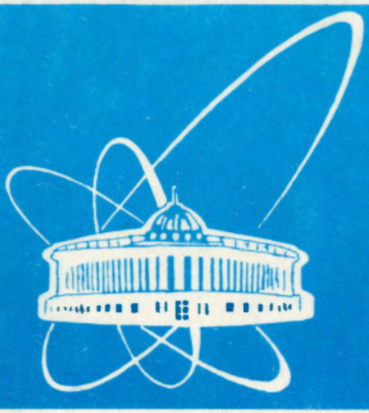

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SPIN-FLUCTUATION LINEWIDTH OF THE 4*f*-ELECTRON CRYSTAL FIELD LEVELS IN CUPRATES

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Спин-флуктуационная ширина уровней $4f$-электронов
в кристаллическом электрическом поле в купратах

Вычислена ширина линии $\Gamma_{cf}(T)$ возбуждений $4f$-электронов в кристаллическом поле в Tm-YBCO соединениях, обусловленная $s-f$ взаимодействием. Расчеты проведены для двухуровневой модели методом двухвременных функцийГрина. Показано, что антиферромагнитные флуктуации в CuO_2 плоскостях важны для объяснения температурной зависимости Γ_{cf}.

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Spin-Fluctuation Linewidth of the $4f$-Electron Crystal Field
Levels in Cuprates

The crystal field excitation linewidth $\Gamma_{cf}(T)$ in Tm-YBCO system is calculated due to $s-f$ interactions. The method of two-time Green function was used in the two-level approximation for crystal field excitations. It is shown that the antiferromagnetic fluctuations in CuO_2 planes are important to explain the temperature dependence of Γ_{cf}.

The investigation has been performed at the Bogoliubov Laboratory of Theoretical Physics, JINR.

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1 Introduction

The effect of sharp reduction of crystal-field (CF) linewidth for $4f$-electrons at the superconducting transition temperature T_c in metallic alloys with rare-earth (RE) impurities (e.g. $Tb_xLa_{1-x}Al_2$) is a well established phenomena [1].

In order to get more information about the spin dynamics in the CuO_2 planes, temperature dependence of linewidth $\Gamma_{cf}(T)$ of CF transitions in RE doped high T_c superconductors has been also investigated [2, 3]. But it was observed that the linewidth sharply decreases at some temperature T_s well above T_c.

The existence of antiferromagnetic (AF) correlations in high-T_c superconducting cuprates is widely accepted [4-8].Suggesting that spin fluctuations provide a primary mechanism for the relaxation of the excited f-electrons, in the present paper we consider the model Hamiltonian of the RE ions and the spins at the Cu2 sites with the indirect-exchange coupling [9]. Using the pseudospin formalism and the method of the two-time Green functions (GF), we have derived the expression for $\Gamma_{CF}(T)$ (similar to that in Ref.1) of the first excited level $\Gamma_4^{(1)}$ RE ion Tm^{3+} in the superconducting $Tm_{0.1}Y_{0.9}Ba_2Cu_3O_{6.9}$ (Tm-$TBCO_{6.9}$)-compound [3]. Using the results of Rossat-Mignod et al. [5] of the temperature dependence of the imaginary part of the magnetic susceptibility of $YBCO_{6.92}$ near the AF wave vector Q_{AF}=(1/2 , 1/2 , 1.6) for the energy $\hbar\omega = 10$ meV , we have made a conclusion that dynamic spin fluctuations in CuO_2 dominate in the line broadening.

For the nonsuperconducting compound Tm-$YBCO_{6.1}$, using spin-wave approximation it has been shown that the main contribution to $\Gamma_{CF}(T)$ arises from a one-magnon process, which means that the spin gap is small compared to the $4f$ level splitting [10].

The paper is organized as follows. In the next Section, we present the model of s-f coupling. In Sec. III we introduce pseudospin formalism and derive the expression for linewidth $\Gamma_{CF}(T)$. In Sec. IV we discuss the numerical results and related works. In Sec. V we present our conclusions.

