ISSN 2072-5981

Magnetic Resonance in Solids

Electronic Journal

Volume **14, 2012**
No. **1, 12101** – 9 *pages*

http://mrsej.ksu.ru

Established and published by Kazan University
Sponsored by International Society of Magnetic Resonance (ISMAR)
Registered by Russian Federation Committee on Press, August 2, 1996
First Issue was appeared at July 25, 1997

© Kazan Federal University (KFU)*

"***Magnetic Resonance in Solids. Electronic Journal***" (**MRS*ej***) is a peer-reviewed, all electronic journal, publishing articles which meet the highest standards of scientific quality in the field of basic research of a magnetic resonance in solids and related phenomena. **MRS*ej*** is free for the authors (no page charges) as well as for the readers (no subscription fee). The language of **MRS*ej*** is English. All exchanges of information will take place via Internet. Articles are submitted in electronic form and the refereeing process uses electronic mail. All accepted articles are immediately published by being made publicly available by Internet (*Editor@ksu.ru*).

Editors-in-Chief

Jean **Jeener** (Universite Libre de Bruxelles, Brussels)
Boris **Kochelaev** (KFU, Kazan)
Raymond **Orbach** (University of California, Riverside)

Executive Editor

Yurii **Proshin** (KFU, Kazan)
Editor@ ksu.ru

Editors

Vadim **Atsarkin** (Institute of Radio Engineering and Electronics, Moscow)
Detlef **Brinkmann** (University of Zürich, Zürich)
Yurij **Bunkov** (CNRS, Grenoble)
John **Drumheller** (Montana State University, Bozeman)
Mikhail **Eremin** (KFU, Kazan)
Yoshio **Kitaoka** (Osaka University, Osaka)
Boris **Malkin** (KFU, Kazan)
Haruhiko **Suzuki** (Kanazawa University, Kanazava)
Murat **Tagirov** (KFU, Kazan)

* In Kazan University the Electron Paramagnetic Resonance (EPR) was discovered by Zavoisky E.K. in 1944.

Spin-magnon relaxation of Yb^{3+}-ions in antiferromagnetic cuprate $Y_{1-x}Yb_xBa_2Cu_3O_{6+y}$

A.A. Vishina [1,*], A. Maisuradze[2]

[1] Kazan Federal University, Kremlevskaya 18, Kazan 420008, Russia

[2] Physik-Institut der Universität Zürich, Winterhurerstrasse 190, ZH-8057, Switzerland

E-mail: alenavishina@gmail.com

(Received October 26, 2012; accepted November 16, 2012)

The spin relaxation of Yb^{3+}-ions due to their coupling to antiferromagnetic spin waves existing in CuO_2 planes in $YBa_2Cu_3O_{6+y}$ compound is reported. It is shown that it results in a strong temperature dependence of electron paramagnetic resonance (EPR) linewidth. The temperature dependence of EPR *g*-factor was also obtained and shows a good agreement with experimental data.

PACS: 76.30.-v, 71.27.+a, 74.72.-h

Keywords: YBCO, electron paramagnetic resonance, rare-earth ions

1. Introduction

The quasi-two-dimensional cuprates such as yttrium barium copper oxide $YBa_2Cu_3O_{6+y}$ (YBCO) whose properties are determined by electrons moving within weakly coupled copper-oxide (CuO_2) layers attract much attention due to their transformation into high-temperature superconductors at high oxygen doping. The YBCO compound is characterized by large superexchange integral between nearest-neighbor Cu sites within the CuO_2 layers ($J \approx 2000$ K [1], $J \approx 1700$ K [2], $J \approx 1400$ K [3]), a rather strong coupling between the layers within a bilayer J_1 ($\delta = J_1 / J \geq 4 \cdot 10^{-2}$ [1], $\delta \geq 7 \cdot 10^{-2}$ [3]), and an extremely small coupling to the next-nearest-layers $J_2 / J \approx 2 \cdot 10^{-5} - 3 \cdot 10^{-4}$ [1, 3].

Among the other techniques electron paramagnetic resonance (EPR) proves to be an effective tool for studying the properties and spin relaxation in cuprate superconductors [4]. The rare-earth ions are used as an EPR-probe due to the fact that the substitution of yttrium by isovalent rare-earth ions having local magnetic *f*-moments does not change the critical temperature T_c or other magnetic properties of the material considerably [5]. We analyze the EPR spectra of the YBCO compound doped by Yb^{3+} ions – $Y_{1-x}Yb_xBa_2Cu_3O_{6+y}$ – at low oxygen doping ($y < 0.15$), while the CuO_2 planes are not yet doped with the oxygen *p*-holes.

The explicit expressions for the coupling of ytterbium ions with the antiferromagnetic (AF) spin waves in CuO_2 planes and the indirect spin-spin interaction between the Yb-ions due to this coupling were obtained in [6]. The contribution of these interaction to EPR linewidth and *g*-factors was also studied. In this article we report the Yb^{3+} ions relaxation due to their coupling with the AF spin waves and the temperature dependence of EPR g-factor.

It was shown in [6] that AF spin waves modes (due to the dipole-dipole interaction between copper ions) have the large energy gaps $\Delta \sim 40 - 90$ K (at the Brillouin zone center) that are much larger than Zeeman energy. That forbids the one-magnon processes to contribute the Yb^{3+} spin relaxation due to the energy conservation law. Hence studying the spin relaxation we should consider the two-magnon processes only.

