

Magnetic Excitation in the Hyperkagome Antiferromagnet Mn_3RhSi

Low- and high-energy inelastic neutron scattering measurements of a hyperkagome antiferromagnet revealed little magnetic specific heat capacity contribution in the enhanced electronic specific heat γ term.

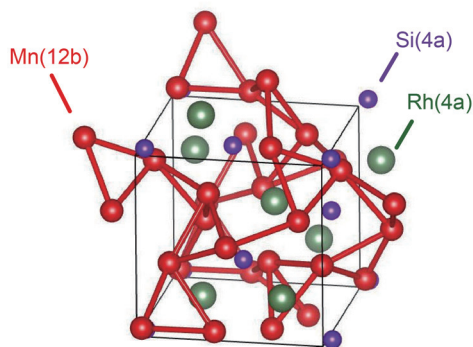


Fig. 1: Mn_3RhSi cubic crystal structure with a lattice parameter of $a = 6.467 \text{ \AA}$ at 293 K. The red bond network is a hyperkagome lattice of the Mn site (12b), where the Mn–Mn bond distance ranges from 2.66 to 2.76 $\text{\AA}$. [Reproduced from Ref. 3]

The hyperkagome antiferromagnetic semimetal Mn_3RhSi lacks spatial inversion symmetry in its β -Mn-type crystal structure (Fig. 1). The material exhibits intriguing magnetic behavior in which magnetic diffuse scattering due to magnetic short-range order is observed in the paramagnetic state up to 720 K, approximately 500 K higher than its Néel temperature of 190 K. The hyperkagome lattice is also found in well-studied β -Mn, which is a known spin liquid candidate and is a heavy Fermion 3d material with an electronic specific heat coefficient (γ) of about 70 mJ/MnK².¹ In ordered β -Mn-type alloys, a quantum critical behavior is observed in the enhanced γ term.² Here, the team of Shin-ichi Shamoto (Comprehensive Research Organization for Science and Society, Japan) studied the magnetic excitation of Mn_3RhSi by low- and high-energy inelastic neutron scattering measurements to elucidate the magnetic contribution to the enhanced γ term. Their research results provided the fluctuating magnetic moment size and the magnetic specific heat capacity at low temperatures for Mn_3RhSi .

In this study, the team measured a 1.65 g Mn_3RhSi single crystal and observed one magnon mode up to the maximum energy, as shown in Fig. 2. The observed intensity in Fig. 3(a) revealed that the magnitude of the magnetic moment of Mn 3d⁵ was approximately 5 μ_B and is almost localized. The magnetic moment of the long-range order state below the Néel point was only 2.6 μ_B at 4 K,⁴ indicating that most of the magnetic moment fluctuates without being ordered. This fluctuation is thought to be due to the geometrical spin frustration of the hyperkagome

lattice. Interestingly, by using a magnetic moment of 2.6 μ_B and the Néel temperature (190 K), the effective exchange interaction can be estimated, yielding a predicted transition temperature of 700 K from the magnetic moment of 5 μ_B based on classical mean field approximation theory. The predicted temperature is very close to the temperature of the magnetic short-range order temperature 720 K mentioned above. The ability to measure low- and high-energy spin fluctuations even with a small crystal has allowed us to better understand mysterious magnetic materials.

Figure 3(b) shows the magnon dispersion of the low-energy mode in Mn_3RhSi . The solid line is fit using the equation $E = E_{\text{top}} \sin^{\alpha}(\pi h)$, where the best fit was obtained with $E_{\text{top}} = 39.5(3) \text{ meV}$ and $\alpha = 0.53(3)$. The peculiar dispersion leads to the magnon specific heat capacity of $C_{\text{mag}} = dU/dT \propto (T/E_{\text{top}})^{3/\alpha}$. As for the electronic specific heat coefficient γ of Mn_3RhSi , the magnon heat capacity becomes small at low temperatures because of the large exponent of $\sim (T/E_{\text{top}})^6$, resulting in little magnon effect on the T -linear electronic specific heat. The team confirmed that the magnon dispersion continues to the low-energy region below 1 meV at SIKa without an appreciable spin gap. The combination of the low- and high-energy inelastic

