Spin and Orbital Magnetic State of UGe_2 under the Pressure.

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The possibility for coexistence of superconductivity (SC) and ferromagnetism (FM) has been long considered theoretically. However, the predominance of spin-singlet SC led to the common belief that SC and FM order are mutually exclusive. Recent experiments discovered the SC and FM coexistence in UGe_2 [1], URhGe [2], and $ZrZn_2$ [3] restoring theoretical interest in the problem. Both the experiment and the theory favor parallel spin pairing magneticaly mediated SC in these materials, and no microscopic material specific theory of SC-FM coexistance exists up to date.

We focus here on the case of UGe_2, for which the SC occurs in the pressure (***P***) range of 10-18 kBar. Very interesting feature of this material is an additional (to FM and SC) phase transition which appears as a jump in the low temperature magnetization [4]. This magnetic moment vs pressure change has been interpreted as a first-order Stoner-like phase transition in spin-only magnetisation due to the sharp double-peak density of states (DOS) in the vicinity of the Fermi level [5]. We show here that the change in the magnetization is associated with the change of the U-atom both orbital and spin magnetic moments and propose a new type of the magnetic phase transition due to the change of the U-atom orbital state in UGe_2 with pressure.

We use LSDA+U electron-electron interaction model with FP-LAPW basis to calculate the total energy and spin/orbital magnetic moments dependence on pressure for a normal state of UGe_2 at T=0. The inclusion of the orbital polarization beyond that provided by LSDA (where it comes from the spin-orbit coupling only) is necessary in order to obtain the values of spin M_S and orbital M_L magnetic moments [6] consistent with experiment.

We do the calculations for different values of the lattice constant ***a*** fixing the ***c/b/a*** - ratios and internal atomic positions as in the

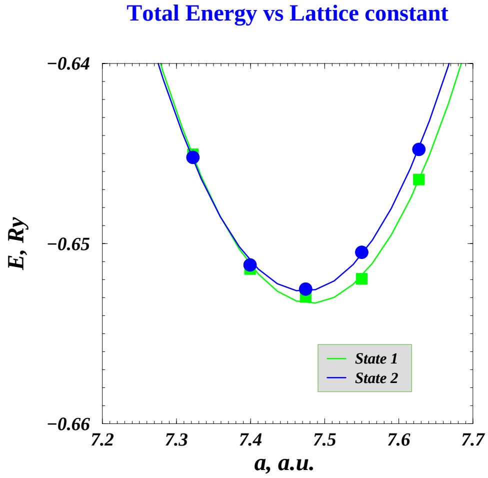

Fig. 1. ***Total Energy*** *vs* lattice parameter ***a***. State 1 (1st solution) is shown in green, and State 2 (2nd solution) is in blue.

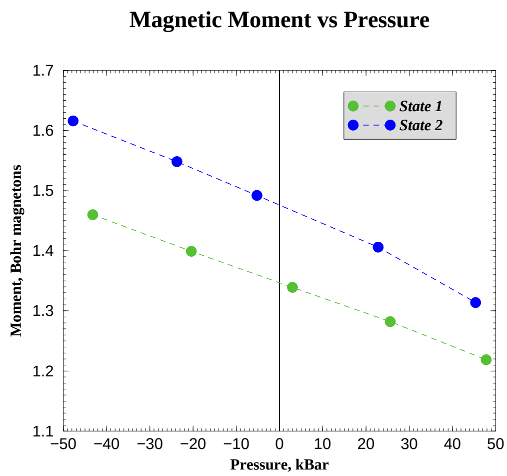

Fig. 2. Total = Spin + Orbital Magnetic Moments.

experiment [7], and use Coulomb-***U*** = 0.7 *eV* and Exchange-***J*** = 0.44 *eV* [6]. We found two LSDA+U solutions (states), for which the total energy ***E*** *vs* ***a*** dependence is shown in Fig.1. The calculated equilibrium ***a*** = 7.48 (State 1)-7.47 (State 2) a.u. are found in good agreement with experimental ***a*** = 7.55-7.63 a.u. values. The total energy difference E(State 1) - E(State 2) < 1 mRy/U-atom and is decreasing with decreasing of a. We consider these two states to be almost degenerate in the accuracy of the calculations.