We start this paper with the necessary brief description of the work [6] in Sec. 2. In the third section we derive the two-magnon part of Yb-Cu interaction Hamiltonian. The Sec. 4 describes the Yb-ions relaxation due to their coupling to AF spin waves and its contribution to the EPR linewidth. The last section gives the temperature dependence of EPR *g*-factor.

2. Spin excitations and electron paramagnetic resonance in two-layer antiferromagnetic system $Y_{1-x}Yb_xBa_2Cu_3O_{6+y}$

It was shown in [1, 2] that four modes of spin waves are formed within the CuO_2 planes at low oxygen doping while the Cu ions are in AF state: two acoustic and two optical ones. In [6] we studied the way dipole-dipole interaction between the copper ions and an external magnetic field (which is always applied in EPR experiments) contributes the energy gaps of the waves. The energy eigenvalues for acoustic modes are

$$\left(\frac{E_{\alpha q}}{2J}\right)^2=\left[1-\gamma_q+2b_{\mathrm{Cu}}^2\left(\gamma_q+\frac{\delta}{4}\right)+\Delta_\alpha\right]\left[1+\gamma_q+\frac{\delta}{2}-\alpha_{xy}\gamma_q\right],$$
$$\left(\frac{E_{\beta q}}{2J}\right)^2=\left[1-\gamma_q+\alpha_{xy}\gamma_q+\Delta_\beta\right]\left[1+\gamma_q+\frac{\delta}{2}-2b_{\mathrm{Cu}}^2\left(\gamma_q+\frac{\delta}{4}\right)\right], \quad (1)$$
$$\Delta_\alpha=2d_3,\qquad \Delta_\beta=-\frac{d_1}{2}+\frac{d_2}{4}+2d_3+\frac{d_4}{2}.$$

The energy eigenvalues for optical modes are given by following expressions

$$\left(\frac{E_{\eta q}}{2J}\right)^2=\left[1+\gamma_q-\alpha_{xy}\gamma_q+\Delta_\eta\right]\left[1-\gamma_q+\frac{\delta}{2}+2b_{\mathrm{Cu}}^2\left(\gamma_q-\frac{\delta}{4}\right)\right],$$
$$\left(\frac{E_{\kappa q}}{2J}\right)^2=\left[1+\gamma_q-2b_{\mathrm{Cu}}^2\left(\gamma_q-\frac{\delta}{4}\right)+\Delta_\kappa\right]\left[1-\gamma_q+\frac{\delta}{2}+\alpha_{xy}\gamma_q\right], \quad (2)$$
$$\Delta_\eta=-\frac{d_1}{2}+\frac{d_2}{4}+2d_3+\frac{d_4}{2},\qquad \Delta_\kappa=2d_3.$$

Here the $b_{\mathrm{Cu}}=\dfrac{B_y}{J(4+\delta)}=-\sin\varphi$, where φ is an angle by which Cu spins are rotated by the external magnetic field; $\gamma_q=1/2\left[\cos(q_xa)+\cos(q_ya)\right]$, $\gamma_{yq}=\cos(q_ya)$; $\alpha_{xy}=\Delta J/J\approx 2\cdot10^{-4}-7\cdot10^{-4}$ is a week planar anisotropy [1, 2], $d_1=3g^2\mu_B^2/Ja^3$, $d_2=3g^2\mu_B^2/Jc^3$, $d_3=3g^2\mu_B^2/4\sqrt{2}Ja^3$, $d_4=3g^2\mu_B^2a^2/JR^5$ with $R=\sqrt{a^2+c^2}$ are the terms due to dipole-dipole interaction between Cu-ions; a = 3.85 Å is the distance between the nearest Cu-ions within the CuO_2 planes and c = 3.38 Å is the distance between the bilayers.

The eigenoperators for the modes have the form

$$\alpha_q=\frac{1}{2}\left\{u_{\alpha q}\left(a_{1q}+a_{2q}+b_{1q}+b_{2q}\right)-v_{\alpha q}\left(a_{1-q}^++a_{2-q}^++b_{1-q}^++b_{2-q}^+\right)\right\},$$
$$\beta_q=\frac{1}{2}\left\{u_{\beta q}\left(a_{1q}+a_{2q}-b_{1q}-b_{2q}\right)-v_{\beta q}\left(a_{1-q}^++a_{2-q}^+-b_{1-q}^+-b_{2-q}^+\right)\right\},$$
$$\eta_q=\frac{1}{2}\left\{u_{q\eta}\left(a_{q1}-a_{q2}+b_{q1}-b_{q2}\right)-v_{q\eta}\left(a_{-q1}^+-a_{-q2}^++b_{-q1}^+-b_{-q2}^+\right)\right\}, \quad (3)$$
$$\kappa_q=\frac{1}{2}\left\{u_{q\kappa}\left(a_{q1}-a_{q2}-b_{q1}+b_{2q}\right)-v_{q\kappa}\left(a_{-q1}^+-a_{-q2}^+-b_{-q1}^++b_{-q2}^+\right)\right\},$$

