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1994 J. Phys.: Condens. Matter 6 3767

(http://iopscience.iop.org/0953-8984/6/20/015)

J. Phys.: Condens. Matter 6 (1994) 3767–3770. Printed in the UK

A possible effect of spin fluctuations on the electric field gradient in Cu–O layers in high-T_c superconductors

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Received 31 August 1993, in final form 2 February 1994

Abstract. A possible effect of spin fluctuations on the electric field gradient in Cu–O layers in HTSCs is studied by the phenomenological antiferromagnetic Fermi-liquid theory of Millis *et al*. Our theoretical analysis suggests that the coupling between the quadrupole charge density and the spin fluctuations in the two-dimensional 'metallic' Cu–O layers is the origin of the temperature dependence of ^{63}Cu NQR frequencies at the Cu(2) sites in $YBa_2Cu_3O_{7-\delta}$.

NMR and Knight-shift measurements have revealed important information about the character of low-energy spin fluctuation in the Cu–O layers in the high-T_c oxides [1,2]. On the basis of these experiments, a number of models has been proposed [2]. One of these is the so-called nearly antiferromagnetic Fermi-liquid model, formulated by Millis *et al* and used by them to explain the NMR experiments on 90 K $YBa_2Cu_3O_{7-\delta}$ [3]. This model was extended later to explain the NMR and Knight-shift measurements on $YBa_2Cu_3O_{6.53}$ [4] and $La_{1.85}Sr_{0.15}CuO_4$ [5], and also the anomalous tunnelling characteristic of the high-T_c oxides [6]. A similar model has been also formulated by Moriya *et al* [7].

It is well known that there are effects of the coupling between the quadrupole charge density and the spin fluctuations in the weakly magnetic and nearly magnetic materials. This effect has been studied in detail both theoretically and experimentally [8,9]. We expect naturally that the same effect would occur in the high-T_c oxides. However, a peculiarity of the high-T_c oxides is that spin fluctuation takes place only in the two-dimensional 'metallic' Cu–O layers, but not in the other 'insulated' layers. So the effect mentioned above is also two dimensional in nature and occurs only in the Cu–O layers i.e. the effect can take place only at the Cu(2) sites and not at the Cu(1) sites.

In [10] the temperature dependence of ^{63}Cu NQR frequencies at the Cu(2) sites in $YBa_2Cu_3O_{7-\delta}$ was reported and the variation in electric field gradients (EFGs) with decreasing temperature was explained as due to lattice compression. In this model we fit the experimental values by a Gaussian function [11]

$$V_Q = V^0 \exp(-bT^2) \tag{1}$$

with $V^0 = 31.6$ MHz and $b = 1.66 \times 10^{-7}$ K^{-2} and where T is the temperature and V_Q is the ^{63}Cu NQR frequency at the Cu(2) sites in $YBa_2Cu_3O_{7-\delta}$. The ^{63}Cu NQR frequency is defined as $e^2Qq/2h$ (q is the total EFG at the Cu(2) sites). In [11] the physical significance of this expression was discussed in detail. Here, we mention that the exponential factor $\exp(-bT^2)$ is an effective Debye–Waller factor, which relates the temperature dependence

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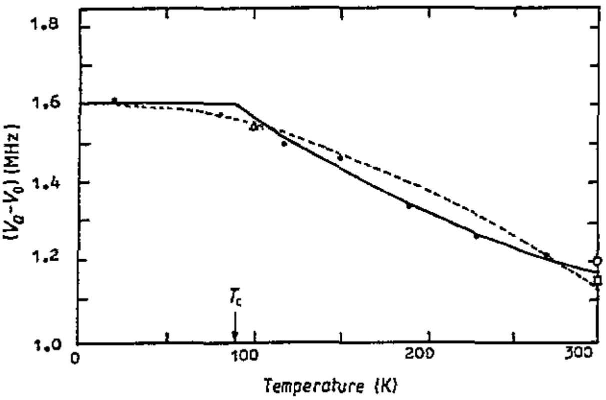

Figure 1. $V_Q - V_0$ versus T: ——, from equations (9)–(12); - - - -, from equation (1); ●, experimental data from [10]; △, experimental data from [14]; □, experimental data from [15]; ○, experimental data from [16].

of the EFG to the vibrational degrees of freedom in the crystal lattice. It is shown in figure 1 by the broken curve. The fit seems to be unsatisfactory. This result seems to indicate that a purely lattice temperature effect of the EFG is not sufficient do describe its temperature dependence.

From the above discussion, we argue that the above-mentioned temperature dependence of V_Q seems to indicate the existence of a coupling between the field gradient, as a quadrupole component of charge density, and the spin-density fluctuation modes.

Here we give a simple argument to show the possible effect of spin fluctuations on the electric gradient at a nucleus due to the conduction electrons. It is often assumed that the EFG q in metals consists of two contributions, i.e.

$$q = q_l + q_{el} \tag{2}$$

where q_l comes from all the positive ion cores surrounding the nucleus of interest and q_{el} represents the deviation in the conduction electron charge density from a cubic distribution.

