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Fermi surface of $CePt_2In_7$: A two-dimensional analog of $CeIn_3$

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We report magnetic quantum oscillations in magnetic fields extending to ∼60 T in single crystals of the body-centered tetragonal antiferromagnet $CePt_2In_7$—recently discovered to exhibit pressure-induced superconductivity at $T_c \approx 2.1$ K. Despite the two-dimensionality of its Fermi surface, the microscopic electronic properties of layered $CePt_2In_7$ are revealed to be more similar to those of cubic $CeIn_3$ than those of layered $CeRhIn_5$. A significant field-induced change in the Fermi surface occurs below $H_m \approx 45$ T in both $CePt_2In_7$ and $CeIn_3$, where it is broken into small pockets with field-dependent effective masses—signaling partial 4*f*-electron involvement in the Fermi surface for $H < H_m$. Since $CePt_2In_7$ and $CeIn_3$ differ only in the dimensionality of their Ce sublattices, an ideal pair of compounds for investigating the effect of dimensionality on superconductivity is realized.

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The series of compounds composed of $CeIn_3$ building blocks (e.g., see Fig. 1) provides a laboratory for studying the effects of dimensionality on the interplay between antiferromagnetism and unconventional superconductivity.[1–5] While pressure-induced superconductivity occurs at a low temperature of $T_c \approx 0.2$ K in cubic $CeIn_3$,[1] this increases to ≈2.1 K in layered $CeRhIn_5$ (Ref. 2) (or ≈2.3 K in $CeCoIn_5$ at ambient pressure[3]). Reduced dimensionality of the Fermi surface and the spin fluctuation spectrum are two factors that are believed to enhance unconventional superconductivity. The former increases the likelihood of nesting-type magnetic instabilities[6] while the latter increases the likelihood of abrupt changes in the degree to which f electrons participate in the Fermi surface volume occurring under pressure and/or magnetic field.[7] A true test of the effect of dimensionality requires a controlled experiment in which the Ce lattice is changed from three dimensional (3D) to two dimensional (2D) while leaving other aspects of the electronic structure unchanged. $CeRhIn_5$ (Ref. 2) was thought to realize this objective as a layered quasi-2D variant of $CeIn_3$, but has since been shown[8–11] to exhibit differences in electronic structure from $CeIn_3$—notably in the degree to which the 4*f* electrons participate in the Fermi surface.

In this Rapid Communication, we report magnetic quantum oscillation measurements on antiferromagnetic body-centered tetragonal $CePt_2In_7$ (Ref. 12)—a pressure-induced layered superconductor exhibiting a comparable transition temperature (≈2.1 K at 3.5 GPa) to layered $CeRhIn_5$. We find that the increased separation between the CeIn layers of $CePt_2In_7$ relative to $CeRhIn_5$ (Ref. 13) (see Fig. 1) leads to an increased two-dimensionality of the Fermi surface topology. In contrast to $CeRhIn_5$, however, quantum oscillations originating from the large conduction-electron-like sections of Fermi surface in $CePt_2In_7$ (exceeding the magnetic Brillouin zone in size) are strongly suppressed below a magnetic-field-induced transition (or crossover) at $\mu_0 H_m \approx 45$ T (for $H \| c$). A plethora of small closed Fermi surface pockets exhibiting field-dependent effective masses are observed below H_m. The close similarity to magnetic-field-dependent effects seen in cubic $CeIn_3$ (Refs. 9,10) suggests that $CePt_2In_7$ comes closer to realizing a 2D analog of $CeIn_3$. We discuss the origin of this similarity and the implications for the relationship between dimensionality and superconductivity in Ce compounds.

Magnetic quantum oscillations are measured using the contactless conductivity technique,[14] which has recently been utilized to probe Fermi surface reconstruction in high-T_c cuprates[15] and pnictides.[16] Single-crystalline platelets of $CePt_2In_7$ of dimensions $\approx 0.7 \times 0.7 \times 0.2\ \mathrm{mm}^3$ are selected and attached to a coil of a few turns that forms part of a tunnel-diode oscillator (TDO) circuit resonating at ≈46 MHz. Magnetic fields of up to 60 T are provided by a pulsed magnetic field system, with the sample and coil rotated *in situ* so as to change the angle θ between the magnetic field H and the crystalline c axis. Temperatures in the range ∼0.5 to 12 K are obtained by controlling the vapor pressure of ^{3}He or ^{4}He liquid, or by use of a heater in He gas. Radio-frequency techniques are sensitive to magnetic quantum oscillations and to phase transitions (or crossovers) affecting the electrical resistivity and/or magnetic susceptibility in strong magnetic fields.[14]