with the coefficients

$$u^2_{\alpha,\beta} = \frac{J}{E_{\alpha,\beta}}\left[1+\frac{\delta}{4}\mp\frac{\alpha_{xy}\gamma_q}{2}\pm b^2_{\text{Cu}}\left(\gamma_q+\frac{\delta}{4}\right)+\frac{E_{\alpha,\beta}}{2J}\right],$$
$$v^2_{\alpha,\beta} = \frac{J}{E_{\alpha,\beta}}\left[1+\frac{\delta}{4}\mp\frac{\alpha_{xy}\gamma_q}{2}\pm b^2_{\text{Cu}}\left(\gamma_q+\frac{\delta}{4}\right)-\frac{E_{\alpha,\beta}}{2J}\right],$$
$$u^2_{\eta,\kappa} = \frac{J}{E_{\eta,\kappa}}\left[1+\frac{\delta}{4}\mp\frac{\alpha_{xy}\gamma_q}{2}\pm b^2_{\text{Cu}}\left(\gamma_q-\frac{\delta}{4}\right)+\frac{E_{\eta,\kappa}}{2J}\right],\tag{4}$$
$$v^2_{\eta,\kappa} = \frac{J}{E_{\eta,\kappa}}\left[1+\frac{\delta}{4}\mp\frac{\alpha_{xy}\gamma_q}{2}\pm b^2_{\text{Cu}}\left(\gamma_q-\frac{\delta}{4}\right)-\frac{E_{\eta,\kappa}}{2J}\right].$$

These spin waves modes all have the energy gaps, which are much larger than Zeeman energy. The smallest of the gaps belongs to the α-mode at the zone center $\mathbf{q}=(0,0)$ and κ-mode at the zone-boundary $\mathbf{q}=(\pi/a,\pi/a)$ and has the value $E_\alpha(0,0)=E_\kappa(\pi/a,\pi/a)\approx 44$ K. One can see that $E_{\alpha 0}\approx 4J\sqrt{d_3}\gg g_{\text{Cu}}\mu_B H_0$. It means that one-magnon processes are not involved in direct exchange between Cu and Yb-ions and studying the Yb-ions relaxation to AF spin waves we should take into account the two-magnon processes only.

Actually there are other interactions contributing the energy gaps. But the main goal of the gaps calculation here was to understand whether they allow or forbid the one-magnon processes to contribute the relaxation. Even dipole-dipole interaction itself gives the gaps large enough to prevent the one magnon processes, so calculation of the other interactions contribution is unnecessary.

Yb^{3+} ions placed between the CuO_2 layers interact with the AF spin waves described above. The Hamiltonian of the interaction for the magnetic field oriented along the y-axis has the following form [6]:

$$H_{\text{YbCu}} = H^{(0)}_{\text{YbCu}} + H^{(1)}_{\text{YbCu}} + H^{(2)}_{\text{YbCu}};$$
$$H^{(0)}_{\text{YbCu}} = 4Ab_{\text{Cu}}Y^y_0 N^{1/2} - Ab_{\text{Cu}}Y^y_0 N^{-1/2}\sum_q\left\{v^2_{q\alpha}+v^2_{q\beta}+v^2_{q\eta}+v^2_{q\kappa}\right\},$$
$$H^{(1)}_{\text{YbCu}} = 2A\sum_q\Big\{F^{ac}_q\left[Y^z_q\left(u_{q\alpha}+v_{q\alpha}\right)\left(\alpha_q+\alpha^+_{-q}\right)+ib_{\text{Cu}}Y^x_q\left(u_{q\alpha}-v_{q\alpha}\right)\left(\alpha_q-\alpha^+_{-q}\right)\right]\tag{5}$$
$$+F^{op}_q\left[Y^z_q\left(u_{q\kappa}+v_{q\kappa}\right)\left(\kappa_q+\kappa^+_{-q}\right)+ib_{\text{Cu}}Y^x_q\left(u_{q\kappa}-v_{q\kappa}\right)\left(\kappa_q-\kappa^+_{-q}\right)\right]$$
$$+iY^y_q\left(1-b^2_{\text{Cu}}\right)^{1/2}\left[F^{ac}_q\left(u_{q\beta}-v_{q\beta}\right)\left(\beta_q-\beta^+_{-q}\right)+F^{op}_q\left(u_{q\eta}-v_{q\eta}\right)\left(\eta_q-\eta^+_{-q}\right)\right]\Big\}.$$

Here $Y^{x,y,z}_q$ is the Fourier-transform of the Yb spin operator; F^{ac}_q and F^{op}_q are form factors for the acoustical and the optical modes:

$$F^{ac}_q = \cos\frac{q_x a}{2}\cos\frac{q_y a}{2},\quad F^{op}_q = \sin\frac{q_x a}{2}\sin\frac{q_y a}{2}.$$

The term $H^{(2)}_{\text{YbCu}}$ quadratic in the boson operators, which is responsible for two-magnon processes, will be described below.

