Theoretical study of fermi surface of $URhIn_5$ with de Hass-van Alphen effect

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Over the last twenty years, heavy fermion compounds [1] from the '115' family have attracted growing experimental attention. These materials follow a XYZ_5 composition, with a lattice structure that can be considered as a particular intermediate between the "infinite layer" XZ_3 geometry of their parent compound, and the "double layer" case with composition: X_2YZ_8. Initial interest in studying material properties upon adding the Y transition metal was prompted by the evolution of superconducting temperature with applied pressure, or with the change from a cubic unit cell into a tetragonal arrangement; and spin/charge correlation analogies with examples from the cuprate family [2].

Experimentally, one notes the appearance of superconductivity when X=Ce or Pu, and its absence when X=U or Np. This difference has been related to the localized vs. itinerant nature of the f electrons, and prompted a variety of experimental investigations [3].

Our work focuses on the $URhIn_5$ example, characterized by an electronic specific heat coefficient of 50 (mJ/K^2mole), and a Néel temperature of 98 (K) [4] with a $\mathbf{Q}$=(1/2,1/2,1/2) AF ground state determined by nuclear quadrupole resonance and neutron scattering experiments [5]. Recent investigations have studied its Fermi surface, by means of the de Haas-van Alphen (dHvA) effect [6].

From previous researches by different groups, a reliable description of 115 materials needs to address various aspects: strong spin-orbit due to the heavy lanthanides/actinides atom X, satisfactory treatment of f electrons, and accurate description of magnetism.

In general, the most comprehensive scheme to handle these aspects work at the level of an all-electron, Dirac equation -based framework, and we present here preliminary results obtained via the Munich Spin Polarized Relativistic Korringa, Kohn, Rostoker (SPRKKR) multiple scattering package [7], in combination with the Supercell K-space Extremal Area Finder (SKEAF) dHvA program [8].

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