Superconductivity and Magnetic Order in $CeRhIn_5$: Spectra of Coexistence

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(Received 27 July 2006; published 22 March 2007)

We discuss the fixed-point Hamiltonian and the spectrum of excitations of a quasi-bidimensional electronic system supporting simultaneously antiferromagnetic ordering and superconductivity. The coexistence of these two order parameters in a single phase is possible because the magnetic order is linked to the formation of a metallic spin density wave, and its order parameter is not associated to a spectral gap but to an energy shift of the paramagnetic bands. This peculiarity entails several distinct features in the phase diagram and the spectral properties of the model, which may have been observed in $CeRhIn_5$. Apart from the coexistence, we find an abrupt suppression of the spin density wave when the superconducting and magnetic ordering temperatures are equal. The divergence of the cyclotron mass extracted from de Haas–van Alphen experiments is also analyzed in the same framework.

DOI: 10.1103/PhysRevLett.98.126406 PACS numbers: 74.70.Tx, 71.27.+a, 75.30.Fv

The interplay between magnetism and superconductivity is a recurrent area of research in condensed matter physics. This interest has been activated in recent years due to the experimental findings of their coexistence in materials based on Ce, particularly in the 1-1-5 $CeMIn_5$ family [1,2]. A prominent member of this family is $CeRhIn_5$, which grows in tetragonal form, alternating $CeIn_3$ and $RhIn_2$ planes along the c crystallographic axis. The structural anisotropy, induces quasi-bidimensionality in the electronic bonding and the Fermi surface, as evidenced in a series of de Haas–van Alphen measurements and band structure calculations [3–5]. At ambient pressure $CeRhIn_5$ becomes an antiferromagnet (AFM) below $T_N \sim 3.8$ K [1], with a small staggered magnetization aligned in the ab plane. Within the standard Doniach's Kondo lattice paradigm, applying pressure in a weak AFM heavy-fermion system opens a route to very interesting effects. As the pressure increases this theoretical scenario predicts the following: (i) a reduction of T_N due to Kondo compensation; (ii) the eventual suppression of the AFM order in a quantum critical point (QCP), which alike other heavy-fermion compounds, would be responsible of the anomalies in the metallic phase; (iii) the setting of unconventional superconductivity. However, all calorimetric [6], NQR [7], transport [8], and susceptibility [9] measurements provide a consistent picture for the pressure-temperature phase diagram (presented schematically in Fig. 1) in conflict with the aforementioned theoretical scenario. Surprisingly, T_N first increases with pressure and it only starts to decrease for pressures higher than 0.7 GPa. Superconductivity (SC) shows up before T_N has gone down to zero, i.e., AFM and SC coexist. Finally, AFM disappears abruptly at $P_c = 1.9$ GPa exactly when $T_N = T_{SC}$, in a first-order transition and before a QCP could have taken place. Despite the lack of a QCP in the pressure-temperature phase diagram, the metallic phase still might be understood in the framework of a quantum criticality if, changing another experimental knob, one could find a QCP nearby in the phase diagram. The natural choice is using a magnetic field to quench the superconductivity, and in that way, continue the point $P_c(H = 0)$ into a line of first-order transitions down to zero temperature, ending with a QCP at H^*_{c2}. A new surprise appeared on this type of experiment [6,10]. For pressures higher than P_c, the AFM reenters applying an in-plane magnetic field $H_m < H_{c2}$. Besides, transport measurements suggest [1,8] that magnetic order in $CeRhIn_5$ may not be associated to a gap in the single-particle spectrum. Actually, the resistivity as a function of the temperature does not show the conventional minimum characteristic of a metal-insulator transition at any temperature. The small anomaly observed in the resistivity close to T_N seems related to a change on the scattering mechanism when the AFM sets in.