Using this Hamiltonian the renormalized Zeeman energy can be written in the form

$$\tilde{B}_{\text{Yb}} = \mu_B H_0\left[g^0_{\text{Yb}} - g_{\text{Cu}}\frac{A}{J}\left(1-\frac{1}{4}v^2_{\text{tot}}\right)\right],\quad v^2_{\text{tot}} = \frac{1}{N}\sum_q\left\{v^2_{q\alpha}+v^2_{q\beta}+v^2_{q\eta}+v^2_{q\kappa}\right\}\approx 0.614.\tag{6}$$

The renormalized g-factors of the ytterbium ions due to their coupling with the AF spin waves were estimated in the following way: for the initial values of the Yb^{3+} g-factors the experimental values of the paramagnetic state $g^0_{\mathrm{Yb}} = g^0_{\parallel} = 3.13$ (for the parallel orientation) and $g^0_{\mathrm{Yb}} = g^0_{\perp} = 3.49$ (for the perpendicular orientation) [7] were used. The compound $Y_{0.98}Yb_{0.02}Ba_2Cu_3O_{6.1}$ is in paramagnetic state at oxygen doping $y = 0.4$ (where the AF state is suppressed, while the symmetry remains tetragonal). In formula (6) we use the typical g-factors of the copper ion in the tetragonal field with the orbital ground state of the type $\left(x^2 - y^2\right)$ which are $g^{\parallel}_{\mathrm{Cu}} = 2.4$ and $g^{\perp}_{\mathrm{Cu}} \approx 2.1$ for the parallel and perpendicular orientations of the external magnetic field, respectively [8]. The exchange coupling between the Cu and Yb ions was found to be $A = -120$ K [6]; we also use $J = 1700$ K [2]. Then the theoretical values of g-factors are $g^{\mathrm{th}}_{\parallel} = 3.27$ and $g^{\mathrm{th}}_{\perp} = 3.61$, which are quite close to the experimental values $g_{\parallel} = 3.23$ and $g_{\perp} = 3.54$.

3. The two-magnon Yb-Cu interaction Hamiltonian

The exchange coupling between the Yb-ions and AF spin waves within the CuO_2-planes has initially the following form:

$$H^{j}_{\mathrm{YbCu}} = A\mathbf{Y}_j \sum_{\rho}\left(\mathbf{S}^a_{j+\rho 1} + \mathbf{S}^b_{j+\rho 2} + \mathbf{S}^b_{j+\rho 1} + \mathbf{S}^a_{j+\rho 2}\right), \tag{7}$$

here ρ corresponds to the positions of the Cu-ions nearest neighboring the j-th Yb^{3+}-ion, $\mathbf{Y}_j$ is the spin of that ion.

Following [6], we assume the field rotates the magnetizations of both sub-lattices slightly toward the y direction by the angle φ. It is convenient then to turn the axes so that the new x-axis is directed along the corresponding magnetizations of the sub-lattices:

$$\begin{aligned} S^a_x &= S'_x \cos\varphi - S'_y \sin\varphi, \\ S^a_y &= S'_x \sin\varphi + S'_y \cos\varphi, \\ S^b_x &= S'_x \cos\varphi + S'_y \sin\varphi, \\ S^b_y &= -S'_x \sin\varphi + S'_y \cos\varphi. \end{aligned} \tag{8}$$

Using the standard Holstein-Primakoff formalism we make the following transformation for the layer:

$$\begin{aligned} S^{xa}_{j1} &= \frac{1}{2} - a^+_{j1}a_{j1}, \quad S^+_{j1} = \left(1 - a^+_{j1}a_{j1}\right)^{1/2} a_{j1}, \quad S^-_{j1} = a^+_{j1}\left(1 - a^+_{j1}a_{j1}\right)^{1/2}, \\ S^{xb}_{j1} &= -\frac{1}{2} + b^+_{j1}b_{j1}, \quad S^+_{j1} = b^+_{j1}\left(1 - b^+_{j1}b_{j1}\right)^{1/2}, \quad S^-_{j1} = \left(1 - b^+_{j1}b_{j1}\right)^{1/2} b_{j1}, \end{aligned} \tag{9}$$

with $S^{\pm} = S^z \mp iS^x$. For the second layer the transformation is the same. Here $a^+,\ a,\ b^+,\ b$ are the boson creation and annihilation operators for the two sub-lattices. Then we perform the Fourier transformation to the reciprocal lattice:

$$a_q = N^{-1/2}\sum_j a_j \exp(i\mathbf{q}\mathbf{r}_j), \qquad b_q = N^{-1/2}\sum_j b_j \exp(i\mathbf{q}\mathbf{r}_j), \tag{10}$$

where N is the number of unit cells in the bilayer.

After these transformations the Hamiltonian has three parts. Two of them, the one not having the boson operators and the one linear in boson operators were given in (5). The term $H^{(2)}_{\mathrm{YbCu}}$ quadratic in the boson operators which is responsible for two-magnon processes has the following form

$$H_{\mathrm{YbCu}}^{(2)} = Ab_{\mathrm{Cu}} \sum_{qq'} Y_{q-q'}^{y} \left\{ \cos\left(\frac{q_x - q'_x}{2} a\right) \cos\left(\frac{q_y - q'_y}{2} a\right) \left(a_{q1}^{+} a_{q'1} + a_{q2}^{+} a_{q'2} + b_{q1}^{+} b_{q'1} + b_{q2}^{+} b_{q'2}\right) \right.$$
$$\left. + \sin\frac{\Delta q_x a}{2} \sin\frac{\Delta q_y a}{2} \left(a_{q1}^{+} a_{q'1} - a_{q2}^{+} a_{q'2} - b_{q1}^{+} b_{q'1} + b_{q2}^{+} b_{q'2}\right) \right\}, \quad (11)$$

