Antiferromagnetism and hot spots in CeIn$_3$

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Introduction. Interest to the phenomenon at quantum critical point (QCP) pervades the current literature on intermetallic compounds. Recently the effect of magnetic fields has been studied in the antiferromagnetic (AFM) CeIn$_3$. The magnetic QCP was found at $B_c = 6$ T. A strong mass enhancement was observed via the de Haas–van Alphen (dHvA) effect for the electron trajectories that cross or pass close to some "hot" spots at the Fermi surface (FS), has been reported and interpreted in terms of strong spin fluctuations at "hot" spots in the strong many-body interactions. It was noted that positions of these "hot" spots coincide with the positions of the necks protruding from the FS for non-magnetic LaIn$_3$. The necks would fall close to the boundary of the AFM Brillouin Zone (BZ) for CeIn$_3$ and must be described by even truncations due to electron reflections at the new BZ. The AFM propagation vector $Q = (\pm a)(1;1;1)$ connects opposite spots on the Fermi surface. Topological changes of the FS geometry near necks, known as the Lifshitz "2.5"-transitions, lead to weak singularities in them dynamics and transport properties. We show that at proper field directions this also affects the dHvA characteristics of "hot" spots.

We consider dHvA effect for the three main orientations in the cubic CeIn$_3$ or LaIn$_3$.

The mass enhancement was reported for two main orientations: B k (110) and B k (111). In the first case the extremal electron trajectory would run across the four necks on the FS. More detailed mass enhancements in Ref. [5] were performed for B k (111). In this case the extremal trajectory does not cross "hot" spots, but may run close if the necks' diameter is large enough. The dHvA mass enhancement at B k (110) when the electron trajectory passes far away from any "hot" spot provides the non-enhanced eective mass value $m_1 = 2.0 m_0$.

To start with, we explain in framework of a simple model, the larger masses for B k (111) by the electron trajectory proximity to the saddle points, where the dHvA eective mass has a logarithmic singularity. If the FS has necks, at certain orientations of the magnetic field the extremal cross-section electron trajectory passes through a saddle point (see Fig. 1).

Model calculations. We take a Fermi surface with axial symmetry along z-axis and narrow necks as shown in Fig. 1. For brevity we omit initially the effects of the AFM ordering and other spin effects on the "bare" electron dispersion chosen as (we set $\eta = 1$)

$$m(k) = 2m_1 + 2t_x [1 - \cos(k_y a)]; \quad (1)$$

where $k_{x,y,z}$ are the momentum components along $x,y,z$ axes and $t_x$ is the transfer integral along $z$ direction.

To describe the neck positions, the Fermi surface $m(k) = m_f$ is given by

$$(k_x^2 + k_y^2) = 2m_1 + 2t_x [1 + \cos(k_z d)] = \tilde{m}_1; \quad (2)$$

where $m_f = \tilde{m}_1$. The neck radius is $k_{neck} = \frac{\tilde{m}_1}{2m_1}$. In CeIn$_3$ and LaIn$_3$ the necks are narrow, $k_{neck} = 1$. The magnetic field $B = B_0$ ($\sin \phi; 0; \cos \phi$) in Fig. 1 directed at angle $\theta = 70.53$ with respect to the z-axis.
would simulate B k (111) in the cubic CeIn$_3$ where the extremal orbitals, as we shall see, run rather close to the other six "hot" spots but do not cross them. Rotate the x-z coordinate axes by the angle $\theta$ to make the direction of an antiferromagnetic edl along the $k_2^0$-axis:

$$
\begin{align*}
  k_x &= k_2^0 \cos \theta + k_1^0 \sin \theta \\
  k_z &= k_2^0 \sin \theta + k_1^0 \cos \theta 
\end{align*}
$$

The dispersion relation (4) in the new variables is:

$$
\begin{align*}
  \langle k^0 \rangle &= \langle k_2^0 \cos \theta + k_1^0 \sin \theta \rangle^2 + \langle k_2^0 \sin \theta + k_1^0 \cos \theta \rangle^2 = 2m_1_l \\
  + 2t_{c1} f 1 \cos (k_2^0 \sin \theta + k_1^0 \cos \theta) g_2
\end{align*}
$$

Electrons move along the quasi-classical trajectories of constant energy and constant $k_2^0$. In the diVA model, only the electron trajectories which encircle the extremal cross-sections $S_{\text{ext}} (k_2^0) = 0$ of the FS are important.