In vivid contrast with quantum critical and quasi–one-dimensional systems, the understanding of the individual AFM or SC states relies on simple but accurate mean-field theories. In this Letter, we propose that a basic comprehension of the microscopic coexistence of AFM and SC

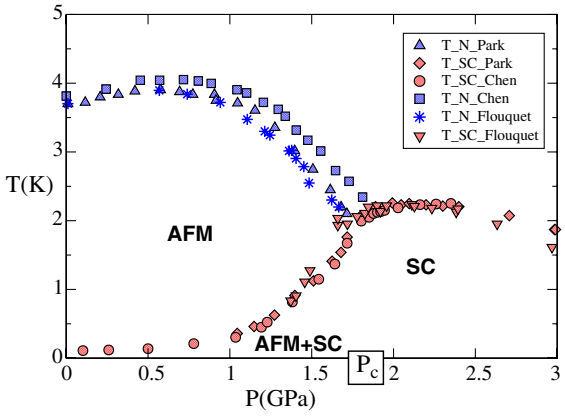

FIG. 1 (color online). Schematic experimental pressure-temperature phase diagram of $CeRhIn_5$ at zero-magnetic field adapted from Refs. [6,9,21].

and the first-order transition between these two phases can also be achieved within a mean-field scenario. We discuss this phenomenon at the microscopic level in terms of a quasi-bidimensional model of interacting electrons proposed by one of us [11–13]. We will enumerate some implications of that model, discussing to what extent they can be related to the phenomenology observed in $CeRhIn_5$.

The model Hamiltonian contains the terms that naturally establish superconductivity and antiferromagnetism.

$$H = H_k + H_V + H_U \tag{1}$$

with

$$H_k = \sum_{k\sigma} \varepsilon(k) c^\dagger_{k\sigma} c_{k\sigma}, \tag{2}$$

$$H_V = \sum_{kq} V_{kq} c^\dagger_{(k+q)\uparrow} c^\dagger_{(-k-q)\downarrow} c_{-k\downarrow} c_{k\uparrow}, \tag{3}$$

$$H_U = \frac{U}{2} \sum_{kk'} c^\dagger_{k\sigma} c^\dagger_{k'-\sigma} c_{k\sigma} c_{k'-\sigma}, \tag{4}$$

where U is a Hubbard on-site repulsion, and V_{kq} the effective interaction in the Cooper channel, which we will take to be attractive. Only s-wave pairing will be considered throughout this Letter. Superconductivity with an order parameter having a symmetry related to V_{kq} is favored by H_V but the presence of a Hubbard repulsion establish a competition, which in terms of the gap is given by $\Delta = \Delta_2 - \Delta_1$, such that

$$\Delta_2 = V {\sum_k}' \langle c^\dagger_{k\sigma} c^\dagger_{-k-\sigma} \rangle, \tag{5}$$

$$\Delta_1 = U \sum_k \langle c^\dagger_{k\sigma} c^\dagger_{-k-\sigma} \rangle, \tag{6}$$

where the prime restricts the summation to states with an energy [measured from the Fermi level (FL)] smaller than a cutoff energy E_c. For those states we assume a very weak momentum dependence of V_{kq}. In the absence of magnetic order and setting a constant density of states at the FL (i.e., far from a logarithmic divergence), the competition between terms favoring and disfavoring the SC is clearly shown in the McMillan-like formula for the critical temperature.

$$T_{SC} = 1.13 E_c \exp\left(\frac{-1}{(V - U^*) D(E_F)}\right), \tag{7}$$

where $U^* = \frac{U}{1 + UD(E_F) \ln(W/E_c)}$.

An essential ingredient of the model is the quasiparticle dispersion relation $\varepsilon(k)$ in the paramagnetic phase taken to set the FL very close to the saddle point of a 2D system of itinerant electrons. Based on first principles calculations, Hall *et al.* [3] find at the FL a sharp peak in the density of states characteristic of a 2D van Hove logarithmic singularity. We have also performed a full first principles calculation of the electronic structure of tetragonal paramagnetic $CeRhIn_5$ using the VASP code [14]. The generalized gradient approximation of Perdew *et al.* [15] for the exchange and correlation was adopted. The results for the experimental lattice parameters [16] are reported in Fig. 2. In Fig. 2(a) we observe, like Hall *et al.* [3], a sharp peak in the density of states near the Fermi level. In addition, in Fig. 2(b) we display the band structure at the vicinity of the Fermi level. We find a saddle point very close to the Fermi level whose dispersion along the z direction (R-X-R in the standard notation) is about 0.3 eV indicating the two-dimensional character of the saddle point singularity. Under these conditions we have, besides the Van Hove singularity in the density of states that favors superconductivity and magnetic order, an important kinematic restriction, namely $\varepsilon(k) = \varepsilon(k + Q)$, where $Q = (\pi/a, \pi/a)$ is the vector connecting two equivalent saddle points within the Brillouin zone. The above restriction determines the gapless nature of the spin-density wave (SDW) like in the charge-density wave (CDW) case proposed by Rice and Scott [17].