At $H = 0$, the Néel transition of $CePt_2In_7$ ($T_N \approx 5.6$ K)[12] is discernible as a kink in the temperature dependence of the TDO resonance frequency shift Δf as shown in the inset to Fig. 2(a)—mostly reflecting changes in the sample skin depth. This feature is dwarfed in magnitude, however, by an inflection point in Δf that occurs at $\mu_0 H_m \approx 45$ T in Fig. 2. The presence of the inflection point at both $T < T_N$ and $T > T_N$ in Fig. 2(a) suggests that H_m originates from an underlying change in the electronic structure distinct from the antiferromagnetic transition. Here, we compare H_m with a similar feature reported at the same field in $CeIn_3$,[17] above which the f electrons have been shown to become entirely decoupled from the Fermi surface[10,19] [occurring well below the antiferromagnetic critical field $\mu_0 H_c \approx 60$ T in $CeIn_3$ (Ref. 18)]. Support for such an interpretation in $CePt_2In_7$ is found on comparing quantum oscillation measurements in each of these materials.

Concentrating initially on the region $H > H_m$ in Fig. 3, the Fermi surface properties of $CePt_2In_7$ can be seen to be similar to those found in other magnetic Ce compounds. Reflecting the behavior of $CeIn_3$,[9] $CeRhIn_5$,[20–22] $CeRu_2Si_2$,[25] and CeB_6 (Ref. 26) in strong magnetic fields, the Fermi surface of $CePt_2In_7$ is found to correspond closely to electronic

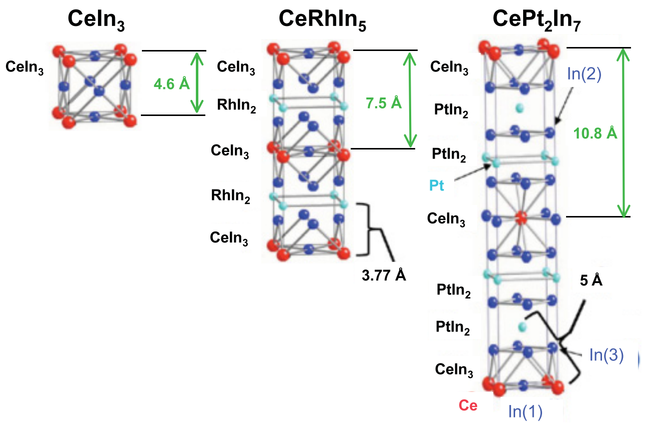

FIG. 1. (Color online) Schematic crystal structures of $CeIn_3$, $CeRhIn_5$, and $CePt_2In_7$ with interlayer spacings indicated.

structure calculations in which the 4f electrons are confined mostly to their atomic cores[12] [see Fig. 3(c)]. As in $CeIn_3$ and $CeRhIn_5$, multiple large sections of Fermi surface are observed in $CePt_2In_7$, yielding quasiparticle effective masses [see Figs. 3(a) and 3(b)] several times heavier than corresponding band masses that are essentially independent of the magnetic field. Mass enhancements of this size are typical for systems in which the 4f electrons are polarized and mostly decoupled from the conduction-electron bands in very strong magnetic fields.[27] On the other hand, the high degree of two-dimensionality [see Fig. 3(c)] of the Fermi surface of $CePt_2In_7$—likely resulting from the large separation between CeIn layers (see Fig. 1)—represents a significant point of departure from those in other Ce compounds. Several large sheets of Fermi surface are observed to have nearly ideal cylindrical forms, yielding θ-dependent magnetic quantum oscillation frequencies that vary approximately as $F \propto 1/\cos\theta$ [see Fig. 3(c)].