After the Bogoliubov transformation to the new creation and annihilation boson operators $\alpha_q^+,\ \beta_q^+,\ \eta_q^+,\ \kappa_q^+,\ \alpha_q,\ \beta_q,\ \eta_q,\ \kappa_q$ by using (3) the quadratic term takes the form

$$H_{\mathrm{YbCu}}^{(2)} = Ab_{\mathrm{Cu}} \sum_{\substack{qq' \\ \varsigma = \alpha\beta\eta\kappa}} Y_{q-q'}^{y} \left\{ \cos\left(\frac{q_x - q'_x}{2} a\right) \cos\left(\frac{q_y - q'_y}{2} a\right) \left[u_{q\varsigma} u_{q'\varsigma} \varsigma_q^{+} \varsigma_{q'} + \nu_{q\varsigma} \nu_{q'\varsigma} \varsigma_{-q'}^{+} \varsigma_{-q} + \delta_{qq'} \nu_{q\varsigma} \nu_{q'\varsigma} \right] \right\}. \quad (12)$$

4. Contribution of the two-magnon processes into EPR linewidth

The contribution of two-magnon processes into the Yb-ions relaxation rate is estimated by the double-time Green functions method described in [9]. The double-time retarded Green function for two operators Y^+ and Y^- ($Y^{\pm} = Y_z \mp iY_x$), which is used here, has the form

$$\left\langle\left\langle Y^{+}(t) \middle| Y^{-}(t') \right\rangle\right\rangle = -i \left\langle \left\{ Y^{+}(t), Y^{-}(t') \right\} \right\rangle \theta(t - t');$$
$$\theta(t - t') = \begin{cases} 1, & t > t', \\ 0, & t < t'; \end{cases}$$

where $Y^{+}(t)$ and $Y^{-}(t')$ are Heisenberg representations of the operators Y^{+} and Y^{-} and $\left\{ Y^{+}(t), Y^{-}(t') \right\}$ is the anti-commutator of these operators.

The Hamiltonian we use has the form

$$\begin{aligned} H &= H_0^{\mathrm{Yb}} + H_0^{\mathrm{Cu}} + H_{\mathrm{YbCu}}^{(2)}; \\ H_0^{\mathrm{Cu}} &= H_{\mathrm{Zeem}}^{\mathrm{Cu}} + \sum_{\substack{q \\ \varsigma = \alpha\beta\eta\kappa}} E_{\varsigma} \varsigma_q^{+} \varsigma_q, \\ H_0^{\mathrm{Yb}} &= B_{\mathrm{Yb}} Y_0^{y}. \end{aligned} \quad (13)$$

Equations of motion for the Green function [9] are

$$\begin{aligned} E\left\langle\left\langle Y^{+} \middle| Y^{-} \right\rangle\right\rangle &= \left\langle \left\{ Y^{+}, Y^{-} \right\} \right\rangle + \left\langle\left\langle \left[Y^{+}, H \right] \middle| Y^{-} \right\rangle\right\rangle, \\ E\left\langle\left\langle \left[Y^{+}, H \right] \middle| Y^{-} \right\rangle\right\rangle &= \left\langle \left\{ \left[Y^{+}, H \right], Y^{-} \right\} \right\rangle + \left\langle\left\langle \left[\left[Y^{+}, H \right], H \right] \middle| Y^{-} \right\rangle\right\rangle, \text{ etc.} \end{aligned} \quad (14)$$

Here we obtain the infinite chain of equations that could be solved in different ways: by decoupling [10] or a special perturbation theory [10, 11]. We use the one proposed by Izyumov [11].

Applying the equations of motion (14) to the Green function we obtain the formulas

$$EG(E) = 1 + \left\langle\left\langle \left[Y^{+}, H \right] \middle| Y^{-} \right\rangle\right\rangle,$$
$$E\left\langle\left\langle \left[Y^{+}, H \right] \middle| Y^{-} \right\rangle\right\rangle = \left\langle\left\langle \left[Y^{+}, H \right] \middle| \left[H, Y^{-} \right] \right\rangle\right\rangle.$$

Substituting the second equation into the first we have the expression for the Green function [11]

$$G(E) = \frac{1}{\left(E - B_{\mathrm{Yb}}\right)} + \frac{1}{\left(E - B_{\mathrm{Yb}}\right)^2} \left\langle\left\langle \left[Y^{+}, H_{\mathrm{YbCu}}^{(2)} \right] \middle| \left[H_{\mathrm{YbCu}}^{(2)}, Y^{-} \right] \right\rangle\right\rangle.$$

On the other hand if we compare it to the Dyson equation [11] (with a yet unknown eigenenergy part $\Sigma(E)$) expansion to the terms of the second order in $\Sigma(E)$

$$G(E)=\frac{1}{E-B_{\mathrm{Yb}}-\Sigma(E)}\approx\frac{1}{E-B_{\mathrm{Yb}}}-\frac{1}{\left(E-B_{\mathrm{Yb}}\right)^2}\Sigma(E),$$

we can see that

$$\Sigma(E)=-\left\langle\left\langle\left[Y^+,H^{(2)}_{\mathrm{YbCu}}\right]\middle|\left[H^{(2)}_{\mathrm{YbCu}},Y^-\right]\right\rangle\right\rangle. \tag{15}$$