2 Model of s-f Interactions

Adopting the model of the one-component AF Fermi-liquid [4], [11] , we can write the model of RE ions and spins $S = 1/2$ at the Cu2 sites in the following form:

$$H = H_{cf} + H_{s-s} + H_{s-f}, \tag{1}$$

where the Hamiltonian of CF for Tm^{3+} ions into the bilayers CuO_2-Tm^{3+}-CuO_2 (Fig. 1) can be presented in the following way:

$$H_{cf} = \sum_{n,i} \omega_n K_{nn}^{(i)} \tag{2}$$

where $K_{mn}^{(i)} = (|m\rangle\langle n|)_i$ are the transitions operators for the n, m levels of the CF of Tm^{3+} ions at the site i, and ω_n is the appropriate energy of the level n. H_{s-s} is the spin Hamiltonian describing doped holes in the CuO_2 plane and spin-spin interactions of the spins $\mathbf{S}_i$ at the copper sites. We are not going to discuss the problem of calculation the dynamical spin susceptibility $\chi(\mathbf{q},\omega)$ for any explicit form of H_{s-s} but adopt some models for $\chi(\mathbf{q},\omega)$ in our numerical calculations.

The Hamiltonian of the s-f interactions describing coupling between spins at Cu2 sites and $4f$-electrons, we present in the following manner:

$$H_{s-f} = -\sum_{i,j} I_{s-f}^{\alpha} J_i^{\alpha} S_j^{\alpha}, \tag{3}$$

where $\mathbf{J}_i$ is the operator of the total angular momentum of the Tm^{3+} ion at site i; $\mathbf{S}_j$ is the operator of the spin at the copper sites j nearest to the site i and I_{s-f}^{α}, in the general case, the anisotropic indirect-exchange coupling constant, $\alpha = (x, y, z)$.

Due to a local character of $4f$-electrons, we ignore the interaction between them and holes in the CuO_2 planes.

3 Calculation of the linewidth in the pseudospin representation

Let us recall that for pollycrystalline samples, in the dipole approximation (for small scattering vectors of neutrons κ), the partial differential cross-section of transversal magnetic inelastic neutron scattering (INS) per ion of RE target can be written as [15]:

$$\left(\frac{d^2\sigma}{d\Omega dE'}\right)_{\perp} = \frac{1}{6}(r_0\gamma)^2 \frac{k'}{k}\left[\frac{g}{2}F(\vec{\kappa})\right]^2 \frac{e^{\beta\omega}}{1-e^{\beta\omega}} \frac{1}{\pi} \mathrm{Im}(\langle J_i^- | J_i^+ \rangle)_{\omega+i\varepsilon}, \tag{4}$$

where $r_0 = \dfrac{e^2}{m_e c^2}$ is the electromagnetic radius of electron, $\gamma = -1.91$ is the magnetic moment of neutron in units of the nuclear magneton $\mu_N = \dfrac{e\hbar}{2m_p c}$, $\vec{\kappa} = \vec{k} - \vec{k}'$, where $\vec{k}$ and $\vec{k}'$ are incident and scattered neutron wave vectors,

respectively, $F(\vec{\kappa})$ is the free-ion form factor, g is the Landé splitting factor and where $\mathrm{Im}(\langle J_i^- | J_i^+ \rangle)_{\omega+i\varepsilon}$ is the Fourier transform of the two-time GF [16].

The ground-state multiplet $^3H_6$ of Tm^{3+} in CF of orthorhombic symmetry D_{2h} splits into 13 singlets [13]: $4\Gamma_1, 3\Gamma_2, 3\Gamma_3$ and $3\Gamma_4$. The wave functions of the irreducible representations Γ_i can be given by [14]:

$$|n\rangle \equiv |\Gamma_i^{(j)}\rangle = \sum_{M=-J}^{J} a_{ij}^{(M)} |M\rangle, \tag{5}$$

where index j represents dimension of the Γ_i, along with

$$J^z|M\rangle = M|M\rangle. \tag{6}$$

Since the first excited level $\Gamma_4^{(1)}$ of CF is non-degenerate and its energy is much lower than the energy of the second one $\Gamma_2^{(1)}$, it is possible to approximate the local CF scheme of Tm^{3+} ions in Tm-$YBCO_{6.9}$ by two levels [1], [3], [13].

