Magnetism without local moments

Novel Itinerant Antiferromagnet TiAu
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Recommended with a commentary by Andy Schofield, University of Birmingham, UK

Two perspectives underpin our understanding of magnetism. In one, the local moment view, we begin with the basic building blocks of the magnet as the magnetic moments carried by the individual atoms. If the degeneracies implicit in an atomic magnetic moment survive the bonding process (and often they do not), the moments almost always develop a long-ranged ordered structure at low temperatures. By contrast, the alternative itinerant view is that of a Stoner-type instability [1] where we begin an unpolarized conduction electron sea which, by virtue of the electron-electron repulsion, develops a local imbalance of up- and down-spins. This reduces correlation energies because of Pauli exclusion albeit at the expense of kinetic energy. In this latter picture, magnetism is truly emergent since it arises from constituent atoms which need not themselves be magnetic. Yet the known examples of itinerant magnets, including the elemental magnets like iron, almost all comprise of magnetic atoms. Only a handful of magnets arise from "non-magnetic" atoms ($ZrZn_2$ and Sc_3In – which has recently been tuned to quantum criticality by the same group as the present work [2]) and these are all ferromagnets. Emilia Morosan's group from Rice University and her coworkers have found the first example of an antiferromagnet made from a compounds of non-magnetic elements: titanium and gold.

The evidence presented by the authors for TiAu being a bulk spin density wave metal is very strong. XPS indicates that the Ti atoms are at or very close to their non-magnetic 4^+ state, so this is not in any sense a local moment system. Yet there is a surprisingly clear signal of antiferromagnetism in the bulk magnetisation showing a transition at 36K (see figure). This is supported by μSR which reveals that the transition is generating small, but again bulk, magnetic fields within the material: this is not a surface or impurity effect. By looking at the specific heat, the authors are also able to deduce the scale of the changes that are accompanying the magnetism. The neutron diffraction data presented in the supporting material indicates a small magnetic moment of $0.15\mu_B$ (much smaller than a typical local moment of $\sim 1\ \mu_B$) per formula unit. The underlying magnetic structure determined from the neutron diffraction results is consistent with a spin-density wave with a Q vector of $(0, \pi/b, 0)$.

This origin of a modulated magnetic structure in a metal is usually understood within Stoner theory by having features in momentum space arising from the Fermi surface shape or from the microscopic interactions. The authors perform density functional calculations and find a strongly nested Fermi surface with a nesting wave-vector close to that of the observed order. As is frequently found with such mean-field theories, the expected size of the moment predicted by theory is over-estimated (here by a factor of around 4) which means a more complete theory must go beyond mean-field.

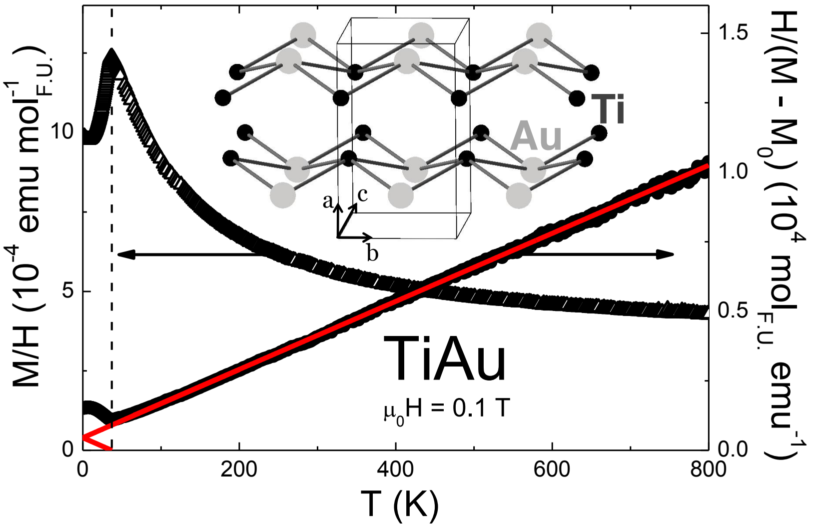

Fig. 1 from arXiv:1409.0811 The inverse susceptibility shows the classic 1/T Curie-Weiss form of local moment magnetism yet the order is small moment and itinerant. That order is modulated along the b-axis.

Indeed, beyond simply its existence, the most fascinating aspect of this system is the clear signature that fluctuation effects are playing a role in the material properties. (In this respect it stands out from chromium which is about as mean-field a spin density-wave system as you can get [3].) As shown in the figure there is a very strongly temperature-dependent susceptibility reminiscent of a local moment system with Curie-Weise behavior. In a local moment picture we would understand these as directional fluctuations of a pre-existing moment. Without an intrinsic moment, what here is fluctuating? In the case of itinerant ferromagnetism this paradox between the appearance of temperature dependences associated with local moments, and ordering scales and sizes of moments being itinerant, have been long understood as being due to strong mode-mode coupling between fluctuations: spin-fluctuation theory [4]. The new example provides us with a poster child of itinerant antiferromagnetism against which we expect theory to provide a quantitative account. Consistent with the significance of spin-fluctuations here is the resistivity. It drops as the magnetism appears showing that, as the Fermi surface is partially gapped by the density, the loss of low-energy carriers is more than compensated for by the reduction in spin scattering. Again a quantitative understanding of this should be possible.

Understanding and characterizing TiAu will give us a starting point to compare and contrast with other unusual magnetic states. The authors compare TiAu with MnSi but the recent observation of spin density-wave order in the high magnetic field ‘nematic’ state of $Sr_3Ru_2O_7$ would be another example [5]. Other potential future directions include tuning the 36K transition to zero temperature to produce a quantum critical point which might be possible via doping.

In summary, this new material provides a fascinating example of the emergence of antiferromagnetism from non-magnetic constituents. It should allow for quantitative theoretical productions which will require going beyond simple mean-field theory so is likely to become a textbook example of the appearance of magnetism in metals.

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