The imaginary part of this eigenenergy part gives the contribution of Yb-Cu interaction into the EPR linewidth. Calculating the energy part we should omit all the divergent terms of the form $\left(E-B_{\mathrm{Yb}}\right)^{-n}$ since they have already been taken into account by the structure of Dyson equation [11]. After the commutators calculation the imaginary part of (15) takes the form:

$$\begin{aligned}
\operatorname{Im}\Sigma(E)=\frac{16A^2\pi}{N^2}\sum_{qq'}\Bigg\{&\cos^2\left(\frac{q_x-q'_x}{2}a\right)\cos^2\left(\frac{q_y-q'_y}{2}a\right)\\
&\times\Big[\left(u_{q\alpha}u_{q'\beta}+v_{q\alpha}v_{q'\beta}\right)^2 n_{q\alpha}\left(1+n_{q'\beta}\right)\delta\left(E-(E_{q'\beta}-E_{q\alpha})\right)\\
&+\left(u_{q'\alpha}u_{q\beta}+v_{q'\alpha}v_{q\beta}\right)^2 n_{q\beta}\left(1+n_{q'\alpha}\right)\delta\left(E-(E_{q'\alpha}-E_{q\beta})\right)\\
&+\left(u_{q\pi}u_{q'\kappa}+v_{q\pi}v_{q'\kappa}\right)^2 n_{q\pi}\left(1+n_{q'\kappa}\right)\delta\left(E-(E_{q'\kappa}-E_{q\pi})\right)\\
&+\left(u_{q'\pi}u_{q\kappa}+v_{q'\pi}v_{q\kappa}\right)^2 n_{q\kappa}\left(1+n_{q'\pi}\right)\delta\left(E-(E_{q'\pi}-E_{q\kappa})\right)\Big]\\
&+\sin^2\left(\frac{q_x-q'_x}{2}a\right)\sin^2\left(\frac{q_y-q'_y}{2}a\right)\Big[\left(u_{q\alpha}u_{q'\pi}+v_{q\alpha}v_{q'\pi}\right)^2 n_{q\alpha}\left(1+n_{q'\pi}\right)\delta\left(E-(E_{q'\pi}-E_{q\alpha})\right)\\
&+\left(u_{q'\alpha}u_{q\pi}+v_{q'\alpha}v_{q\pi}\right)^2 n_{q\pi}\left(1+n_{q'\alpha}\right)\delta\left(E-(E_{q'\alpha}-E_{q\pi})\right)\\
&+\left(u_{q\beta}u_{q'\kappa}+v_{q\beta}v_{q'\kappa}\right)^2 n_{q\beta}\left(1+n_{q'\kappa}\right)\delta\left(E-(E_{q'\kappa}-E_{q\beta})\right)\\
&+\left(u_{q'\beta}u_{q\kappa}+v_{q'\beta}v_{q\kappa}\right)^2 n_{q\kappa}\left(1+n_{q'\beta}\right)\delta\left(E-(E_{q'\beta}-E_{q\kappa})\right)\Big]\Bigg\}.
\end{aligned} \tag{16}$$

Here n_q is magnon Bose-Einstein distribution $n_{q\varsigma}=\left[\exp\left(E_{q\varsigma}/k_BT\right)-1\right]^{-1}$.

Using the formulas (4) and neglecting the dipole-dipole terms we can substitute the terms of the form $\left(u_{q\alpha}u_{q'\beta}+v_{q\alpha}v_{q'\beta}\right)^2$ by

$$\left(u_{q\alpha}u_{q'\beta}+v_{q\alpha}v_{q'\beta}\right)^2\approx\frac{1}{2}\left[1+\frac{(2J)^2}{E_{q\alpha}E_{q'\beta}}\left(\left(1+\frac{\delta}{4}\right)^2-\left(\gamma_q+\frac{\delta}{4}\right)\left(\gamma_{q'}+\frac{\delta}{4}\right)\right)\right]. \tag{17}$$

In order to obtain the analytical formula for $\operatorname{Im}\Sigma(E)$ by (16) we use the linear dispersion law for the eigenenergies $E_{\varsigma q}\approx\upsilon q$, where $\upsilon=\sqrt{2}Ja$. It is reasonable since the EPR experiments were made at low temperatures where magnon frequencies are small enough to use the linear approximation typical for all antiferromagnets. Using this approximation and neglecting the small E term (which is the frequency of Fourier transformation and is of the order of Zeeman frequency, and for EPR-experiments is much smaller than the magnons frequencies (1)) we can replace the δ-functions

