{\mu_0 \mu_B},$$

where B_f is the effective field acting on the nucleus.

Using Eq. (2), we want to compute numerically the coefficients a and b for various doping levels x in Li. From the value of x , we have to compute

$$\delta = \frac{E_F - E_s}{k_B T}$$

and insert that value of δ in Eq. (2), which is the only variable. To do that, we assume that each Li atom is transformed into a Li^+ ion and thus takes away one hole from the CuO_2 plane. The results of our calculations are given in Fig. 1 where we plot the relative

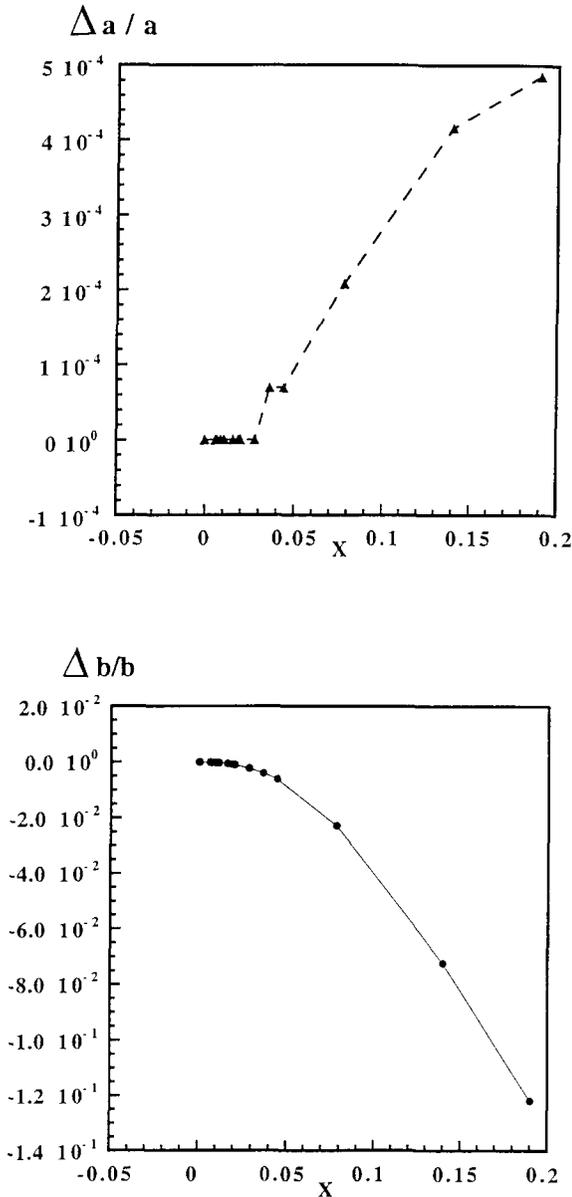


Fig. 1. Relative variation of the slope a (a), and the ordinate b (b) of the law $a(\ln(1/T)) + b$, with the Li concentration x .

position of a (Fig. 1(a)) and b (Fig. 1(b)) with x between 0 to 0.2, i.e. δ between 0 to 3. We see that the slope a is insensitive to x , for $x < 0.03$, and that the relative variation of b is negligible, for $D = 3$ eV.

The experiments have been done for the following values of x : $x = 0.0062, 0.0072, 0.016$ and 0.019 ; with an oxygen concentration of 7.01 ± 0.02 constant for all x , and the critical temperature of the samples are such

that $89 \text{ K} < T_c < 91 \text{ K}$ [2]. We see that for this doping range, the slope a and also b are practically constant. To fit the calculated value a to the experimental one, we need the two quantities D and B_f . D is taken as 3 eV which is an experimental value taken from photo-emission data [6]. For B_f , we fit the calculated value of a with the experiment for $x = 0.019$, for which we have a maximum of experimental points. This leads to $\alpha = 3.96 \times 10^{29} \text{ J T}^{-2}$; then $B_f = 4.6 \text{ T}$.

