Incommensurate spin excitations in BiCu$_2$PO$_6$

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We report detailed inelastic neutron scattering experiments on the newly discovered spin-1/2 ladder compound BiCu$_2$PO$_6$. Our measurements were performed on the C5 DUALSPEC triple axis spectrometer at the Canadian Neutron Beam Centre at Chalk River Laboratories. BiCu$_2$PO$_6$ has an orthorhombic unit cell, space group Pnma with $a = 11.755$, $b = 5.16$, $c = 7.79$ at 6 K. The ladder legs and rungs oriented along the crystallographic $b$ and $c$ axis respectively [Fig. 1]. Frustration is introduced by competing nearest ($J_1$) and next-nearest-neighbour ($J_2$) antiferromagnetic interactions on the ladder leg.

Experiments were carried out on a 4.5 g single crystal grown using the traveling floating zone method. The sample was mounted in the (0kl) scattering plane and the spectrometer was operated at a fixed final energy of 14.56 meV, using a focusing pyrolytic graphite monochromator (PG) and graphite analyzer with a horizontal collimation sequence of [33'-48'-51'-144']. Two sets of PG filters were placed in the scattered beam to eliminate higher order reflections. Temperature control was provided by a closed cycle cryostat with a base temperature of 6 K. All data was corrected for higher-order wavelength neutrons in the incident beam monitor. In-tensities were placed on an absolute scale by normalization with the integrated intensity of a transverse acoustic phonon measured near the (004) Bragg peak.

The spin excitation spectrum in BiCu$_2$PO$_6$ was mapped out through a series of constant momentum transfer scans. Throughout the Brillouin zone we observe two steeply dispersing modes. Representative scans are shown in Fig. 2.

The inelastic intensity decreases with increasing temperature and vanishes above 60 K, corresponding with the turnover observed in the magnetic susceptibility. Extensive sampling of $q$-values throughout reciprocal space enabled the construction of a map of the dynamic structure factor $S(q, \omega)$ shown in Fig. 3.

No evidence for elastic magnetic scattering was found indicating the absence of magnetic long-range order in BiCu$_2$PO$_6$. Two branches of long-lived magnetic excitations disperse along both the $b^*$ and $c^*$ directions. The modes are gapped throughout the Brillouin zone and the excitation minimum occurs at an incommensurate wavevector. The excitation bandwidth was observed to be $\sim 12$ meV along the ladder leg, $b^*$ direction and $\sim 2$ meV along the ladder rung, $c^*$ direction.

Our neutron scattering data are consistent with a $J_1$-$J_2$-$J_4$ two-leg ladder model including small interladder exchange $J_3$. Competing interactions $J_1$ and $J_2$ drive the dynamic correlations to an incommensurate wavevector.

FIG. 1. (a) Schematic representation of the crystal structure of BiCu$_2$PO$_6$. (b) Perspective view of the ladder unit in the $bc$ plane. Along the chains Cu$^{2+}$ ions interact via NN exchange $J_1$ and NNN exchange $J_2$. The chains are coupled along the $c$ axis via superexchange interactions $J_3$ and $J_4$.

FIG. 2. Representative constant-$q$ scans collected on C5, at $T = 6$ K and $T = 90$ K.

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FIG. 3. Map of the dynamic structure factor $S(q, \omega)$ measured at $T = 6 \text{ K}$. Neutron scattering intensities were corrected for higher order wavelength contamination in the incident beam monitor and the isotropic $\text{Cu}^{2+}$ form factor. Intensity maps were constructed by linear interpolation of a series of constant-$q$ scans.

In contrast to the single triply degenerate excitation normally observed in spin ladders, we observe two-branches of excitations. The appearance of two modes may be due to the presence of significant anisotropic interactions which split the degeneracy of the triplet in zero field.