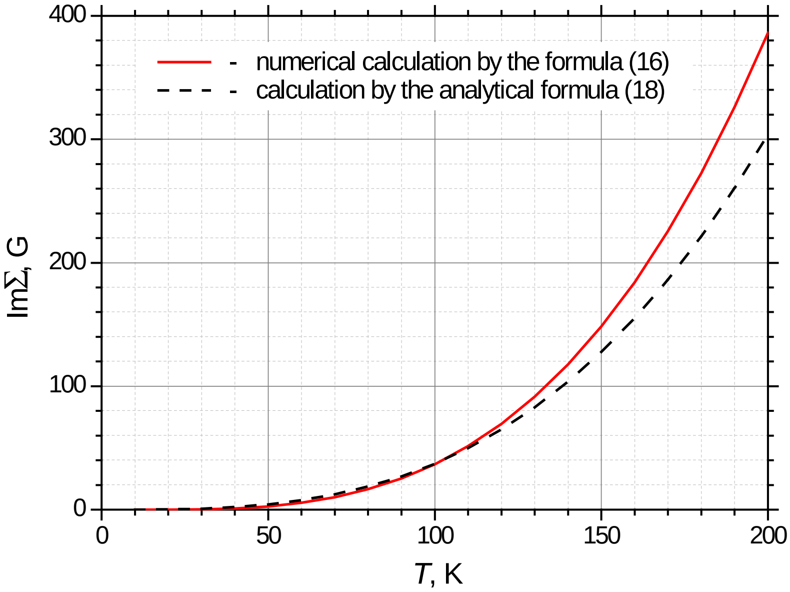

Figure 1. The contribution of the two-magnon processes into EPR linewidth. Solid line describes the numerical calculation by the formula (16), dashed line is the calculation by the analytical formula (18).

in (16) by $\delta(q-q')/\upsilon$. We also suppose $\exp(E_{q\varsigma}/k_BT)\gg 1$, which allows us to replace $n_{q\varsigma}$ by $\exp(-E_{q\varsigma}/k_BT)$. Now using (16) and (17) we have

$$\operatorname{Im}\Sigma(E)=\frac{16A^2a^4}{\pi\upsilon}\int_0^\infty dqq^2\left[1+\frac{4J^2(1-\gamma_q)\left(1+\gamma_q+\frac{\delta}{2}\right)}{\upsilon^2q^2}\right]\exp\left(-\frac{\upsilon q}{k_BT}\right),$$

which, after the γ_q expansion and the integral calculation, takes the form

$$\operatorname{Im}\Sigma(T)\approx\frac{16A^2}{\pi J}\left(\frac{k_BT}{J}\right)^3. \qquad (18)$$

Calculating (18) for $T=40$ K (which is the lowest temperature used in EPR experiments for $Y_{1-x}Yb_xBa_2Cu_3O_{6+y}$ [7]) we can see that at low temperatures contribution of two-magnon processes into the EPR line is negligible $\Sigma\approx 1$ G. But it increases substantially with temperature (see Fig. 1).

The numerical evaluation of (16) with the explicit form of $E_{\varsigma q}$ taken into account shows that the approximations we made in the analytical formula are good enough to closely describe the more accurate values of $\operatorname{Im}\Sigma(T)$ (see Fig. 1).

5. Temperature dependence to EPR g-factor

Using the Hamiltonian $H^{(2)}_{\mathrm{YbCu}}$ given above (12) we obtain its contribution into the EPR *g*-factors for the ytterbium ions. The part of $H^{(2)}_{\mathrm{YbCu}}$ which doesn't contain the magnon operators has already been taken into account in (6). We now consider the other part, quadratic in magnon operators, which defines *g*-factors' temperature dependence. After we put $q=q'$ the renormalized Zeeman energy due to $H^{(2)}_{\mathrm{YbCu}}$ can be written in the following form

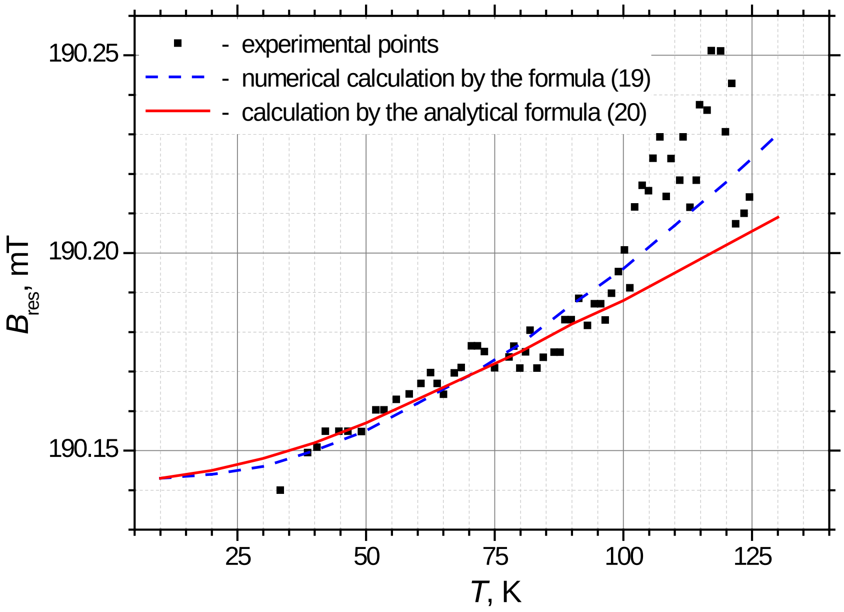

Figure 2. Temperature dependence of the resonance field (for $H \perp c$) in $YBCO_{6.1}$ with 2% of Yb: experimental points are marked by squares, dashed line gives the numerical calculation by the formula (19) for $g^0_{\text{Yb}} = g^0_\perp = 3.4$ and solid line is the calculation by the analytical formula (20).