Let us define the wave functions of the ground state of H_{cf} by:

$$|-\rangle \equiv |\Gamma_3^{(1)}\rangle = a_{31}^{(6)}|6\rangle + a_{31}^{(2)}|2\rangle, \tag{7}$$

and the first excited one as

$$|+\rangle \equiv |\Gamma_4^{(1)}\rangle = a_{41}^{(5)}|5\rangle + a_{41}^{(3)}|3\rangle + a_{41}^{(1)}|1\rangle, \tag{8}$$

respectively. Then, it is possible to introduce an operator of pseudospin σ^{α} whose components satisfy the following relations:

$$\sigma^z|\pm\rangle = \pm\frac{1}{2}|\pm\rangle \qquad \text{and} \qquad \sigma^{\pm}|\mp\rangle = |\pm\rangle. \tag{9}$$

In this pseudospin representations H_{cf} can be written as:

$$\hat{H}_{cf} = \omega_0 \sum_i \sigma_i^z \tag{10}$$

where $\omega_0 = \omega_+ - \omega_- = 11.8$ meV is the energy of the first excited CF level.

By expanding the components of the total angular momentum $\mathbf{J}$ into the basical operators of the components of pseudospin, H_{s-f} can be written as

$$H_{s-f} = -\sum_{i,j}\{I_{ij}^{zz}[A \cdot S_j^z + B \cdot \sigma_i^z S_j^z] + \tag{11}$$
$$+\frac{1}{2}I_{ij}[C \cdot (\sigma_i^- S_j^- + \sigma_i^+ S_j^+) + D \cdot (\sigma_i^+ S_j^- + \sigma_i^- S_j^+)\},$$

where the coefficient are

$$A = \frac{1}{2}\{6(a_{31}^{(6)})^2 + 2(a_{31}^{(2)})^2 + 5(a_{41}^{(5)})^2 + 3(a_{41}^{(3)})^2 + (a_{41}^{(1)})^2\} \approx 1.05$$

$$B = 5(a_{41}^{(5)})^2 + 3(a_{41}^{(3)})^2 + (a_{41}^{(1)})^2 - 6(a_{31}^{(6)})^2 - 2(a_{31}^{(2)})^2 \approx -0.38$$
$$C = a_{31}^{(6)} a_{41}^{(5)} \sqrt{12} + a_{31}^{(2)} a_{41}^{(1)} \sqrt{40} \approx 2.44$$
$$D = 6 a_{41}^{(3)} a_{31}^{(2)} \approx 1.69$$

Keeping only the resonance terms, H_{s-f} becomes

$$\tilde{H}_{s-f} = -\frac{1}{2} \sum_{i,j} \tilde{I}_{ij} (\sigma_i^- S_j^+ + \sigma_i^+ S_j^-), \tag{12}$$

where $\tilde{I}_{ij} = I_{ij} D$ and $I_{ij}^{xx} \approx I_{ij}^{yy} = I_{ij}$.

The differential cross section (4) in terms of the pseudospin operators can be written as:

$$\left(\frac{d^2\sigma^i}{d\Omega d\omega} \right)_\perp \propto \frac{e^{\beta\omega_0}}{1 - e^{\beta\omega_0}} \frac{1}{\pi} \mathrm{Im} \langle\langle \sigma_i^- | \sigma_i^+ \rangle\rangle_{\omega_0 + i\epsilon}. \tag{13}$$

Using the technique of differentiating with respect to two times, t and t', in the equation-of-motion method for the two-time GF $\langle\langle \sigma_i^-(t), \sigma_i^+(t') \rangle\rangle$, we find:

$$(\omega - \omega_0)^2 \langle\langle \sigma_i^- | \sigma_i^+ \rangle\rangle_\omega = -2\langle \sigma^z \rangle (\omega - \omega_0) + \sum_{j,j'} \tilde{I}_{ij} \langle\langle \sigma_i^z S_j^- | \sigma_i^z S_{j'}^+ \rangle\rangle_\omega \tilde{I}_{ij'}. \tag{14}$$

Since the s-f coupling is very weak, we consider only the second order terms which are allowing for by the decoupling:

$$\langle \sigma_i^z(t) S_j^-(t) \sigma_i^z S_{j'}^+ \rangle \simeq \langle \sigma_i^z(t) \sigma_i^z \rangle \langle S_j^-(t) S_{j'}^+ \rangle \simeq \frac{1}{4} \langle S_j^-(t) S_{j'}^+ \rangle. \tag{15}$$

In this approximation we neglect the longitudinal relaxation :

$$\langle \sigma_i^z(t) \sigma_i^z \rangle \simeq \langle \sigma_i^z \sigma_i^z \rangle = \frac{1}{4}. \tag{16}$$