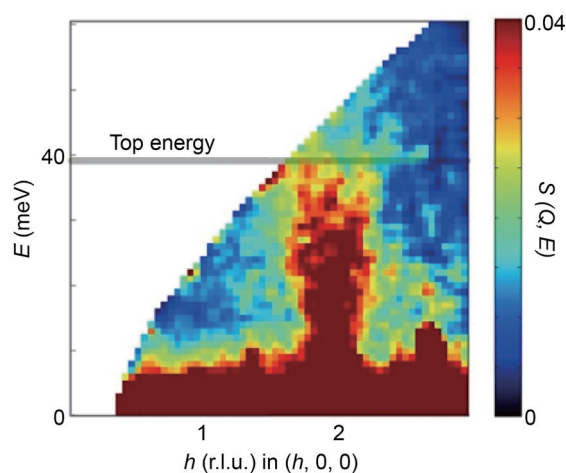


Fig. 2: Dynamical structure factor divided by the Bose factor $\{n(E) + 1\}$ in the low-Q region measured with $E_i = 95 \text{ meV}$. The single-crystal scattering intensity at $T = 6 \text{ K}$ is averaged vertically in the range of $-0.2 < k < 0.2$ and $-0.2 < l < 0.2$ (r.l.u.). The horizontal scattering plane is $[h, 0, 0]$ – $[0, k, k]$. The top energy of the low-energy magnon mode is shown by a solid line. [Reproduced from Ref. 3]

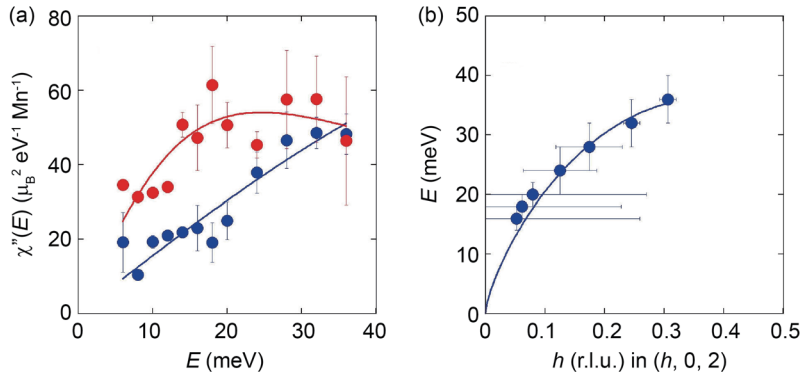


Fig. 3: (a) The dynamical spin susceptibilities are plotted as a function of energy at $T = 6$ K (blue open circles) and 200 K (red closed circles). (b) Magnon dispersion observed at $T = 6$ K. Solid lines are used to aid with visual inspection. [Reproduced from Ref. 3]