We assume that an electron in the Bloch state k as a Hartree–Fock solution gives a field gradient at the Cu(2) nuclear site. The total EFG due to the conduction electrons q_{el} is then given by

$$\begin{aligned} q_{el} &= T\sum_{\sigma}\sum_{k} q_k G^{\sigma}(k) \\ G^{\sigma}(k) &= \frac{1}{[G^{\sigma}_{HF}(k)]^{-1} - \Sigma^{\sigma}(k)} \end{aligned} \tag{3}$$

where k is the four vector $k = (k_0, \boldsymbol{k})$ with $k_0 = (2n+1)\pi T$, n being an integer, and T is the temperature in the energy units (so that $k_B = 1$). $G^{\sigma}(k)$ is the one-particle Green function, and $G^{\sigma}_{HF}(k)$ the Green function within the Hartree–Fock approximation. $\Sigma^{\sigma}(k)$ is the self-energy correction. We now study the self-energy correction due to the transverse spin fluctuations:

$$\sum_{sf}^{\sigma} = TI^2\sum_{q}\chi^{-\sigma\sigma}(q)G^{-\sigma}(k+q) \simeq I^2\Big(T\sum_{q}\chi^{-\sigma\sigma}(q)\Big)G^{-\sigma}(k) \tag{4}$$

where I is the intra-atomic exchange interaction constant and $\chi^{-\sigma\sigma}(q)$ is the transverse dynamical susceptibility. Then

$$G^{\sigma}(k) \simeq G^{\sigma}_{\mathrm{HF}}(k) + \left(I^2 T \sum_q \chi^{-\sigma\sigma}(q)\right) G^{\sigma}_{\mathrm{HF}}(k) G^{-\sigma}(k) G^{\sigma}(k) \tag{5}$$

and we obtain

$$q_{\mathrm{el}} \simeq q_{\mathrm{el}}^{\mathrm{HF}} + K S_{\mathrm{L}}^2(T) \tag{6}$$

with

$$q_{\mathrm{el}}^{\mathrm{HF}} = T \sum_{\sigma} \sum_{k} q_k G^{\sigma}_{\mathrm{HF}}(k)$$

$$K = \tfrac{2}{3} N_0^2 I^2 \sum_{\sigma} \sum_{k} q_k G^{\sigma}_{\mathrm{HF}}(k) G^{-\sigma}(k) G^{\sigma}(k)$$

$$S_{\mathrm{L}}^2(T) = \frac{3}{2N_0} T \sum_q \chi^{-+}(q)$$

where N_0 is the number of Cu(2) sites and $S_{\mathrm{L}}^2(T)$ is the mean square local amplitude of the spin fluctuation. According to the self-consistent renormalization theory [9],

$$S_{\mathrm{L}}^2(T) = \frac{A}{\chi(Q)} + B \tag{7}$$

where A and B are temperature-independent constants $\chi(Q)$ is the temperature dependence of the staggered susceptibility. Thus, from equations (2), (6) and (7) we obtain

$$q \simeq q_0 + K' + \frac{K''}{\chi(Q)} \tag{8}$$

with $K' = KB$, $K'' = KA$ and $q_0 = q_1 + q_{\mathrm{el}}^{\mathrm{HF}}$.

Equations (6) and (8) give a simple argument to show how q_{el} is influenced by the spin fluctuations and can be related to the staggered susceptibility.

From a more detailed theory [8, 9] we have

$$V_{\mathrm{Q}} = V_0 + V'/[1/\chi(Q) + d] \tag{9}$$

where V_0 represents the contributions from the ion cores, the antishielding effect and the valence electrons of the Cu(2) ion that are treated by the Hartree–Fock approximation, and V' and d are constants. It is obvious that the behaviour of the temperature dependence of the ^{63}Cu NQR frequencies is closely related to the staggered susceptibility $\chi(Q)$.

The $\chi(Q)$-value is calculated from the phenomenological antiferromagnetic Fermi-liquid theory [3]:

$$\chi(Q) = \chi_0 (L/L_0)^2 \tag{10}$$

where χ_0 is the static susceptibility and L is the spin correlation length which is assumed to vary with temperature as [12, 13]

$$L^2(T) = L^2(0)[T_{\mathrm{x}}/(T + T_{\mathrm{x}})]. \tag{11}$$

The parameters T_x, $L(0)/L_0$ and χ_0 have been determined by fitting NMR data [3]. For 90 K $YBa_2Cu_3O_{7-\delta}$, the values are $T_x = 115$ K, $L(0)/L_0 = 5.5$, $\chi_0/u_B^2 = 3$ states eV^{-1} Cu(2), when $T \leqslant T_c$ and

$$L^2(T) = L^2(0)[T_x/(T_c + T_x)]. \tag{12}$$

In figure 1 we plot $V_Q - V_0$ against T. The experimental points in figure 1 are from [10, 14–16]. The solid line represents a least-squares fit of the theoretical equations (9)–(12) with the experiment. The following values are used for the parameters: $V_0 = 30$ MHz, $V' = 0.0822$ MHz eV Cu(2)/states and $d = 0.0315$ eV Cu(2)/states.

Our theoretical analysis fits the experimental results excellently and suggests strongly that the coupling between the quadrupole charge density and the spin fluctuations in the two-dimensional 'metallic' Cu–O layers is the predominant origin of the temperature dependence of ^{63}Cu NQR frequencies at the Cu(2) sites in $YBa_2Cu_3O_{7-\delta}$.

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