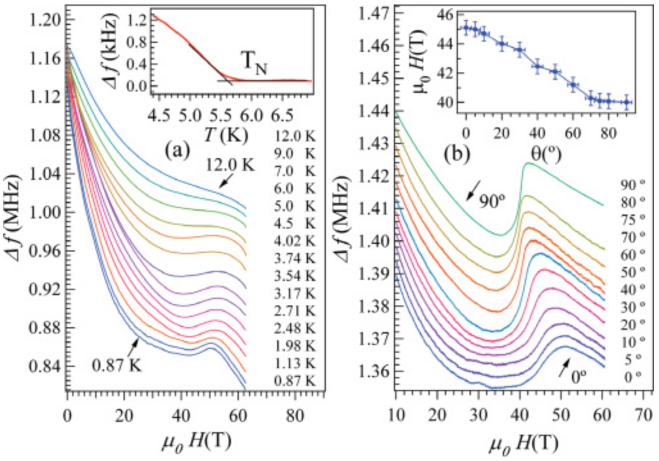

FIG. 2. (Color online) (a) Magnetic-field dependence of the change in resonance frequency Δf of the TDO oscillator for a sample of $CePt_2In_7$ with H oriented along the c axis, revealing an inflection point at $\mu_0 H_m \approx 45$ T that becomes weaker with increasing T as indicated. The inset shows Δf as a function of T at $H = 0$, evidencing T_N. (b) Δf as a function of field at $\approx$0.5 K for different angles θ between H and the c axis. The sample is rotated from H along [001] to [100]. The inset shows the angular dependence of H_m.

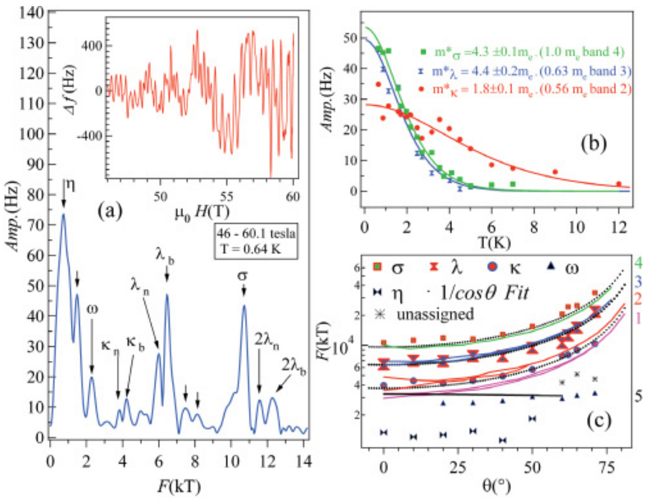

FIG. 3. (Color online) (a) Fourier transform (noise floor ∼5 Hz) of the oscillations in $CePt_2In_7$ for $H > H_m$ with the raw data (after background polynomial subtraction) shown in the inset, revealing different frequencies and harmonics corresponding to large Fermi surface sections. The harmonic ratio ($A_2/A_1 \sim e^{-\pi/\omega_c\tau}$) of λ suggests $\omega_c\tau \sim 4$—too large for the strong suppression of the high frequencies below ∼45 T to be attributed only to disorder. The peaks around 8 kT likely correspond to harmonics of κ. Subscripts "n" and "b" refer to proposed minimum "neck" and maximum "belly" cross sections of warped Fermi surfaces. (b) T dependences of the prominent peaks with fits to the Lifshitz-Kosevich T dependence $R_T = X/\sinh X$ (where $X = 2\pi^2 m^* k_B T/\hbar e B$), yielding effective masses as indicated (Ref. 29). Band masses are shown in parentheses. (c) θ dependence of the prominent Fourier peaks, where θ is the angle between H and the c axis. Solid lines correspond to electronic structure calculations in which the 4f electrons are confined to their atomic cores (Ref. 12), shown in Fig. 5(a) (the bands being labeled 1, 2, . . . ,5), while dotted lines represent $F \propto 1/\cos\theta$ fits indicating consistency with 2D Fermi surface sheets. We associate κ with bands 1 and/or 2 and λ, σ, and ω with bands 3, 4, and 5, respectively. η may correspond to the kidney-shaped section (not shown here owing to its relatively small cross section $\approx 0.5 k_B T$) from band 5 [near the edge of the Brillouin zone in Fig. 5(a)]—its small size making it sensitive to details of the band structure model.

Quite a different picture of the Fermi surface of $CePt_2In_7$ emerges on considering the low-magnetic-field regime ($H < H_m$ in Fig. 4). Signals from the large conduction-electron sections of Fermi surface are strongly suppressed, giving way instead to a plethora of low frequencies. Consistent with a change in electronic structure, the oscillations can be seen to become attenuated as the field $H_m \approx 45$ T is approached from both above and below H_m in Figs. 3 and 4. Below H_m [see Fig. 5(b)] the effective masses of several Fermi surface sections are found to be magnetic-field dependent.