It results in the following equation for the GF:

$$\langle\langle \sigma_i^- | \sigma_i^+ \rangle\rangle_\omega = -\frac{2\langle \sigma^z \rangle}{\omega - \omega_0 - \Sigma_i(\omega)/(-2\langle \sigma^z \rangle)}, \tag{17}$$

where in the self-energy operator

$$\Sigma_i(\omega) = \frac{1}{4} \sum_{j,j'} \tilde{I}_{ij} \langle\langle S_j^- | S_{j'}^+ \rangle\rangle_\omega \tilde{I}_{ij'}. \tag{18}$$

The summation runs over the j, j' copper sites in the neighbouring CuO_2 planes and

$$\langle \sigma^z \rangle \simeq -\frac{1}{2} \mathrm{th} \left(\frac{\omega_0}{2kT} \right). \tag{19}$$

The linewidth $\Gamma_{cf}(T)$ is determined by the imaginary part of the self-energy operator

$$\Gamma_{cf}(\omega_0) = \coth \left(\frac{\omega_0}{2kT} \right) \mathrm{Im} \{ \Sigma_i(\omega_0 + i\varepsilon) \}. \tag{20}$$

Translational invariance allows the spatial Fourier transformation:

$$\langle\langle S_j^- | S_{j'}^+ \rangle\rangle_\omega = \frac{1}{N} \sum_{\mathbf{q}} e^{i\mathbf{q}(\mathbf{R}_j - \mathbf{R}_{j'})} \langle\langle S^- | S^+ \rangle\rangle_{\mathbf{q},\omega}, \tag{21}$$

and (19) becomes:

$$\Gamma_{cf}(\omega_0) \propto \coth \left(\frac{\omega_0}{2kT} \right) \sum_{\mathbf{q}} |F(\mathbf{q})|^2 \mathrm{Im} \{ \chi^{-+}(\mathbf{q}, \omega_0 + i\varepsilon) \}. \tag{22}$$

where the imaginary part of the dynamical spin susceptibility in the CuO_2 planes is given by :

$$\mathrm{Im}\chi^{-+}(\mathbf{q}, \omega_0) \equiv -\mathrm{Im} \langle\langle S^- | S^+ \rangle\rangle_{\mathbf{q},\omega_0} \equiv \chi''_{-+}(\mathbf{q}, \omega_0), \tag{23}$$

and

$$F(\mathbf{q}) = 8 \cos\left(\frac{aq_x}{2}\right) \cos\left(\frac{bq_y}{2}\right) \cos\left(\frac{cq_z}{6}\right) \tag{24}$$

is the form factor reflecting the local symmetry of the Tm^{3+} ion in the $TmBa_2Cu_3O_7$ unit cell with the lattice constants a, b and c (Fig. 1).

4 Numerical Results and Discussion

At the present time, there is no well justified model for spin susceptibility in the CuO_2 planes. Therefore we have used some experimental data and a theoretical model for $\chi''(\mathbf{q}, \omega)$ in our numerical calculations to compare them with the results of the experiment [3] on $\Gamma_{cf}(T)$ in an effort to elucidate spin dynamics in the CuO_2 planes.

4.1 Millis–Monien–Pines (MMP) model

Let us consider first the phenomenological model of AF Fermi liquid proposed by Millis, Monien and Pines [4], where the dynamical spin susceptibility $\chi^{+-}(\mathbf{q}, \omega)$ is given by the formula:

$$\chi_{AF}(\mathbf{q}, \omega) = \frac{\chi_Q}{1 + \xi^2(\mathbf{Q} - \mathbf{q})^2 - i(\frac{\omega}{\omega_{SF}})}, \tag{25}$$

where χ_Q is the static spin susceptibility at the AF wave vector $\mathbf{Q} = (\pi/a, \pi/a)$, $\xi(T)$ is the temperature dependent AF correlation length, and $\hbar\omega_{SF}$ is a typical energy scale for the AF spin dynamics.

Though the MMP model was introduced to describe the nuclear magnetic resonance (NMR) experiments in the region of a very low frequency of order of μeV, we suggest that it can be used also in the range of $\hbar\omega \simeq 12$ meV.

