MAGNETIC RESONANCE IN LOW DOPED
$Cu_{1-x}M_xGeO_3$ WITH DIFFERENT TYPE OF
3D AFM ORDERING

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Abstract: We report a symmetry analysis and a calculation of the frequency-field dependencies of different 3D AFM states for the underdoped $Cu_{1-x}M_xGeO_3$. Our consideration based on the supposition about existence or absence of structural distortions, which result into an alternation of the AFM exchange along magnetic chains. Two types of wave vectors $k_{AF}=(0,1,1/2)$ and $k_{SP}=(1/2,0,1/2)$ were considered. The existence or absence of displacements of the copper ions does not result in appearance of Dzyaloshinskii-Moriya antisymmetric interaction along chains. However, such an interaction between chains presents in all AFM phases. It is shown that spin wave spectrum contains two acoustical and two exchange branches. Surprisingly, that frequency of exchange mode possesses the same magnitude ~20 cm$^{-1}$ as the gap energy of the triplet state. The role of exchange modes for coexisting dimerized and 3D-AFM states has been discussed.

Key words: Magnetic resonance, symmetry analysis, Dzyaloshinskii-Moriya interaction, structural phase transition, 3D AFM ordering, spin-Peierls state.

1. INTRODUCTION

Competing ground states and quantum criticality present a special interest of modern physics of strongly correlated systems and most of emergent materials [1, 2]. The lightly doped $Cu_{1-x}M_xGeO_3$ has demonstrated a competition of a dimerized spin-Peierls (SP) phase and a 3D AFM phase, which replace each other under temperature decrease [3-5]. The microscopic mechanism of this replacement and phase coexistence (phase separation) could be a subject of magnetic resonance spectroscopy.

The most interesting features of the phase diagram of $Cu_{1-x}M_xGeO_3$ de-
velop in a region of the small doping concentration (less than 3%). In this region the 3D AFM ordering realizes on the background of the SP structure distortions (D-AFM). The SP-phase precedes its appearance so that \( T_N < T_{SP} \). High level doping (more than 3%) leads to a suppression of SP-distortions and development of a U-AFM phase. Recent studies of the \( Cu_{1-x}Mg_xGeO_3 \) [6-9] revealed that AFM ordering changes from D-AFM to U-AFM discontinuously in the region of critical concentrations close to \( x_0 = 0.027 \pm 0.001 \). Such changing is typical for the first order phase transition. The ion magnetization, Néel temperature, the atomic displacements, changes discontinuously.

However, elastic neutron scattering studies show that SP-phase, for instance, in \( Cu_{1-x}Si_xGeO_3 \) with \( x \) less than 1% coexists with the AFM ordering at the temperatures below \( T_N \) [3, 10]. Furthermore, in the work [11] an EPR-signal in \( Cu_{1-x}Mg_xGeO_3 \) was observed at temperatures less than Néel one. Authors considered this fact as a manifestation of more complicated phase composition in the samples, which supposes a small admixture of the paramagnetic phase also. All of this evidences about presence of a complex phase separation in the lightly doped \( Cu_{1-x}M_xGeO_3 \) in the vicinity of Néel temperature under temperature decrease.

We are going to explore of high frequency properties of all type AFM phases and SP-phase to justify its participation in phase-separated regions. Triplet excitations are representatives of SP-phase and exchange modes of magnetic resonance can serve as fingerprints of AFM order.

It is necessary to make a comment about exchange modes. Onset of 3D AFM order in \( Cu_{1-x}M_xGeO_3 \) implies intra-chain and inter-chain spin ordering. Thus, four sub-lattices model is a minimal model for description of this type of ordering. The exchange modes of magnetic resonance are an analogue of optic phonons. These modes can appear only if magnetic cell contains more then two magnetic sublattices. Such kinds of excitations were discovered, for instance, in \( CuCl_2 \cdot H_2O \) [12] a classical compound of antiferromagnetism in which for the first time in early 50-th were observed antiferromagnetic resonance and spin-flop magnetic phase transition. Spin oscillations of exchange modes violate of the 3D AFM ordering and their gaps define by production of intra- and inter-chain exchange interactions like \( (J_x/J_y)^{1/2} \). One can show that such kind of excitations will destroy of boundaries between SP- and AFM-phase if they coexist in the sample.

We provide a symmetry analysis and a calculation of the frequency-field dependencies of the different 3D AFM states for the underdoped \( Cu_{1-x}M_xGeO_3 \). Our consideration based on the supposition about existence or absence of structural distortions, which result into an alternation of the AFM exchange along magnetic chains. Two types of wave vectors...