The SDW order parameter is given by

$$\gamma_\sigma = U \sum_k \langle c^\dagger_{k\sigma} c_{k+Q-\sigma} \rangle, \tag{8}$$

with $\gamma_\sigma = -\gamma_{-\sigma} = \gamma$. The resulting quadratic Hamiltonian is solved by a Bogoliubov transformation

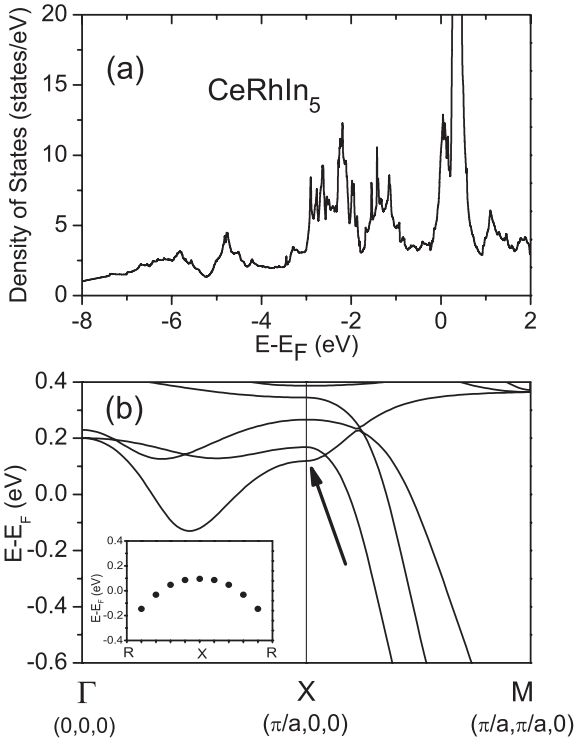

FIG. 2. Calculated electronic structure of paramagnetic $CeRhIn_5$. (a) Density of states and (b) band structure. The arrow indicates a saddle point singularity at the X point of the Brillouin zone. The inset shows the variation of the saddle point energy along the z R-X-R direction [it crosses the Fermi level at approximately the $(\pi/a, 0, 0.6\pi/c)$ point].

and the SC and SDW order parameters obtained self-consistently. The Hamiltonian eigenvalues are obtained by solving:

$$\begin{vmatrix} \varepsilon_k - E_k & -\gamma_\uparrow & -\Delta & 0 \\ -\gamma_\uparrow & \varepsilon_{(k+Q)} - E_k & 0 & -\Delta \\ -\Delta & 0 & \varepsilon_{-k} - E_k & \gamma_\downarrow \\ 0 & -\Delta & \gamma_\downarrow & \varepsilon_{-(k+Q)} - E_k \end{vmatrix} = 0.$$

The four solutions are $E_1 = -E_-$, $E_2 = -E_+$, $E_3 = E_-$, $E_4 = E_+$, where $E_\pm(k) = \sqrt{\varepsilon(k)^2 + \Delta^2} \pm \gamma$. Notice that for a 1D or 2D nested system $\varepsilon(k) = -\varepsilon(k+Q)$ and therefore $E_\pm(k) = \pm\sqrt{\varepsilon(k)^2 + \Delta^2 + \gamma^2}$.