Using the same transformation of the variables in the corresponding integrals like in Appendix C of Ref. [4], we find:

$$\Gamma_{cf}(\omega_0) \propto \coth\left(\frac{\omega_0}{2kT}\right)\frac{\chi_0(T)}{\Gamma(T)}(2\tilde{I}_1 - \tilde{I}_3), \tag{26}$$

where

$$\tilde{I}_1 = 4\int_0^{1/2} dx \int_0^{1/2} dy \frac{1-\cos(2\pi x)}{\{x^2+y^2+\eta^2\}^2 + (\frac{\omega}{\omega_{SF}})^2},$$

$$\tilde{I}_3 = 8\int_0^{1/2} du \int_0^{(1/2)-u} dv \frac{1-\cos(4\pi u)}{\{2u^2+2v^2+\eta^2\}^2 + (\frac{\omega}{\omega_{SF}})^2}, \tag{27}$$

where $\eta = \frac{1}{2\pi}\left(\frac{a}{\xi}\right)$, $\chi_Q = \frac{\sqrt{\beta}\chi_0}{4\pi^2\eta^2}$, $\beta \approx \pi^2$ and $\omega_{SF} = \frac{4\pi\Gamma}{\beta^{1/2}}\eta^2$, where $\chi_0(T)$ is the strong temperature dependent static spin susceptibility at $q = 0$, and $\hbar\Gamma(T)$ is a weakly temperature dependent spin-fluctuation energy of the electronic system.

As the value of the $(2\tilde{I}_1 - \tilde{I}_3)$ changes only by 5% and the value of the $\hbar\Gamma(T)$ by 7% in the considered temperature range $75 < T < 170K$, in this approximation the main contribution to the temperature dependence of $\Gamma_{cf}(\omega_0)$ comes from $\chi_0(T)$. The latter one can be exctracted from the temperature dependent spin part of the Knight shifts ${}^{\alpha}K_S(T)$, $\alpha = (63, 89, 17)$. Using the result of $\chi_0(T)$ from Ref. [4] and experimental result of Knight shift $-\Delta K(T)$ from Ref. [7], in this approximation, we get theoretical curves (short and large dashed line, respectively, in the Fig.3), which are not consistent with experimental results [3] for linewidth $\Gamma_{CF}(T)$.

By considering another model for dynamical spin susceptibility the authors of Ref. [10] have concluded that the temperature dependence of the linewidth $\Gamma_{CF}(T)$ is determined by the temperature dependence of the uniform static susceptibility $\chi_0(T)$. But this assumption has not permitted them to obtain a good agreement between their theoretical curve and experimental data [3].

4.2 Models for $\chi(\mathbf{q},\omega)$ based on experimental studies

According to the experimental results obtained by Rossat–Mignod et al. [5], [17], magnetic scattering in metallic phase of YBCO -system remains concentrated around the AF-rod, and there is no sign of any incommensurability. The spin excitation spectrum is isotropic in the metallic state ($\chi^{zz} = \chi^{xx}$) and the dynamical structure factor can be written as:

$$S(\mathbf{Q},\omega) = \frac{2}{\pi}\frac{1}{1-e^{-\hbar\omega/(kT)}}\mathrm{Im}\chi(\mathbf{Q},\hbar\omega). \tag{28}$$

By assuming that the line shape of magnetic intensity is of the Gaussian-type and using the value of the full width at half maximum (FWHM) i.e. "q-width" $\Delta q = 0.27$ in $2\pi\sqrt{2}/a$ units [5] in $YBa_2Cu_3O_{6.92}$ at $T = 150$K at the energy $\hbar\omega = 10$meV , we can estimate a contribution to the line-width from AF spin fluctuations by the ratio:

$$\gamma = \frac{\int d^2\dot{q}|F(\mathbf{q})|^2\chi''(\mathbf{Q},\omega)}{\int d^2q|F(\mathbf{q})|^2\int d^2q\chi''(\mathbf{Q},\omega)} \simeq 0.16 \tag{29}$$

where the $\mathbf{q}$-integration is done over the first B.Z. Since the spin susceptibility at $\mathbf{q} = \mathbf{Q}$ is much larger than at $q = 0$ (e.g. in the MMP model $\chi''(\mathbf{Q},\omega)/\chi''(0,\omega) \simeq \beta(\xi/a)^4 \simeq 300$), we propose that the main contribution to the linewidth arises from the AF spin fluctuations, estimated by (29).