To compare this value of B_f to measurements of the Knight shift of ^7Li in other compounds, we used Ref. [10]. We find a value of $B_{\text{eff}}^{\text{atom}} = 12.2 \text{ T}$ for a free Li atom as deduced from atomic beam measurements. When the Li nucleus is in a solid, the effective field becomes $B_f = \xi B_{\text{eff}}^{\text{atom}}$, the factor ξ is used to account for any deviation in hyperfine coupling from free-atom behavior. ξ is estimated to have values typically between 0.1 and 0.8 for simple metals. A value of $\xi = 0.4$ is given for metallic lithium. Taking our value of $B_f = 4.6 \text{ T}$ deduced from experiment, we find $\xi = 0.38$ which is in very good agreement with the estimations given in Ref. [10]. Fig. 2 shows the theoretical curve (Eq. (4)) with $B_f = 4.6 \text{ T}$ and $b = 618.5 \text{ ppm}$ and the experimental points for all values of x [2]. Because we do not know the various contributions χ_0 to the magnetic susceptibility, b is an adjusted parameter.

As a conclusion, we note, that we have computed the magnetic susceptibility of a Fermi liquid of itinerant electrons in a two-dimensional periodic potential in the normal state. When the Fermi level lies near a van Hove singularity, we predict a susceptibility $\chi(T)$ linear in $\ln(1/T)$. $\chi(T)$ is practically independent of the relative position of the Fermi level $\delta = (E_F - E_s)/(k_B T)$ as long

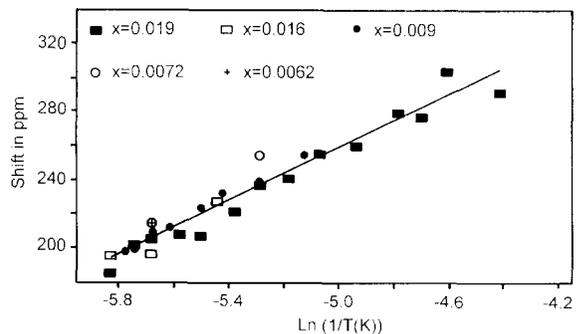


Fig. 2. Variation of the Knight shift ΔK in ppm with $\ln(1/T)$. Full line: calculation; experimental points: (■) $x = 0.019$, (□) $x = 0.016$, (●) $x = 0.009$, (○) $x = 0.0072$, (+) $x = 0.0062$.

as $\delta < 0.2$. These calculations explain very well the experimental results obtained by Sauv et al. [2] on the Knight shift of ^7Li in YBaCuO. The agreement is particularly good on two points:

(1) the value of the slope a is fitted without adjustable parameters. D and B_f are taken from other experiments, (2) the slope a and the ordinate at the origin b are independent of the Li concentration x , for $x < 2\%$.

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References

- [1] K. Sauv, M. Nicolas and J. Conard, *Physica C* 223 (1994) 145.
- [2] K. Sauv, J. Conard and M. Nicolas, *Physica C* 235–240 (1994) 1731.
- [3] J. Bok and J. Labbé, *C.R. Acad. Sci.* 305 (1987) 555.
- [4] J. Labbé and J. Bok, *Europhys. Lett.* 3 (1987) 1225.
- [5] L. van Hove, *Phys. Rev.* 89 (1953) 1189.
- [6] A. Bansil, M. Lindros, K. Gofron and J.C. Campuzano, *J. Phys. Chem. Solids* 54 (1993) 1185.
- [7] Z.X. Shen, D.S. Dessau, B.O. Well and D.M. King, *J. Phys. Chem. Solids* 54 (1993) 1169.
- [8] A.M. Clogston, V. Jaccarino and Y. Yafet, *Phys. Rev. A* 134 (1964) 650.
- [9] J. Labbé, *Phys. Rev.* 158 (1967) 647.
- [10] J.C. Carter, L.H. Bennett and D.J. Kahan, *Metallic shifts in NMR*, *Progress in Material Science*, vol. 20 (Pergamon, Oxford, 1977).