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Half-metals: Systems with Correlated Electrons

Halbmetalle: stark korrelierte Systeme

Half-metals show a particular type of magnetism in nature, and an unusual electronic property: they are metallic for one spin channel, and insulating or semiconducting for the opposite one. Half-metallicity can be easily understood: exchange splitting may cause one spin channel to overlap with another set of bands giving a metallic channel, while the Fermi level lies within the gap of the other insulating channel, forming a half-metallic ferromagnet (HMF). Because the insulating channel has filled bands, and there are an integral number of electrons in the unit cell, the spin moment is integer. Whenever local moments in a half-metal are oriented in opposite directions, with a non-zero net spin moment, one can talk about half-metallic ferrimagnets. In the extreme limit of a zero spin-moment, when the number of up and down spins is equal, a half-metallic anti-ferromagnetic (HMAF) state is formed. Since there is no symmetry connection between up and down spins it is qualitatively different from the usual anti-ferromagnet. In many regards ferri- or anti-ferro- half-metals behave like HMF: they are metallic with 100% spin-polarized transport, but have no Stoner continuum. These properties make the half-metals possible candidates to what we call today "Spintronics": electronics based on the manipulation of spins.
Band structure calculation, in the framework of Local Density Approximation (LDA) of Density Functional Theory (DFT) explains this peculiar behaviour. One of the shortcomings of DFT-LDA approach resides in a non adequate description of electron-electron interaction. This kind of interaction is frequent in nature, and in some materials can be of the order of the bandwidth which makes the material to be called correlated (W/U=1).
Nowadays, in the field of strongly correlated electron systems, the Weiss' molecular field has been extended to be able to describe local quantum (temporal) fluctuations between the possible quantum states. This recently emerged theory called "Dynamical Mean Field Theory" (DMFT) becomes exact in the limit of large spatial dimensions or more appropriately in the limit of large lattice coordination. However, phenomena depending on dimension are missed in a local mean-field approach but can be restored step by step using cluster expansions. A cluster expansion such as the Variational Cluster Approximation (VCA) is a promising tool which reincorporates the short-range correlations which are neglected in the local mean-field approach. In our work we study many-body and finite temperature effects in half-metallic materials, in the framework of LDA+DMFT/VCA. For a large number of HMF with the gap in the minority spin channel, we showed that many-body interactions give rise to "non-quasiparticle" states (NQP), situated above the Fermi level, (Fig. 1) which contributes in a destructive way to the 100% spin polarization of the bulk half-metallic state.
In addition, we can raise an interesting question concerning the coexistence of superconductivity and half-metallic magnetism. Since the HMAF has a vanishing spin moment there is no obstacle (macroscopic magnetic field) for superconductivity to appear in the metallic channel. Thus, HMAF would provide the first example of the single-spin superconductivity. Whether superconductivity and half-metallic magnetism might coexist is still an open question, nevertheless there is no doubt concerning the necessity to develop many-body methods to treat correlated electrons in general and half-metals in particular.

Presentation

L. Chioncel was born in Oradea, Romania in 1972. Following a BSc. in Physics (1995) and MSc. (1996) in Solid State Physics from "Babes-Bolyai" University Cluj-Napoca, Romania, he carried out a PhD (1999) in Solid State Physics at the same university, benefiting from several research stages at the CNRS Grenoble, France, and Max-Planck Institute for Solid State Physics Stuttgart, Germany. In 1996 he started his academic career as an assistant and then as a junior lecturer at Oradea University, Romania. From 2000 to 2005 he was a junior researcher in the Netherlands where he performed a PhD in Theoretical and Computational Physics followed by a brief Postdoc at the Radboud Universtiy Nijmegen. In January 2005 he became a university assistant at the Institute for Theoretical Physics – Computational Physics at the TU Graz.

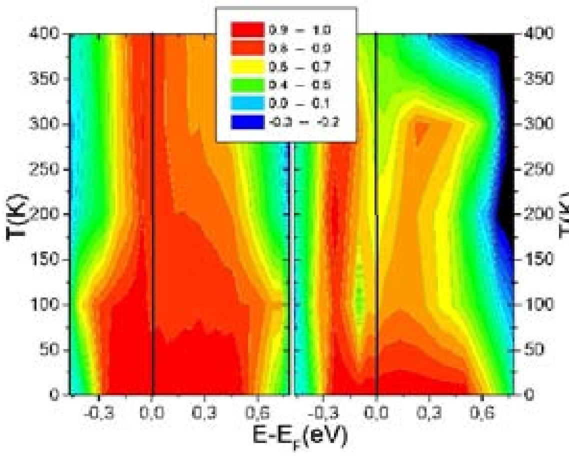

Fig.1. Finite temperature spin polarization of the half-metallic ferrimagnet FeMnSb computed for different values of the Coulomb interaction U=2eV (left), U=4eV (right). The asymmetry around Fermi energy is due to the existence of NQP states. The effect is more visible for larger values of the local Coulomb interaction (L. Chioncel et al. PRL, 96, 137203, 2006).

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Halbmetalle weisen eine besondere magnetische Ordnung auf und besitzen eine unübliche elektronische Konfiguration: eine Spinrichtung zeigt metallischen Charakter, die andere ist hingegen halbleitend oder gar isolierend. Man kann das so verstehen: Exchange splitting kann in einem Spinkanal zu einem Überlappen mit anderen Bändern führen und diesen somit metallisch leitend werden lassen. Die Fermi-Energie des anderen Spinkanals liegt hingegen in einer Lücke und das führt zu einem halbmetallischen Ferromagneten (HMF). Andere Formen des Magnetismus wie Ferri- oder Antiferromagnetismus sind ebenso möglich. Diese Eigenschaften zusammen mit der Möglichkeit voller Spinpolarisierung macht diese besondere Klasse von Materialien zu geeigneten Kandidaten für die „Spintronik": eine Klasse von elektronischen Bauteilen, die auf der Manipulation des Spins beruhen. Natürlich sieht die Realität etwas anders aus und reelle Materialien weisen auf Grund von endlicher Temperatur und Korrelationseffekten eine signifikant niedrigere Spinpolarisierung auf. Mittels kombinierter materialspezifischer und vielkörperphysikalischer Rechnungen untersuchen wir diese Depolarisationseffekte, die von essenzieller Bedeutung für zukünftige Anwendungen in der Spintronik sind.