Berthier et al. [6] have recently measured the temperature dependence of the NMR relaxation rates

$$({}^{\alpha}T_1T)^{-1} \propto \sum_{\mathbf{q}} |{}^{\alpha}A(\mathbf{q})|^2\frac{\chi''(\mathbf{q},\omega_n)}{\omega_n} \tag{30}$$

in $YBa_{1.93}Sr_{0.07}Cu_3O_{6.92}$ where ω_n is the NMR frequency and $|{}^{\alpha}A(\mathbf{q})|^2$ is squared modulus of the Fourier-transfered hyperfine coupling constants for different nuclear sites $\alpha = (63, 17, 89)$. This dependence for ^{63}Cu can be approximated with good accuracy for $T > 75$K by:

$$({}^{63}T_1T)^{-1} \simeq a(T-75)^b\exp[c(T-75)], \tag{31}$$

where the parameters have the values $a \simeq 0.08$ $s^{-1}\cdot K^{-b-1}$, $b \simeq 1.27$, $c \simeq -0.02$ K^{-1} .

According to Horvatić et al. [6], the temperature dependence of $({}^{63}T_1T)^{-1}$ and $\chi''(Q_{AF}, \hbar\omega \simeq 10$ meV) are quite similar in the considered temperature range. Therefore we can assume that the temperature dependence of the sum over $\mathbf{q}$ in (22) due to our estimation (29) corresponds to (31), i.e.

$$\sum_{\mathbf{q}} |F(\mathbf{q})|\chi''(\mathbf{q},\omega) \propto ({}^{63}T_1T)^{-1}. \tag{32}$$

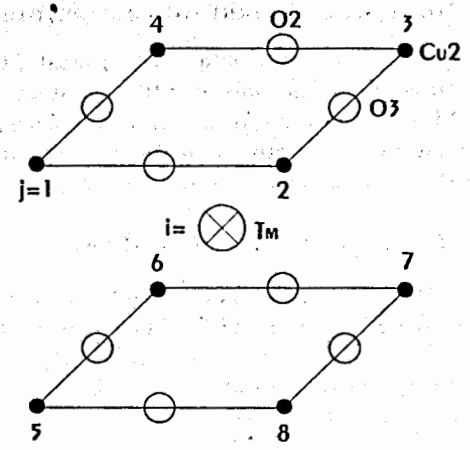

Fig. 1.
Positions of ions in CuO_2-Tm-CuO_2 bilayer.

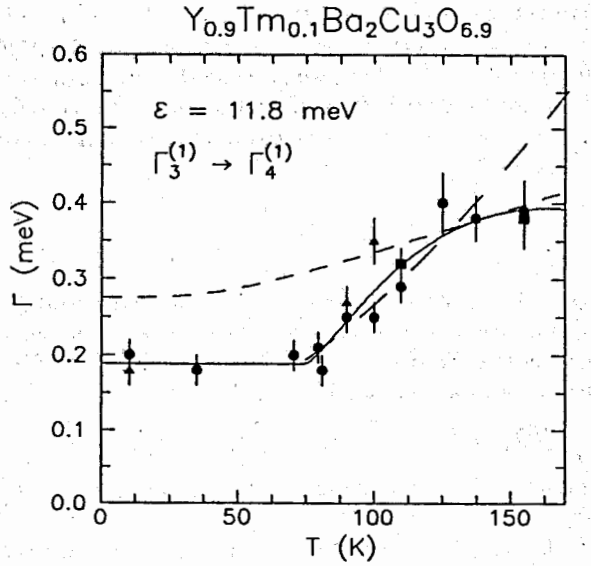

Fig. 2.
Temperature dependence of the linewidth for CF excitation $\Gamma_3^{(1)} \rightarrow \Gamma_4^{(1)}$ (ε = 11.8meV) of the Tm^{3+} ion in Tm-$YBCO_{6.9}$: points – experimental data [3], curves – theoretical results for some models of $\chi(\mathbf{q},\omega)$ (see text).