Were the layered structures in Fig. 1 an important factor in determining the f-electron contribution to the Fermi surface, we would expect the greatest degree of similarity to exist between $CePt_2In_7$ and $CeRhIn_5$. However, the evidence presented in Figs. 4 and 5 suggests very different behaviors for these two compounds. Unlike $CePt_2In_7$, $CeRhIn_5$ undergoes no significant change in its electronic structure upon varying the magnetic field. No inflection in Δf is observed in $CeRhIn_5$, nor are the effective masses observed to be magnetic-field

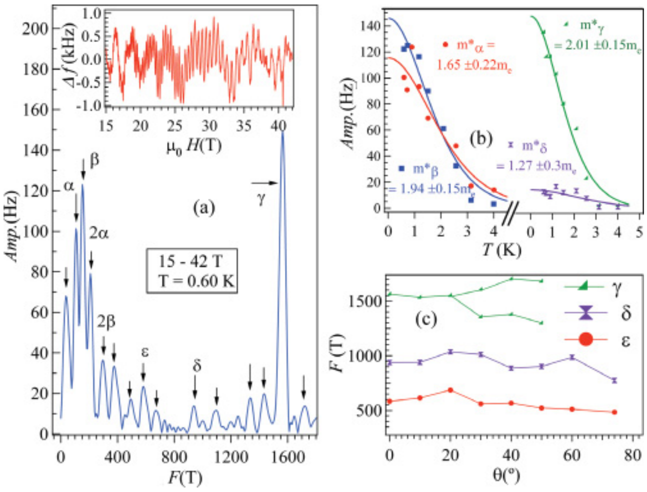

FIG. 4. (Color online) (a) Fourier transform (noise floor ∼5 Hz) of the magnetic quantum oscillations observed in $CePt_2In_7$ for $H < H_m$ with the actual oscillations (after background polynomial subtraction) shown in the inset, revealing a plethora of frequencies corresponding to multiple small Fermi surface pockets. Only frequencies easily isolated as a function of T and/or θ are labeled. The peaks labeled α and β are poorly resolved (and their harmonics tentatively labeled), and so cannot be unambiguously identified with separate sets of oscillations. (b) The measured T dependences of the prominent Fourier peaks together with fits to the Lifshitz-Kosevich T dependence term R_T so as to extract their quasiparticle effective masses. (c) Field-angle dependence of the prominent Fourier peaks.

dependent.[13,20] Indeed, $CeRhIn_5$ is often regarded as being ideally representative of a Kondo lattice system (with integer valence[28]) in which the f electrons do not participate in the Fermi surface volume once the f moments are antiferromagnetically coupled[13,20] or polarized in strong magnetic fields.[19,24] Characteristic of such Kondo lattice behavior is the continued observation of conduction band orbits in weak magnetic fields,[13,19,20] in contrast to $CePt_2In_7$ and $CeIn_3$.

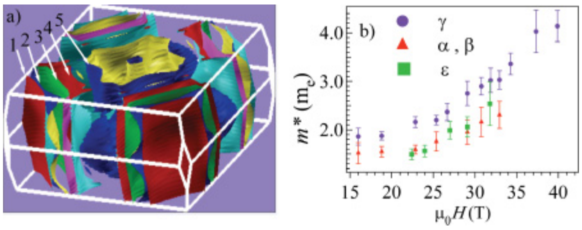

FIG. 5. (Color online) (a) Fermi surfaces sheets labeled 1,2, . . . ,5 from the band calculation in Ref. 12. Here, the Fermi surface is presented in the body-centered tetragonal Brillouin zone for which the unit cell contains one Ce atom. (b) H dependence of the effective masses for $H < H_m$ obtained by performing Fourier transforms over reduced intervals in H. In the case of the α and β orbits, separate frequencies cannot be resolved upon reduction of the H interval, causing the fitted value to be a mixture of α and β, which have similar effective masses in Fig. 4(b).

On comparing all three compounds, the greatest degree of similarity exists between $CePt_2In_7$ and pure $CeIn_3$, which are at the opposite extremes of interlayer separation in Fig. 1. Both compounds undergo qualitatively similar inflections in f at similar values of the magnetic field[17] (i.e., H_m), and both undergo a breakup of the Fermi surface topology below H_m with little evidence for magnetic breakdown tunneling across the gaps associated with antiferromagnetic ordering. The emergence of new frequencies with field-dependent effective masses together with the strong attenuation of signals originating from the large conduction-band-like Fermi surfaces at low fields in both $CePt_2In_7$ and $CeIn_3$ are consistent with an increased f-electron participation in the Fermi surface.

