A surprising discovery about the magnetic interactions in a Kagome layered topological magnet

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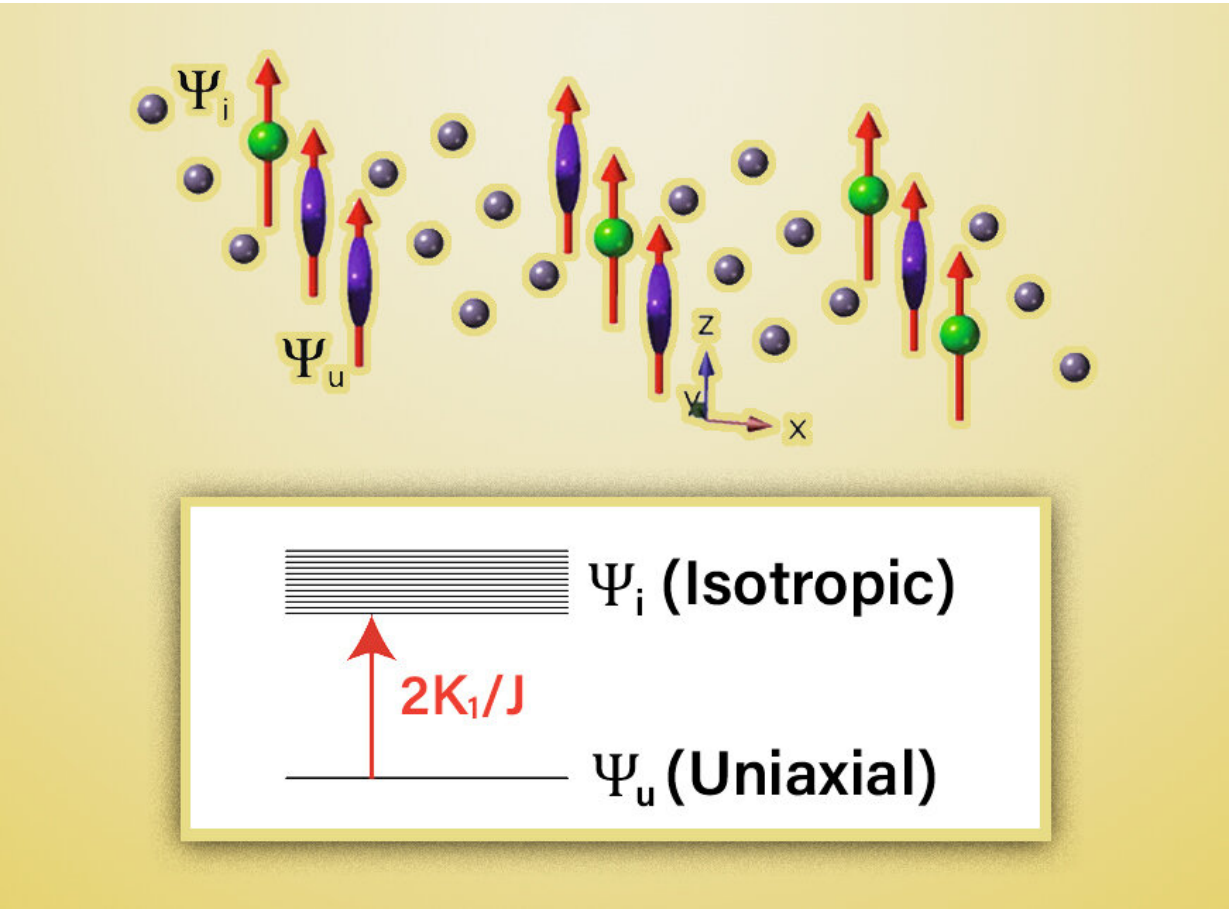

The uniaxial Tb ions have elongated electronic orbitals (shaped like ellipsoids) and the Tb moment points along the ellipsoid due to spin-orbit coupling. The isotropic Tb ions have spherically shaped orbitals, so spin-orbit coupling gives no preference for the moment direction. The image shows that Tb atoms are either ellipsoidal (purple) or spherical (green) at intermediate temperatures (on some

time scale). The number of spherical Tb ions determines when the transition occurs. Credit: U.S. Department of Energy Ames National Laboratory

A team from Ames National Laboratory conducted an in-depth investigation of the magnetism of $TbMn_6Sn_6$, a Kagome layered topological magnet. They were surprised to find that the magnetic spin reorientation in $TbMn_6Sn_6$ occurs by generating increasing numbers of magnetically isotropic ions as the temperature increases.

Rob McQueeney, a scientist at Ames Lab and project lead, explained that $TbMn_6Sn_6$has two different magnetic ions in the material, terbium and manganese. The direction of the manganese moments controls the topological state, "But it's the terbium moment that determines the direction that the manganese points," he said. "The idea is, you have these two magnetic species and it is the combination of their interactions which controls the direction of the moment."

In this layered material, there is a magnetic phase transition that occurs as the temperature increases. During this phase transition, the magnetic moments switch from pointing perpendicular to the Kagome layer, or uniaxial, to pointing within the layer, or planar. This transition is called a spin reorientation.

McQueeney explained that in Kagome metals, the spin direction controls the properties of topological or Dirac electrons. Dirac electrons occur where the magnetic bands touch at one point. However, magnetic order causes gapping at the points where the bands are touching. This gapping stabilizes the topological Chern insulator state. "So you can go from a Dirac semimetal to a Chern insulator just by turning the direction of the moment," he said.

As part of their $TbMn_6Sn_6$ investigation, the team performed inelastic neutron scattering experiments at the Spallation Neutron Source to understand how the magnetic interactions in the material drive the spin reorientation transition. McQueeney said that the terbium wants to be uniaxial at low temperatures, while the manganese is planar, so they are at odds.

According to McQueeney, the behavior at very low or very high temperatures is as expected. At low temperatures, the terbium is uniaxial (with electronic orbitals shaped like an ellipsoid). At high temperatures, the terbium is magnetically isotropic (with a spherical orbital shape), which allows the planar Mn to determine the overall moment direction.

The team assumed that each terbium orbital would gradually deform from ellipsoidal to spherical. Instead, they found both types of terbium exist at intermediate temperatures, however the population of spherical terbium increases as the temperature increases.

"So, what we did was we determined how the magnetic excitations evolve from this uniaxial state into this easy plane state as a function of temperature. And the long-standing assumption of how it happens is correct," said McQueeney.

"But the nuance is that you can't treat every terbium as being exactly the same on some timescale. Every terbium site can exist in two quantum states, uniaxial or isotropic, and if I look at a site, it's either in one state or the other at some instant time. The probability that it's uniaxial or isotropic depends on temperature. We call this an orbital binary quantum alloy."

The study is published in the journal *Nature Communications*.

More information: S. X. M. Riberolles et al, Orbital character of the

spin-reorientation transition in $TbMn_6Sn_6$, *Nature Communications* (2023). DOI: 10.1038/s41467-023-38174-5

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