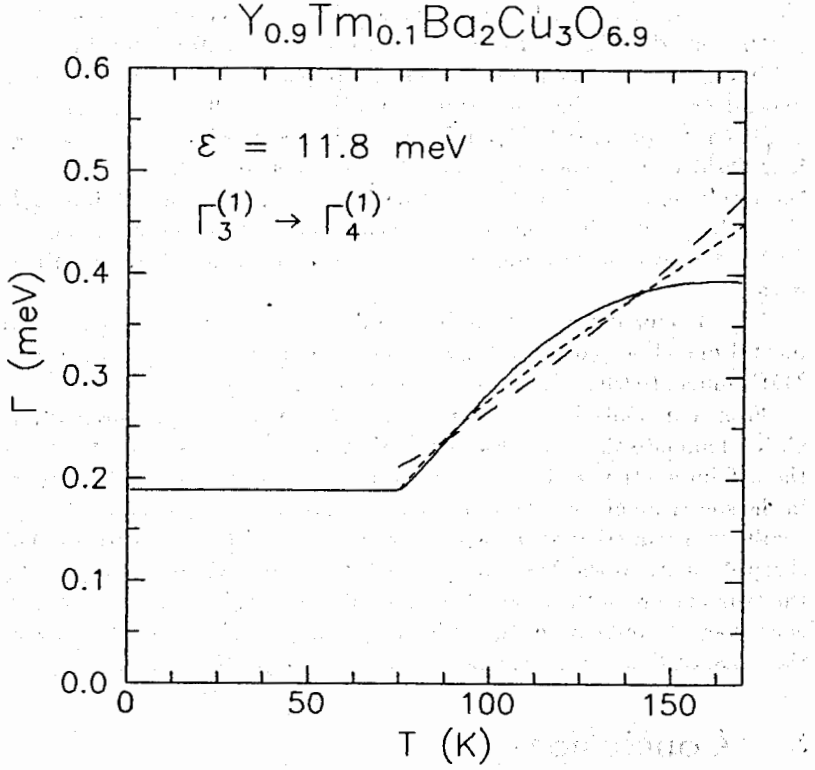

Fig. 3.
Comparison of theoretical results for $\Gamma_{CF}(T)$: based on MMP model [4] with different $\chi_0(T)$ (large [4] and short dashed line [7]), and experiments for NMR relaxation rate $1/(T_1T)$ for ^{63}Cu [6] (full line).

By introducing a constant component Γ_0 of linewidth which is not caused by dynamic spin fluctuations, we find the following expression for the linewidth:

$$\Gamma_{cf}(T) = \Gamma_0 + A\mathrm{coth}\left(\frac{\omega_0}{2kT}\right)(^{63}T_1T)^{-1}, \qquad (33)$$

The best agreement with the experimental data [3] can be obtained for the parameter values $\Gamma_0 = 0.189 \pm 0.008$ meV and $A = 0.019 \pm 0.002$ a.u.

In Fig.2 the full line represents our theoretical results (33) for temperature dependence of the linewidth $\Gamma_{cf}(T)$. If we adopt that $\sum_{\mathbf{q}}|F(\mathbf{q})|^2\chi''(\mathbf{q},\omega) \propto^{89} (T_1T)^{-1}$ we get the result which is represented by long-dashed line. For the temperature independent $\chi''(\mathbf{q},\omega)$ one can get the result represented by the short-dashed line. Experimental data [3] are shown by points (different symbols means different energy of incident neutrons). One can see that only the full line is in agreement with experimental data.

Fig. 3 compares our theoretical results for $\Gamma_{CF}(T)$ by using the experimental model of $\chi(\mathbf{q},\omega)$ (full line - the same as in Fig.2) and by using the MMP model (dashed lines - see above given discussion).

From our analysis one can conclude that dynamic spin fluctuations in CuO_2 dominate the line broadening. Excited f-electrons can relax through the s-f interaction with the Cu- spin system. Opening of a pseudo-gap E_g in the spectrum of spin excitations observed in neutron experiments [5], [17] results in a reduction of the low-energy spin fluctuations and corresponding sharp decrease in the linewidth for CF excitation with energy $\hbar\omega_0 < E_g$ at the temperature of the onset of the gap. If the energy of CF $\hbar\omega_0 > E_g$, there is no sharp decrease in the linewidt that permits one, in principle, to measure the value of E_g by using compounds with different RE doped ions.

5 Conclusions

In the present paper we have proposed a model describing the relaxation of CF excitations for $4f$-electrons in cuprates due to spin fluctuations on Cu-sites . A general expression (22) for Tm^{3+} in (Y-Tm)BCO-compound has been derived and estimations for $\Gamma_{CF}(T)$ has been done for some models of dynamical spin susceptibility $\chi(\mathbf{q},\omega)$.