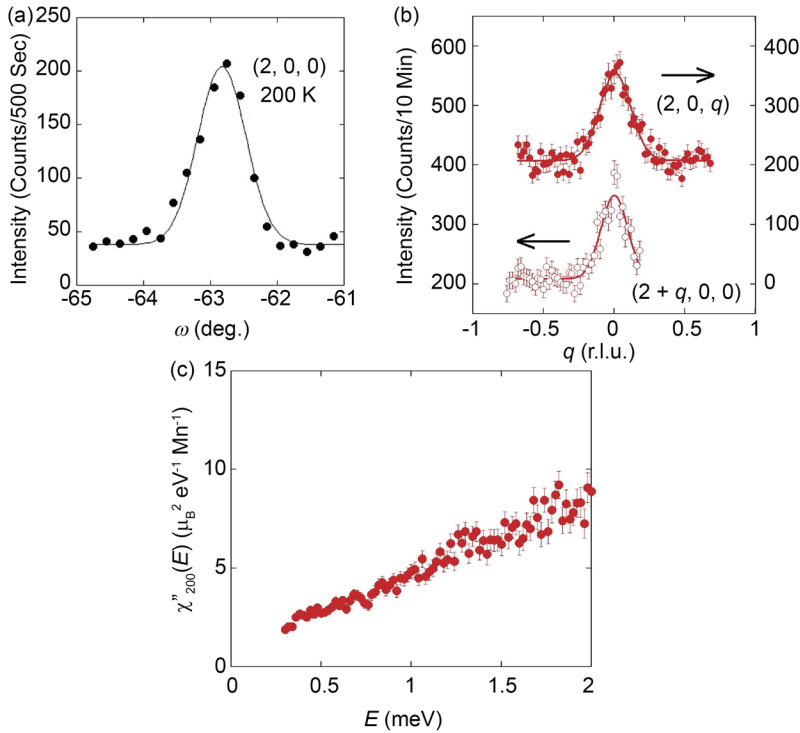


Fig. 4: (a) ω -scan at $(2, 0, 0)$ of the Mn_3RhSi crystal. (b) The constant-energy q -scan in $(2 + q, 0, 0)$ (open circles) and $(2, 0, q)$ (closed circles) of $E = 1$ meV at $T = 200$ K. The horizontal scattering plane is $[h, 0, 0] - [0, 0, l]$. (c) Low-energy Q -integrated local dynamical spin susceptibility $\chi''_{200}(E)$ at $Q = (2, 0, 0)$ measured at $T = 200$ K. [Reproduced from Ref. 3]

neutron scattering measurements of a hyperkagome antiferromagnet revealed how magnetic excitation can contribute to the magnetic specific heat capacity in the enhanced electronic specific heat γ term. (Reported by Shin-ichi Shamoto, Comprehensive Research Organization for Science and Society, Japan)

This report features the work of Shin-ichi Shamoto and his collaborators published in Phys. Rev. Research 6, 033303 (2024).

ANSTO SIKA – Cold Neutron Triple-axis Spectrometer

- Neutron Inelastic Scattering
- Materials Science, Condensed-matter Physics

References

1. H. Nakamura, K. Yoshimoto, M. Shiga, M. Nishi, K. Kakurai, J. Phys.: Condens. Matter **9**, 4701 (1997).
2. H. Yamauchi, D. P. Sari, Y. Yasui, T. Sakakura, H. Kimura, A. Nakao, T. Ohhara, T. Honda, K. Kodama, N. Igawa, K. Ikeda, K. Iida, D. Ueta, T. Yokoo, M. D. Frontzek, S. Chi, J. A. Fernandez-Baca, K. M. Kojima, D. Arseneau, G. Morris, B. Hitti, Y. Cai, A. Berlie, I. Watanabe, P.-T. Hsu, Y.-S. Chen, M. K. Lee, A. E. Hall, G. Balakrishnan, L.-J. Chang, S. Shamoto, Phys. Rev. Research **6**, 013144 (2024).
3. S. Shamoto, H. Yamauchi, K. Iida, K. Ikeuchi, K. Kaneko, Y.-S. Chen, S. Yano, P.-T. Hsu, M. K. Lee, A. E. Hall, B. Geetha, L.-J. Chang, Phys. Rev. Research **6**, 033303 (2024).
4. H. Yamauchi, D. P. Sari, I. Watanabe, Y. Yasui, L.-J. Chang, K. Kondo, T. U. Ito, M. Ishikado, M. Hagihara, M. D. Frontzek, S. Chi, J. A. Fernandez-Baca, J. S. Lord, A. Berlie, A. Kotani, S. Mori, S. Shamoto, Commun. Mater. **1**, 43 (2020).