The existence of heavy and field-dependent effective masses in antiferromagnetic $CeIn_3$ has been attributed to its weak mixed valence (i.e., with a $4f$-electron occupancy of $n_f \approx 0.97$),[10] in which the $4f$ electrons contribute small pockets of holes to the Fermi surface inside the antiferromagnetically ordered phase below H_m.[9,10,19] Immediately preceding depopulation of the small f pockets at H_m, a strong field-induced upturn in their effective mass is observed in $CeIn_3$.[10] Residual hybridization (permissible within the antiferromagnetic phase in a mixed-valence picture) is believed to be responsible for field-dependent masses being seen on neighboring conduction band Fermi surface sections—the "hot spots" in Ref. 18 being a notable example. While the base temperature of the ^{3}He refrigerator limits the maximum observable m^* in $CePt_2In_7$, the field-induced upturn in m^* found for several orbits followed by the disappearance of these orbits above H_m mirrors the behavior observed in $CeIn_3$ under similar experimental conditions.[9,18] Such similarities signal a partial f-electron participation in the Fermi surface of $CePt_2In_7$ for $H < H_m$ that ceases once $H > H_m$. Sections α and β provide possible candidates for f-electron pockets in $CePt_2In_7$. Their Fermi velocity $v_F = \sqrt{2e\hbar F}/m^* \approx 2 \times 10^4$ ms^{-1} (at 33 T) is found to be significantly lower than that $v_F \approx 1.5 \times 10^5$ ms^{-1} of the regular conduction band sections in the high-field regime ($H > H_m$).

While hybridization between the $4f$ and conduction electrons is important in all of these materials, one structural factor that causes $CeRhIn_5$ to stand out from the other two systems and which may cause f-f hopping to be superseded by hybridization, is the close proximity between the $4f$ sites and the transition metal ion M (where M = Rh in the case of $CeRhIn_5$).[12] The interlayer Ce-M separation of 3.8 Å is comparable to the Ce-Ce separation of 3.6 Å in $CeRhIn_5$, implying that the hybridization between the $4f$ electrons of Ce and the $4d$ electrons of Rh is of similar importance to f-f hopping within the CeIn layers.[12] In $CePt_2In_7$, by contrast, the interlayer Ce-M separation is increased to 5.0 Å, implying that hybridization between the $4f$ and $5d$ electrons is relatively unimportant.[12] The resulting likeness of the local crystalline environment of the $4f$ electrons in $CePt_2In_7$ to that in cubic $CeIn_3$ could be a factor in causing their electronic properties to be similar—i.e., both exhibit magnetic-field-dependent Fermi surfaces below a characteristic field H_m that is the same in the two compounds and only weakly anisotropic with respect to the orientation of the field in $CePt_2In_7$ [see Fig. 2(b)].

Of all the layered Ce compounds exhibiting superconductivity, $CePt_2In_7$ therefore comes closest to realizing a 2D analog of a 3D compound—in this case $\mathrm{CeIn_3}$. *f*-electron Fermi surface participation is similar to the extent that both $\mathrm{CePt_2In_7}$ and $\mathrm{CeIn_3}$ exhibit field-dependent effective masses followed by an abrupt change in the electronic structure at the same field. These similarities may be linked to the negligible hybridization between the 4*f* electrons of Ce and 5*d* electrons of Pt in $\mathrm{CePt_2In_7}$.[12] Given the enhancement of fluctuations often found in low-dimensional materials, one intriguing possibility therefore is that dimensionality is the single most important factor in elevating the superconducting transition temperature of $\mathrm{CePt_2In_7}$ relative to $\mathrm{CeIn_3}$.

While reduced dimensionality is also likely to be the dominant reason for the increase in T_c from $\mathrm{CeIn_3}$ to $\mathrm{CeRhIn_5}$, we can now appreciate that attempts to understand the microscopic origins for this increase have been complicated by differences in hybridization with M affecting the electronic structure. Our study shows that this complication does not exist between $\mathrm{CePt_2In_7}$ and $\mathrm{CeIn_3}$, enabling future experiments to more accurately target the microscopic mechanism by which reduced dimensionality causes an order of magnitude increase in T_c over that in $\mathrm{CeIn_3}$.

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