The effective electron mass is determined by:

$$
2 \left( k_2^0 \right)^2 = \frac{P \left( 2m_1 + 2t_{c1} \left[ \left[ 1 + \cos (k_2^0 d \sin \theta) \right] \right] \right)}{2m_1 \left( 1 + 2t_{c1} \left[ 1 + \cos (k_2^0 d \sin \theta) \right] \right)}
$$

and the integration limit $k_{\text{eq}} (\theta)$ is the solution of the equation $k_2^0 (k_{\text{eq}} (\theta)) = 0$. The extremal electron trajectory passes through the saddle point $S_{\text{ext}} (k_2^0) = 0$. The extremal trajectory runs along the saddle point if in addition to the Eqs. (4), the condition $k_2^0 (k_{\text{eq}} (\theta)) = 0$ is satisfied. From (4), one finds the critical tilt angle $\theta$ (for the necks at $k_{\text{eq}} (\theta) = 0$) corresponding to a jump of the diVA frequency. For lower the electron trajectory does not pass through the saddle point. At higher tilt angles the electron trajectory over the necks comes to the next BZ.

Consider the case of a narrow neck. Introducing $k_{\text{eq}} (\theta) = 0$ in Eq. (4), return in (4) to the integration over $k_2^0 : d k_2^0 = d k_2 \cos \theta$. Expanding $v_2 (k_2^0)$ near $k_{\text{eq}} (\theta)$ at close to $\theta = 0$, one obtains:

$$
\begin{align*}
  m (\theta) &= \frac{2}{d} \left( \frac{m_1}{t_{c1}} \right) 1^{\text{st}} Z \frac{d \pi}{2 + \frac{2}{d} \left( \frac{m_1}{t_{c1}} \right)}
\end{align*}
$$

where $m (\theta) = (2 \pi \left( \frac{m_1}{t_{c1}} \right) 1^{\text{st}} Z \frac{d \pi}{2 + \frac{2}{d} \left( \frac{m_1}{t_{c1}} \right)}}$ is logarithmically divergent as

$$
\begin{align*}
  m (\theta) &= (2 \pi \left( \frac{m_1}{t_{c1}} \right) 1^{\text{st}} Z \frac{d \pi}{2 + \frac{2}{d} \left( \frac{m_1}{t_{c1}} \right)}
\end{align*}
$$

For B k z-axis in Fig.1 the diVA oscillations in the model of Eq. (1) only measure the central ("belly") cross-section and the thickness of the "neck". Should we return to the cubic case and B k (111), the extremal trajectories cross none of the six "hot" spots in Fig.3 but numerically run rather close to them (the deviation of the trajectory from the center of the "hot spot" is given by $\theta = 19^\circ$). Thus, it becomes a question how broad are the necks to lead to a significance enhancement.

From the diVA data on LaIn$_3$ (Fig. 4 of Ref. [10]) we know the neck and "belly" cross-section areas: $k_{\text{neck}} a = 0.02$ and (for the spherical FS) as depicted by (diVA) $a = 0.02$. Taking the value $d = 1.0$ in Eq. (1), we find the cubic lattice, this gives $k_{\text{neck}} d = 0.03$ and $d = 0.06$. The saddle points in LaIn$_3$ appear at the angle $\theta = 58^\circ$. Hence, the necks in nonmagnetic LaIn$_3$ are too narrow to affect the diVA effects and mass for B k (111).

In CeIn$_3$ the "belly" radius $k_r$ is very close to the one in LaIn$_3$, while the neck cross-section area depends on the AFM order parameter and the value of magnetic edl in addition, the bands become spin split, see below). At edl $B = 15T$, the diVA frequency from the neck (the "belly") is about 3 times larger than in LaIn$_3$, while which would give $k_{\text{neck}} d = 0.55$ and $d = 0.10$. It is still rather far from the tilt angle $\theta = 19^\circ$ (however, according to Refs. [10]) the neck radius is considerably higher. Then the neck radius may reach and overpass the critical value $k_r = 1.0$ when $\theta = 0$ for the extremal orbit to pass through the saddle point at the edl B k (111). There are no data on the edl dependence of the neck radius in CeIn$_3$ so far.

If B is perpendicular to the plane in Fig.1 for our model (1), the extremal trajectory would run along the FS shown in Fig.1. The mass enhancement would be determined by the neck's width $m = 2m_1 \left( 1 + 2t_{c1} \left[ 1 + \cos (k_2^0 d \sin \theta) \right] \right)$. In the cubic CeIn$_3$ this would correspond to B k (111): four necks' singularities would provide strong mass enhancement, as stated in Ref. [11]. Strictly speaking, the diVA frequency for the (4) FS should be observable only at strong band splitting, as we discuss below.

