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**Bilateral International Exchange Program (BIEP, invite) report**

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(Year/Month/Day) \_2008/12/17\_\_\_\_\_

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**Research Project**

Title	Spin wave spectrum for SrCu <sub>2</sub> (BO <sub>3</sub> ) <sub>2</sub>
Duration	2008/08/01-2008/12/28

During my stay in Kyoto I have started a new problem: the calculation of the excitation spectrum of the quasi two-dimensional S=1/2 dimer system SrCu<sub>2</sub>(BO<sub>3</sub>)<sub>2</sub>. This material has been interesting – among many other phenomena – for showing magnetization plateaus. The ground state is a singlet (two-dimensional network of orthogonal singlet bonds) separated by a finite excitation gap from the excited triplet states. It is known from inelastic neutron scattering and high field electron spin resonance (ESR) measurements that the gap is about 35 K, and the ratio of the antiferromagnetic intra-dimer (J) and inter-dimer (K) coupling is K/J~0.67. SrCu<sub>2</sub>(BO<sub>3</sub>)<sub>2</sub> shows magnetization plateaus at m/m<sub>sat</sub>=1/8, 1/4 and 1/3. Recently, Prof. Hagiwara and his group in Osaka University measured the ESR spectra in very high magnetic fields. My aim was/is to calculate the ESR and the momentum-dependent spectra in the model system (the Shastry-Sutherland) lattice, and eventually provide an insight into the experimentally measured spectrum.

One explanation to these plateaus is a field induced “metal-insulator” transition of magnetic excitations. When magnetic field reaches a critical value the energies of lowest lying states cross and triplet excitations condense. As the frustration reduces the kinetic energy of

the triplet excitations, the repulsive interaction becomes dominant and the excitations form a magnetic crystal, with a commensurate spin density wave order in the plateaus.

To have a better understanding on the  $1/3$  plateau, we performed a spin wave like calculation and determined the excitation spectrum. As a first step we carried out a variational calculation in the dimer-bond basis, keeping all the 4 states (1 singlet and 3 triplets) for each dimer, assuming that the unit cell in the  $1/3$  plateau state consist of 6 dimer bond. Out of those 6 dimers, two are fully magnetic  $S_z=1$  triplets (with magnetization pointing in the direction of the magnetic field), while the spin configurations on the remaining 4 dimers are a linear combination of the singlet and  $S_z=0$  triplet states, which allows the dimers to produce a finite staggered magnetization to “screen” the  $S_z=1$  triplets. The value of staggered magnetization on these dimers is the variational parameter  $\lambda$ , which measures the mixing of the  $S_z=0$  triplet to the singlet state on the bond. We calculated the expectation value of the Hamiltonian operator containing first and second nearest neighbor interaction as well as a Zeeman term and minimized the energy according to the  $\lambda$  parameter.

In the spin wave calculation we kept the same basis, and let the  $S=1$  dimers and polarized states condensate according to the previously described pattern. As an excitation we imagined the three noncondensed states on each dimer (each of them described by a Holstein-Primakoff-like boson), which can clearly interact between the dimers, resulting in 18 modes. We determined the spin wave spectrum and found a mode softening at the two end-points of the  $1/3$  plateau. Our preliminary results are very promising: the main fetures of the measured spectra seems to be captured by our method. As a next step we would like to introduce Dzyaloshinskii-Moriya and third-neighbor or ring-exchange like interactions to have a better quantitative agreement with the experimental data, as well as to understand the nature of possible instabilities (super-solid phases) at the boundary of the  $1/4$  and  $1/3$  plateaus.