We show in Fig. 2 the total magnetic moment dependence on P for the States 1,2. There is ~0.2-0.25 μ_B difference in the total M between these two states. Then, we can associate our results with Fig.2(b) of [4] assuming that the change in M occurs as system moves from State 2 to the State 1 under the applied pressure. This is further justified since the magnetic states of UGe_2 are shown experimentally to switch in the applied field of 5T meaning that they are extremely close in energy.

We plot in Fig. 3 partial f-electron DOS for State 1 (top) and State 2 (bottom) at the equilibrium value of a. The major difference between States 1 and 2 is seen to come from the difference between the orbital occupation of the states in the vicinity of the Fermi level: State 1 has spin-up m_L =0 level occupied; and State 2 has spin-up m_L=-1 occupied. It provides us with a sudden change in M_L at State 2 to State 1 phase transition, causing a step-like change in the total M under the applied pressure.

We point out that the measurements of M_L/M_S - ratio pressure dependence could be a good way to examine further the origin of the magnetic states in UGe_2 as it is shown to change sharply from State 2 (2.1) to State 1 (1.9) in our calculations and can be measured by polarized neutron diffraction experiments.

Finally, we will discuss the effect of "orbital" phase transition on Fermi surface pressure dependence and will analyze its possible implications on the SC-pairing mechanism.

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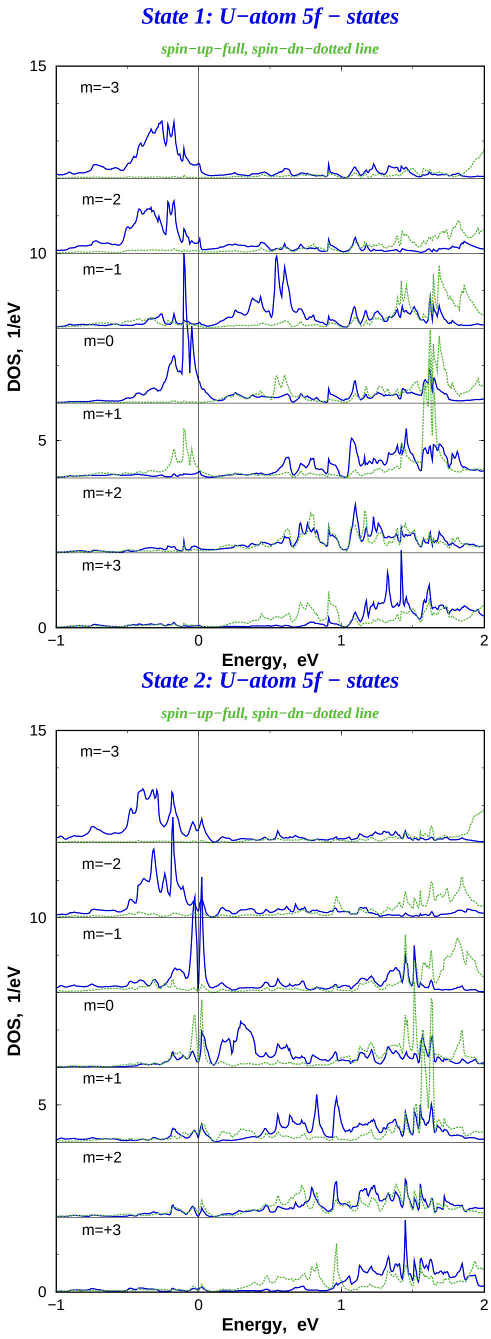

Fig. 3. Spin and Orbitally resolved U-atom 5f-DOS for the State 1 (top) and 2 (bottom).

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