CeIn$_3$ and other REIn$_3$. The FSs in CeIn$_3$ are now known in some detail. The two most remarkable features are comm on with nonmagnetic LaIn$_3$: 1) a practically spherical FS sheet (denoted as (diVA) LaIn$_3$) with the diameters in the k-space close to the AFM vector $Q = (-a/2; 1/2; 1/2)$ and "neck" extractions from FS sheet (4) toward an outer FS sheet. The diVA orbits and FS's for necks were labeled as (j); their sizes vary among the REIn$_3$ group [12]. A detailed analysis of the diVA oscillations from the electron-positron annihilation experiments in the paramagnetic phase of CeIn$_3$ and the localized character of the Ce electrons [13,14,15]. The moment $J = 5/2$ in the cubic environment is split into the quartet, $g$, and the Kramers' doublet $J = 7/2$; J is responsible for the AFM ordering in CeIn$_3$. The propagating vector $Q$, corresponds to the staggered magnetization, $S (Q)$, aligned antiferromagnetically perpendicular to the adjacent (111)
ferromagnetic plane. Magnetic anisotropy seems to be weak and is neglected in what follows.

CeIn$_3$ is a moderate HF material with the Somm erfeld constant $\gamma = 130$ mK. At an ambient pressure the Neel temperature is $T_N = 10$ K. The staggered magnetization is close to the value $0.71$ K expected for localized $\gamma$ doublet (see in Ref. [4]). The AFM state can be suppressed by applied pressure $P_c = 26$ kbar. In the vicinity of this pressure the existence of AFM order and superconductivity has been reported. The magnetic QCP in CeIn$_3$ was found at the CDW at $610$ K. As it was said above, the authors claim strong many-body effects at “hot” spots on the FS sheet (d).

AFM order in CeIn$_3$. For comm on antiferromagnets strong enough applied $\delta$ destroys the Neel state by aligning staggered moment parallel to the CDW. For CeIn$_3$ $T_N = 10$ K looks already rather low, so that one may attempt to apply the Landau mean-field approach.

$$F(T; B) = a(T; T_N) S^2 + h S + \frac{B^2}{2} S^2 + \frac{B^2}{2} S^2$$

(10)

where $S$ is the local spin component along the staggered magnetization vector (only terms independent of the crystal anisotropy left in Eq. (10)). From Eq. (10) the quadratic dependence on $T_N$ ($B = T_N$) immediately follows, reproducing the results in Ref. [4] with high accuracy. This agrees with the assumption that the magnetic anisotropy is indeed low. The dHvA mass for the $(110)$ sheet away from the Fermi surface is also rather low: $m = 2 m_0$. Therefore, we assume that AFM order and the phonon data studied in Ref. [4] are only weakly linked to other fundamental features of CeIn$_3$: i.e., the $(1)$ and $(4)$ FS pieces are weakly coupled to the Fermi electrons. Next question is whether one can explain $T_N = 10$ K for CeIn$_3$ via the RKKY mechanism with the help of $(1)$-sheet only. The dHvA signal of the $(1)$-sheet equals to the Q valley value and, hence, is not provided by the Fermi surface of the AFM. It is, also, important to demonstrate that RKKY interaction is zero. It is, also, known that paramagnets that paramagnetic effects in CeIn$_3$ are not dramatically different from the rest of REIn$_3$ family. From Ref. [10] it follows that $S = S_0$ at $T = 0$.

Energy spectrum near hot spots on non-zero $B$ and $\delta$. Introduce the exchange term $J S_1 S_2$ between itinerant and localized spins. This exchange leads to the RKKY interaction between localized spins. It can be estimated as $J = \gamma_0 T_N$, where $\gamma$ is the density of states at the Fermi level. Assuming that only the $(1)$-parts of the electron spectrum contribute to the RKKY interaction we obtain $J = 3000$ K. This gives $J = 170$ K. Therefore, at all $B$, $J = B$.

The effective magnetic field acting on electrons is

$$B_{\text{eff}} = B + JS_k$$

(11)

where $S_k$ is the local spins' component parallel to $B$. Let $S_1$ and $S_2$ be the two perpendicular (in absence of anisotropy) unit vectors of Pauli matrices for the directions of $S_1$ and $B$ correspondingly. Then with $\frac{Q}{Q} = \text{AFM propagation vector}$, the new energy spectrum in AFM phase is determined by two equations for the electronic states $k, k = Q$:

$$E_1 = \frac{k}{k + Q} + \frac{\mu B_{\text{eff}}}{2}$$

$$E = \frac{k + Q}{2} + \frac{\mu B_{\text{eff}}}{2}$$

(12)

Multiplying both equations by $k$ and excluding $k + Q$, one obtains the equation in the spin space:

$$E_1 S = \frac{k}{k + Q} + \frac{\mu B_{\text{eff}}}{2}$$

$$E = \frac{k + Q}{2} + \frac{\mu B_{\text{eff}}}{2}$$

(13)