The system is solved self-consistently for an effective half bandwidth at ambient pressure of W_0 and the phase diagram for $V = 4W_0$, $E_c = 0.7W_0$, $n = 0.92$ electrons and $U = 2.25W_0$, $U = 2.50W_0$, and $U = 2.75W_0$, is presented in Fig. 3. To simulate the effect of the pressure we have considered a linear variation of the bandwidth with the pressure and a bandwidth independent electron-electron interaction U. These assumptions have been found to be reasonable with a first principles calculation using the SIESTA code [18] taking Ni as a benchmark. Also, for simplicity, a constant V interaction and hole concentration independent of pressure are assumed. The results of our model agree qualitatively with the experimental findings depicted in Figs. 1 and 3(d). We indeed find a competition between SDW and SC but, as seen experimentally, they can coexist in a non-negligible region of the phase diagram. In addition, the SDW disappears abruptly when the two critical temperatures became equal, i.e., the SDW transition temperature cannot be lower than the superconducting one. This numerical result is similar to the analytical finding by Bilbro and McMillan [19] concerning superconductivity and martensitic transformation in A15 compounds.

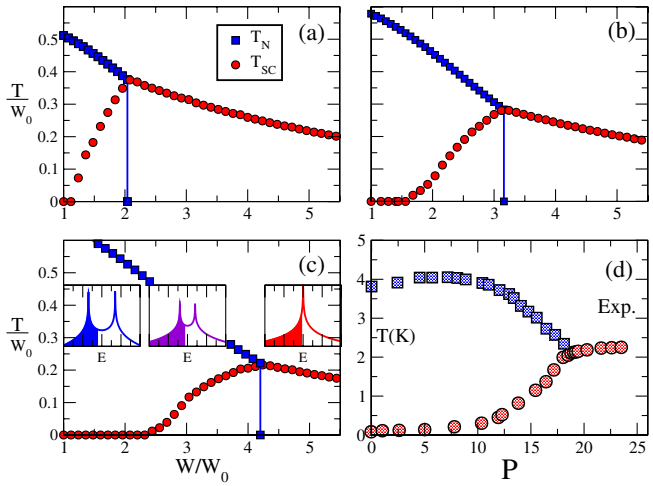

FIG. 3 (color online). Phase diagram (temperature versus pressure) obtained using the model Hamiltonian (1) and a two-dimensional band structure with the FL close to a saddle point. The variables are in units of the half bandwidth W_0. T_N and T_{SC} stand for the SDW and SC critical temperatures, respectively. Panels (a), (b), and (c) are the calculated results for the parameters given in the text and $U = 2.25W_0$, $U = 2.50W_0$, and $U = 2.75W_0$ respectively. The inset in panel (c) indicates the metallic DOS in the three (SDW, SDW + SC, and SC) different regimes. The shaded area indicates occupied levels. Panel (d) represents the experimental results of Ref. [9].

The proximity of the FL to a saddle point is an ingredient of model (1) necessary for the formation of the metallic SDW. We ask ourselves whether in $CeRhIn_5$ there is experimental evidence for such a proximity. A recent de Haas–van Alphen study [4] shows a divergence in the cyclotron mass at a pressure $P_{c2} \sim 2.4$ GPa, accompanied with a change in the quasi-2D Fermi surface. Those experiments were performed for values of magnetic fields and pressures in which the system is AFM. Following Park *et al.* P_{c2} is very close to the pressure at which T_N would extrapolate to zero in absence of SC (see upper inset in Fig. 4). The cyclotron mass in a 2D electronic system $m_c = (\hbar^2/2\pi)[\partial A(E)/\partial E]$ where A is the area enclosed in the isoenergetic contour line $E(k) = E$. Close to the 2D Van Hove singularity one expects the cyclotron mass to diverge logarithmically. Actually, the precise functional form has been computed in Ref. [20] and found to be

$$m_c = m_{c0}\left(C + D\ln\frac{E_{\mathrm{VHS}}}{|E_F - E_{\mathrm{VHS}}|}\right). \tag{9}$$

In a tetragonal crystal structure C and D are numbers nearly independent of the pressure and m_{c0} is the cyclotron mass at the bottom of the band. The divergence is driven by