$$\tilde{B}_{\text{Yb}} = \mu_B H_0 \left[g^0_{\text{Yb}} - g_{\text{Cu}} \frac{A}{J} \left(1 - \frac{1}{4} v^2_{\text{tot}} - \frac{1}{4} \sum_{\substack{q \\ \varsigma=\alpha,\beta,\eta,\kappa}} \left\{ \left(u_{q\varsigma} + v_{q\varsigma} \right)^2 n_{q\varsigma} \right\} \right) \right],$$
$$\left(u_{q\varsigma} + v_{q\varsigma} \right)^2 = \left(1 + \frac{\delta}{4} \right) \frac{J}{E_{\varsigma k}}. \tag{19}$$

To calculate the sum in (19) we make the same approximations we did above for $\operatorname{Im}\Sigma(T)$ (see Sec. 4) but take the energy gaps as the lower limits of the integrals. It gives us the following approximate analytical expression:

$$\tilde{B}_{\text{Yb}} = \mu_B H_0 g_{\text{eff}}(T),$$
$$g_{\text{eff}}(T) = g^0_{\text{Yb}} - g_{\text{Cu}} \frac{A}{J} \left\{ 1 - \frac{1}{4} v^2_{\text{tot}} - \frac{1}{4} \frac{k_B T}{\pi J} \left[\exp\left(-\frac{E_\alpha(0,0)}{\sqrt{2} k_B T} \right) + \exp\left(-\frac{E_\beta(0,0)}{\sqrt{2} k_B T} \right) \right] \right\}. \tag{20}$$

We use the values of the energy gaps $E_{\alpha,\beta}(0,0)$ obtained by (1) ($E_\alpha = 44$ K, $E_\beta = 109$ K). At $T = 40$ K the contribution of temperature-dependent part is negligible and it raises slightly with temperature. The calculated value of the *g*-factor at $T = 40$ K ($g^{\text{th}}_\perp = 3.61$) is a little higher than the experimental one ($g^{\text{exp}}_\perp = 3.54$). To compare the temperature dependence we shift the theoretical points down by choosing $g^0_{\text{Yb}} = g^0_\perp = 3.4$ in (19) instead of $g^0_{\text{Yb}} = g^0_\perp = 3.49$ (which doesn't change the temperature dependence itself), see Fig. 2. Along with the analytically obtained result we also show the more accurate numerical calculation by the formula (19).

As can be seen theoretical temperature dependence shows a good agreement with the experimental data.

6. Results and conclusions

The contribution of the two-magnon processes to Yb-Cu interaction and EPR linewidth was considered. It is shown that these processes result into strong temperature dependence of the EPR linewidth, and being negligible at low temperatures give the considerable input as the temperature rises. The temperature contribution to EPR *g*-factor was also obtained which fits nicely the experimental data.

Acknowledgments

We thank Prof. B.I. Kochelaev for the valuable discussions. This work was supported by the Swiss National Science Foundation, the SCOPES grant No. IZ73Z0_128242, and partially by the Ministry of Education and Science of the Russian Federation.

References

1. Vettier C., Burlet P., Henry J.Y., Jurgens M.J., Lapertot G.. Regnault L.R., Rossat-Mignod J. *Phys. Scr.* **29**, 110 (1989)
2. Rossat-Mignod J., Regnault L.P., Vettier C., Burlet P., Henry J.Y., Lapertot G. *Physica B* **169**, 58 (1991)
3. Shamoto S., Sato M., Tranquada J.M., Sternlieb B.J., Shirane G. *Phys. Rev. B* **48**, 13817 (1993)
4. Kochelaev B.I., Teitel'baum G.B. *Superconductivity in Complex Systems*, edited by K.A. Müller and A. Bussmann-Holder, Springer-Verlag, Berlin Heidelberg, pp. 203-266 (2005)
5. Hor P.H., Meng R.L., Wang Y.Q., Gao L., Huang Z.J., Bechtold J., Forster K., Chu C.W. *Phys. Rev. Lett.* **58**, 1891 (1987)
6. Vishina A.A., Maisuradze A., Shengelaya A., Kochelaev B.I., Keller H. *J. Phys.: Conf. Ser.* **394**, 012014 (2012)
7. Maisuradze A., Shengelaya A., Kochelaev B.I., Pomjakushina E., Conder K., Keller H., Müller K.A. *Phys. Rev. B* **79**, 054519 (2009)
8. Abragam A., Bleaney B. *Electron Paramagnetic Resonance of Transition Ions*, Clarendon Press, Oxford (1970)
9. Zubarev D.N. *Sov. Phys. Uspekhi*. **3**, 320-345 (1960)
10. Bonch-Bruevich V.L., Tyablikov S.V. *The Green Function Method in Statistical Mechanics*, North Holland Publishing Co. (1962)
11. Izyumov Yu.A., Katsnelson M.I., Skrabin Yu.N. *The Magnetism of Collective Electrons*, PhysMatLit, Moscow (1994) (*in Russian*)