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Physics Letters A 334 (2005) 453–459
PHYSICS LETTERS A
www.elsevier.com/locate/pla

Uranium nitride—a spin polarized weak itinerant electron antiferromagnet with strongly correlated electrons

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Received 24 November 2004; accepted 30 November 2004
Available online 18 December 2004
Communicated by V.M. Agranovich

Abstract

A brief survey of anomalous properties of uranium nitride—a collinear metallic antiferromagnet with NaCl-structure is presented and argued that it must be regarded as a weak antiferromagnet with polarized itinerant electrons. It is shown that this new weak itinerant antiferromagnet appears to be a very simple magnetic system, well understood within the Fermi liquid picture of spin polarized 5*f*-electrons, and may be used as a model to study basic problems of strongly correlated systems.

PACS: 71.27.+a; 75.40.Gb; 76.20.+w

Keywords: Itinerant antiferromagnetism; Fermi liquid; Relaxation; Spin fluctuations

1. Introduction

Weak itinerant electron magnets being at the edge of magnetic instabilities exhibit strong electron correlations and represent a class of simple model systems to investigate novel physical phenomena. First, they have relatively low critical (Curie or Néel) temperatures which may be tuned to absolute zero by applying, e.g., rather moderate hydrostatic pressure, thus opening a possibility to investigate quantum critical phenomena, etc. [1]. Second, due to their proximity to a magnetic instability at low temperatures fluctuations of their magnetic order parameter—spin fluctuations (SF)—dominate over the Fermi quasiparticle excitations not only in the vicinity of the phase transition but also down to the low temperatures [2,3]. Third, SF having a diffusive or overdamped nature occupy an essential part of the phase space (e.g., the Stoner, continuum in the ballistic regime) and may give rise to

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0375-9601/$ – see front matter
doi:10.1016/j.physleta.2004.11.052

giant averaged amplitudes of zero-point SF [4,5]. This in turn may result in strong spin anharmonicity and in the break down of a simple Gaussian picture where SF are viewed as a gas of independent collective excitations [2,3]. The concept of strong spin anharmonicity has given novel trends to SF thermodynamics and kinetics, where fluctuations are treated as non-Gaussian and relaxate due to non-linear multi-mode scattering processes [6].

However, not so many weak itinerant electron magnets are well understood up to now. Among them we should mention classical weak itinerant ferromagnets Ni_3Al, $ZrZn_2$ and MnSi with the Curie temperatures 41 K, 28 K and 29.5 K and ordered atomic magnetic moments $0.075\mu_B$, $0.15\mu_B$, and $0.4\mu_B$, respectively [2,3].

A quite new candidate is uranium nitride UN, which for a long time was considered as a perspective nuclear fuel [7], that is probably why not so many efforts were focused on its magnetic properties. Uranium nitride is a metallic antiferromagnet with the Néel temperature [8] $T_N \approx 53$ K and the ordered moments on uranium atoms $\mu_S \approx 0.75\mu_B$. It has a cubic NaCl-structure with the ferromagnetic order inside the uranium (001) planes, which are ordered antiferromagnetically with the magnetization parallel to the antiferromagnetic wavevector $(0, 0, 1)$.

In the present Letter we argue that uranium nitride is a new example of a weak itinerant antiferromagnet, where, unlike chromium, antiferromagnetism arises due to the spin polarization of electronic subbands rather than due to the Fermi surface nesting. We present a novel approach based on the Fermi liquid concept to describe this spin polarized antiferromagnetic compound and to show that this simple magnetic system may be used as a model to study basic problems of physics of strongly correlated systems.

2. Electron properties of UN

Among the uranium compounds with the NaCl-structure UN has probably the smallest lattice constant (at $T \approx 300$ K) $a_0 = 4.890$ Å [3] and the spacing between uranium atoms $d_{\mathrm{U}} = 3.450$ Å [9], which is close to the critical U–U interatomic distance $d_c = 3.5$ Å following from the Hill's plot [10] and pointing to the non-local character of the $5f$-electron orbits of uranium.

Photoemission measurements directly indicate the itinerant nature of $5f$-electrons forming a relatively narrow band with a bandwidth $W \approx 1$ eV [9], which is located in the vicinity of the Fermi level and hybridized with the $6d$-electron bands. The values of the Fermi energy and the density of $5f$-electrons measured in [9,11] were $\varepsilon_F \approx 0.78$ eV and $n_f \approx 2.2 \pm 0.5$ electrons per U atom. The latter value is close to the value $n_f = 2.45$ electrons per U atom resulting from the electron band structure calculation [12], where the mass of $5f$-electrons was estimated to be $m \approx 7.42 m_e$, m_e being the mass of a free electron. Electron density measurements [9,11] also indicate non-integer occupation of $5f$-orbitals of uranium atoms, intermediate between $5f^2$ and $5f^3$, which suggests the delocalization of $5f$-electrons. Another indication of the itinerant nature of $5f$-electrons is the change in the peak of $5f$-electrons observed in the photoemission spectrum when the period of the crystal lattice is doubled below the Néel temperature [9].

Itinerant $5f$-electrons make a significant contribution to the electronic specific heat $c_e = \gamma T$ with a coefficient [13] $\gamma = 49.6\,\mathrm{mJ\,K^{-2}\,mol^{-1}}$, which corresponds to the electron density of states at the Fermi surface [9] $\sim 20\ \mathrm{eV^{-1}}$ (U atom)$^{-1}$ and considerably exceeds the value [13] $3.1\ \mathrm{mJ\,K^{-2}\,mol^{-1}}$ for ThN, an isostructural analog of UN with unfilled $5f$-shells.

Uranium nitride exhibits metallic conductivity [8]. Its resistivity increases with temperature monotonically from $\rho = 1.18\ \mu\Omega\,\mathrm{cm}$ in the low-temperature limit to $\rho = 78.6\ \mu\Omega\,\mathrm{cm}$ at $T_N = 53$ K and $\rho = 150\ \mu\Omega\,\mathrm{cm}$ at $T = 300$ K. At the magnetic transition point $T = T_N$, the $\rho(T)$ curve has a bend, which is usually attributed to a change in the Brillouin zone at the Néel point.

Such a behavior of the resistivity is usually attributed to scattering of conduction electrons by SF [8] playing a significant role up to the Fermi degeneracy temperature $T_F \approx \varepsilon_F / k_B \approx 9.05 \times 10^3$ K, which considerably exceeds the melting point $T_m \approx 3000$ K of UN [14].

All elastic moduli in UN below the Néel temperature have clearly manifested anomalies $\sim 10\%$, which are associated with the onset of a magnetic order and strong magnetoelastic coupling [8].