Coexistence of superconductivity and antiferromagnetism in CeRhIn$_5$; Model Hamiltonian and ab-initio calculations.

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Abstract. The finite temperature phase diagram of CeRhIn$_5$ as a function of pressure and magnetic field has three main highlights: a) the competitive coexistence of metallic antiferromagnetism and superconductivity, b) the abrupt disappearance of antiferromagnetism when the Neel and superconducting temperatures become equal at a critical pressure $P_c$ and c) the reentrance of the antiferromagnetic phase in a range of pressures larger than $P_c$ when a magnetic field is applied. Based on first-principles band structure calculations, we propose a quasi-two-dimensional model of interacting electrons, which reproduces, at the mean-field level, the central features of the phase diagram.

1. Introduction
The increasing interest in the family of CeMIn$_5$ compounds does not come exclusively from the heavy-fermion nature of its low-energy excitations. Rather, it is their capability to illustrate different aspects of the competition and coexistence of superconducting (SC) and antiferromagnetic (AFM) phases in the proximity of a quantum critical point, what has caught the attention of the solid state community. Specifically, the temperature vs pressure phase diagram of CeRhIn$_5$ (see Fig. 1) has been determined, with extremely consistent results, using several experimental techniques, namely: low-temperature calorimetry [1, 2], resistivity [3], nuclear quadrupole resonance [4] and ac-susceptibility [5]. Coexistence has been also found in the family of compounds CeRh$_{1-x}$Co$_x$In$_5$ with $x = 0.1, 0.2, 0.4$ [6] [7], with a similar behavior under the application of pressure.

The purpose of this work is discussing how the conditions that favor coexistence of a SC and AFM impose restrictions in the low-energy band structure, which in turn are observed in ab-initio calculations on the compound. In addition, other phenomenological implications, mainly the enhancement of both the cyclotron and specific heat masses of the electronic liquid under pressure, may have been experimentally observed in CeRhIn$_5$.

2. Coexistence of antiferromagnetism and superconductivity
Inspired by the phenomenology of CeRhIn$_5$, we will consider a model of interacting electrons based in the following assumptions: 1.) The electrons contributing to the SC and the AFM will be treated in equal footing and considered equivalent. 2.) The Hamiltonian contains terms
favoring both the SC and AFM instabilities. 3.) The Hamiltonian is solved within a mean-field approach. 4.) The dispersion relation satisfies, for some section of the Fermi surface, the condition $\varepsilon(k + Q) = \varepsilon(k)$. The starting point is therefore the following model: [8, 9]:

$$H = \sum_{k, \sigma} \varepsilon(k) c_{k, \sigma}^\dagger c_{k, \sigma} + \sum_{k, q} V_{kq} c_{(k + q)\uparrow}^\dagger c_{(-k - q)\downarrow}^\dagger c_{-k\downarrow} c_{k\uparrow}$$

$$+ \frac{U}{2} \sum_{k, k'} c_{k, \sigma}^\dagger c_{k', -\sigma}^\dagger c_{k, \sigma} c_{k', -\sigma}$$

$H_V$ favors SC with an order parameter having a symmetry related to the effectively attractive $V_{kq}$ but the presence of of the Hubbard repulsion $U$ forbids SC at arbitrarily low values of $V_{kq}$ and in turn favors the SDW. What kind of quasiparticle $\varepsilon(k)$ favor the coexistence of both phases for the same electrons? To avoid a gapped SDW, which will turn the system insulating at temperatures close to $T_N$ and would not facilitate the coexistence, we consider a dispersion relation satisfying $\varepsilon(k + Q) = \varepsilon(k)$ [8, 10], which are associated to the presence of extended saddle points connected by the antiferromagnetic Q vector.

To make connection between the model phase diagram and the experimental pressure-temperature one, we need to know the relation between the parameters of the model and the pressure. Specifically, the dependence of the bandwidth in which the density of states shows a logarithmic divergence is crucial. To this end, we have computed the pressure dependence of the effective bandwidth of the Van Hove singularity $W$ and the on-site interaction $U$ using first-principles calculations in two planar benchmark systems, the layers of Ni(100) and Ni(111). We used the SIESTA code for this calculations [11]. We find that $W$ increases linearly and $U$ is nearly constant in that range of pressures. We assumed a $V$ independent of pressure. The results are presented in Fig. 2 (a). With these dependencies, we have plotted different theoretical phase diagrams, for different values of $U$. The results are presented in Fig. 2 (b) in comparison with the experimental phase diagram by Chen et al [5].

As discussed in Ref. [9] the enhancement of the cyclotron [13] (see Fig. 3) and specific heat masses [14] are compatible with the existence of a VHS close to the FL.

3. Band structure calculations.
Our band structure calculations for CeRhIn$_5$ (GGA implemented in VASP [15] and performed in the paramagnetic phase) show, in accordance with previous results [12], a peak in the DOS.
Figure 2. (a) Pressure dependence of the bandwidth W and the on-site interaction in a layer of Ni(100) used as a benchmark system. W is the typical energy scale in which the density states has a logarithmic dependence, and here we study the dependence of this scale on the pressure. In the inset pressure dependence of the inter-atomic distance. (b) Comparison of our results with $V = 4W_0$, $E_c = 0.7W_0$, $n = 0.92$ electrons and $U = 2.25, 2.50$ and $2.75W_0$. $W_0$ is the bandwidth at ambient pressure (upper panel and lower panel on the left) with the experimental phase diagram of reference [5] (lower panel on the right).

Figure 3. Cyclotron mass ($m_c$) as a function of pressure. Triangles are the experimental values from Ref. [13] showing the $m_c$ divergence close to $P \sim 2.4$ GPa, where the magnetic order disappears. The solid line is a fit to the theoretical model. Close to a Van Hove singularity the cyclotron mass diverges logarithmically as the difference between $E_F$ and the $E_{vhs}$ vanishes (see lower inset). According to the model this energy difference is proportional to $T_N$ and its pressure dependence can be extracted, for instance, from Ref. [2](see upper inset).

close to the FL. Furthermore, due to the quasi-2D character of the material a saddle point is observed along the $(\pi/a, 0, q_z)$ dispersing along $c^*$ and crossing the FL at a value of $q_{zc} \sim 0.25c^*$. At this mean-field level this implies that the order will be incommensurate in the z direction with a modulation vector of $2q_{zc}$. The magnetic order of CeRhIn$_5$ is incommensurate along the $c^*$ crystallographic axis however the experimental value for the modulation vector is 0.297.

Finally, when treated beyond mean-field theory, the presence of a saddle point in $\varepsilon(k)$ has further interesting implications. Using RG techniques [16, 17] it is possible to demonstrate that $V_{kq}$ has electronic origin and d-wave is the more likely order-parameter symmetry of the SC phase. The analysis of the self-energy shows unambiguously non-Fermi Liquid behavior.
Figure 4. Low-energy electronic structure of CeRhIn$_5$ along Γ-X-M i.e. $q_z = 0$ (left panel) and
$q_z = 0.3\pi/c$ (central panel). (Upper right panel) DOS (lower right panel) energy of the saddle
point as a function of $q_z$.

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