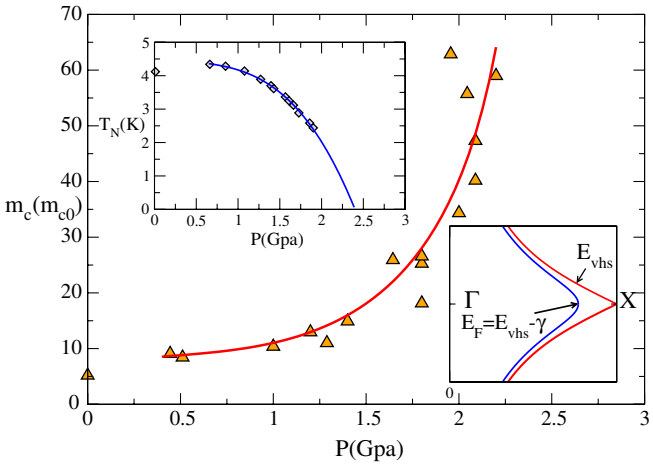

FIG. 4 (color online). Cyclotron mass (m_c) as a function of pressure. Triangles are the experimental values from Ref. [4] showing the m_c divergence close to $P \sim 2.4$ GPa, where the magnetic order disappears. The solid line is a fit to the theoretical model. Close to a Van Hove singularity the cyclotron 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. [6] (see upper inset).

the denominator in the argument of the logarithm which in our model is $E_F(\gamma) - E_{\mathrm{VHS}} \sim \gamma(P) \sim T_N(P)$. In other words, in model (1), m_c is enhanced as the AFM vanishes because the FL in the SDW approaches the saddle point at X (see the inset in Fig. 4). To elucidate if the experimental results are compatible with this argument and with expression (9), we have extracted the pressure dependence of T_N, fitting the experimental data in Ref. [6] (see upper inset in Fig. 4 to a cubic polynomial law in $(P_{c2} - P)$ in the range of pressures between $P = 0.65$ and $P = 2.4$ GPa. We do not attempt to justify physically this fit here, since our only goal is extracting an analytic expression for $T_N(P)$ for the range of pressures of interest, to insert it in (9). The results are presented in the main panel of Fig. 4. Our model reproduces reasonably well these experimental findings.

Within this model, we expect an anomaly in the specific heat at T_N, which is not associated to a SDW spectral gap but to the entropy released when the magnetic order disappears. The electronic part of the specific heat is

$$C_V^{e-} = -2\beta \sum_{i,k} E_i(k) \frac{\partial f_k}{\partial E_i(k)} \times \left(E_i(k) + \frac{\beta}{2\sqrt{\varepsilon(k)^2 + \Delta^2}} \frac{d\Delta^2}{d\beta} + \beta \frac{d\gamma}{d\beta} \right), \qquad (10)$$

where $i = 3, 4$. The second term inside the parenthesis gives the SC anomaly at T_C and the third term gives the antiferromagnetic anomaly at T_N. The SC anomaly is much weaker in the coexisting phase, because the FL lies in a depression of the density of states [see central graph on the panel (c) of Fig. 3] created by the underlying SDW, while in the purely SC phase the FL is very close to a divergence in the density of states (right graph). Remarkably, this enhancement has been also observed in calorimetric measurements on $CeRhIn_5$ [6].

To summarize: beyond the detailed boundary shape in the phase diagram of $CeRhIn_5$ we have identified two unequivocal, clear-cut features of the phenomenology of the $CeRhIn_5$ compound, namely; coexistence and abrupt disappearance of AFM when $T_N = T_{\mathrm{SC}}$. The essential ingredient in the model is the metallic SDW, favored for the proximity of Fermi level to a Van Hove logarithmic singularity in the density of states. The gapless nature of the SDW implies the lack of a metal-insulator transition at, or close to, T_N as shown by resistivity measurements. The kinematic conditions needed for the metallic SDW to be formed seem to be present in $CeRhIn_5$ as shown by the logarithmic divergence of the cyclotron mass.

We appreciate very much discussions with G. Gomez-Santos, H. Suderow, and S. Vieira. Financial support of the Spanish Ministry of Science (Ramon y Cajal contract and Grant No. BFM2003-03372) is acknowledged.

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