The four energy branches from (13)

$$E_{k1} = \frac{k}{k + Q} + \frac{\mu B_{\text{eff}}}{2} + J^2 S^2$$

(14)

If the vector $Q$ exactly connects two opposite necks in Fig. 1, one obtains near the necks

$$E_{k1} = \frac{k}{k + Q} + \frac{\mu B_{\text{eff}}}{2} + J^2 S^2$$

(15)

Above $B_c$ the two branches go over into the Zeeman splitting with the effective field from Eq. (11) and $S_0 = 1$. For convenience, we normalize $Q_k = j + j = 1$. Then substituting Eq. (11) to (15) we obtain

$$E_{k1} = \frac{k}{k + Q} + \frac{\mu B_{\text{eff}}}{2} + J^2 S^2$$

(16)

The AFM order adds new features to the electron dispersion and the Fermi surface of the model. With signs $\text{sign}$ there are now two branches shown in Fig. 2. For the sign $(+)$ the dHvA experiment at $B > B_c$ would see the decrease of the peaks' width as compared to the bare spectrum (i.e., without AFM order). If $k^2 = 3m_1 < J$, these spins in the $(1)$-part of the FS are completely destroyed, as shown in Fig. 2, otherwise, these peaks would only be narrowed. For the sign $(-)$ the peaks' width increases due to AFM ordering.

The authors of Ref. [4] have used the width of the peaks $\approx 12$ of the orbit circumference. This is close to the data of Ref. [8] but disagree with the estimations of Ref. [8]. Using data of Ref. [8] we would get comparable to $J$. So, one may indeed relate the mass enhancement mechanism for $B_k$ (111) described above to the broadening of the gap between two outer $(+)$ trajectories in Fig. 2. This broadening depends on the magnetic field as described by Eq. (16). At $J = 170$ K and $B = 60T$ this term is $0.4J$. The estimates we have done for $J$ show that it is realistic to account for the observed mass enhancement at $B_k$ (111). On the other hand, we must repeat that there are no experimental data for a quantitative $t$ because so far no attempt has been made to account for the band splitting and the $\delta$ dependence of the dHvA frequencies corresponding to the orbitals on the Fermi surface (the necks).
Band splitting and the dHvA experiments. At high magnetic field (above \( B_c \)) the effective Zeeman splitting \( |\beta_j| = 1 \) results in the spin dependence of the energy spectrum and of the neck width. The Zeeman splitting makes the necks thicker for one spin component and thinner for the other, which leads to the spin-dependence of the effective mass, as mentioned above. This spin dependence can be observed for both (110) and (111) magnetic field directions. In particular, for the direction \( B_k (111) \) the saddle point logarithmic divergence of the effective mass is possible for only one spin component (sign (-) in Fig. 2). With further increase of magnetic field (assuming \( J > 0 \)), this spin component ceases to contribute to the dHvA signal with this frequency at all since the electron trajectories start to leave the (d)-sheet of the FS. This can be experimentally verified. At \( B_k (110) \) one expects similar behavior, except the (-) spin component at this field direction, ceases to contribute to old dHvA frequency at lower \( B < B_c \) than at \( B_k (111) \). At \( B < B_c \) the splitting of the energy spectrum remains, but now \( \beta_j = 1 \). Though, in Ref. 3 the spin dependence (or the band splitting) of the effective mass was not studied, it has been observed rather definitely in CeIn₃ under pressure.

More remarkable effect for \( B_k (110) \) is that the two signs in Eq. 13 would correspond to two different dHvA frequencies. If one of the necks is broken (sign (+) in Fig. 2), one of the dHvA frequencies corresponds to the trajectory encircling the (d)-sheet of the FS. If the utmost importance are the dHvA experiments measuring explicitly the frequency (les) from the trajectories on the FS as a function of the field (for \( B_k (111) \), i.e. along the direction of the neck), that would conf use the whole band structure of the AFM CeIn₃, constructed in this paper.

To summarize, by making use of the peculiar shape of the energy spectrum of CeIn₃ in terms of spherical (d) and neck-like (\( \parallel \)) Fermi surfaces, we have constructed the full (T-B) phase diagram for antiferromagnetism in this compound in agreement with the experiments. We have analyzed the interplay between antiferromagnetism and external magnetic field at the neck positions and semiquantitatively explained the observed enhancement of the electron effective mass at the so-called "hot spots". We have phasified the magnetic phase transition between magnetic CeIn₃ and normal CeAl₃. It was our intention to show that the details of the Fermi surface topology are important for CeIn₃, although the magnetic quantum criticality in other heavy fermion materials may bear the universal character. A few straightforward experiments are suggested to verify the above ideas.

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