We cannot explain a sharp decrease of $\Gamma_{cf}(T)$ observed experimentally for Y-$TmBa_2Cu_3O_{6.9}$ [3] by employing the MMP-model [4] for $\chi(\mathbf{q},\omega)$ as well as considering the temperature-dependent NMR relaxation rate $1/(T_1T)$ for ^{89}Y [6]. To fit the experimental data [3] one has to adopt that AF spin fluctuations measured by inelastic neutron scattering [5] at $\hbar\omega_0 \simeq 10meV$ [9] or by NMR relaxation rate $1/(T_1T)$ for ^{63}Cu [6] give an essential contribution to $\Gamma_{cf}(T)$, as justified by our estimation (29). Unfortunately , we cannot

present at this time a full self-consistent calculation for the linewidth $\Gamma_{cf}(T)$ (22) , since now there is no reliable theory of the dynamical spin susceptibility in strongly correlated electronic systems which cuprates belongs to .

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References

[1] P.Fulde, M.Loewenhaupt, Advances in Physics, **34** (1986) 589;
R.Feile, M.Loewenhaupt, J.K.Kjems, H.E.Hoenig,
Phys.Rev.Lett., **47** (1981) 610.

[2] U.Walter , E.Holland-Moritz , A.Severing , A.Erle ,
H.Schmidt , E.Zirngiebl ,
Physica C **153 - 155** (1988) 170-171;
P.Allenspach, A.Furrer, P.Bruesch, P.Unternaehrer,
Physica B **156 - 157** (1989) 864-866;
A.T.Boothroyd, A.Mukherjee, D.McK. Paul, Jones Rutherford Appleton Laboratory Report 1993, RAL-93-050, A 314.

[3] E.A.Goremychkin, R.Osborn and A.D.Taylor,
JETP Lett., **50** (1989) 380;
R.Osborn, E.A.Goremychkin, Physica C, **185 - 189** (1991) 1179.

[4] A.J.Millis, H.Monien, D.Pines, Phys.Rev. B **42** (1990) 167;
H.Monien, D.Pines, M.Takigawa, Phys.Rev. B **43** (1991) 258;
A.J.Millis,H.Monien,Phys.Rev.B **45** (1992) 3059.

[5] J.Rossat-Mignod, L.P.Regnault, C.Vettier, P.Bourges, P.Burlet, J.Bossy, J.Y.Henry, G.Lapertot,
Physica C, **185 - 189** (1991) 86; Physica B,**180 - 181**(1992)383;

[6] C.Berthier, J.A.Gillet, T.G.Auler, Y.Berthier, M.Horvatić, P.Ségransan, J.Y.Henry, Physica Scripta **48** (1993) 1-6;
M.Horvatić, T.Auler, C.Berthier, Y.Berthier, P.Butaud, W.G.Clark, J.A.Gillet, P.Ségransan, Phys.Rev. B **47** (1993-II) 3461

[7] H.Alloul, T.Ohno, P.Mendels, Phys.Rev.Lett., **63** (1989) 1700
(Fig. for sample x=1-ε).

[8] B.J.Sternlieb, G.Shirane, J.M.Tranquada, M.Sato, S.Shamoto, Phys.Rev. B **47** (1993) 5320.

[9] Ž.Kovačević, N.M.Plakida, JETP Lett. **57** (1993) 249–252.

[10] V.L.Aksenov, V.V.Kabanov, Phys.Rev. B **49** (1994).

[11] F.C.Zhang, T.M.Rice, Phys.Rev. B **37** (1988) 3759.

[12] V.L.Aksenov, E.A.Goremychkin, T.Frauenheim, Fiz.Met. Matallov. **55** (1983) 496.

[13] E.A.Goremychkin, A.V.Belushkin, J.Mayer, A.Yu.Muzychka, I.Natkaniec, I.L.Sachin, R.Osborn, A.D.Taylor, Proceedings of the Int. Sem. on HTSC, Dubna, 1989. World Scientific, V. 21 (1989) 324-331.

[14] P.Allenspach, A. Furrer, P.Brüesch, R.Marsolais, P.Unternährer, Physica C, **157** (1989) 58-64.

[15] Yu.A.Izyumov, Soviet Phys. Uspekhi **80** N 1 (1963) 40-59; W.Marshall, S.W.Lovesey, "Theory of Thermal Neutron Scattering", Oxford at Clarendon Press, 1971, p.169.

[16] D.N.Zubarev, Soviet Phys. Uspekhi **71** N 1 (1960) 71-116;

[17] J.Rossat – Mignod, L.P.Regnault, P.Bourges, P.Burlet, C.Vettier, J.Y.Henry, "Neutron Scattering Study of the High-T_c Superconducting System $YBa_2Cu_3O_{6+x}$",CEN-Saclay 1993.

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