

Pressure-induced Lifshitz transition in CsV_3Sb_5 evidenced by the quantum oscillation measurements

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CsV_3Sb_5 exhibits a unique double-dome superconducting phase diagram under pressure, closely linked to its distinctive charge density wave (CDW) order evolution and corresponding Fermi surface reconstruction. The intricate interplay between CDW and superconductivity has garnered significant research interest, particularly in finding experimental methods to investigate Fermi surface evolution under pressure. Here, by measuring the quantum oscillation signals in in-plane resistivity and thermoelectric effect of CsV_3Sb_5 at various pressures, we reveal for the first time that the Fermi surface of CsV_3Sb_5 undergoes an abrupt change around 0.4 GPa. This phenomenon may be associated with alterations in the interlayer modulation within the CDW state, which is consistent with our density functional theory calculations. Furthermore, we observe the presence of a Dirac band that may move away from the Fermi energy as pressure increases. Our findings offer crucial insights into the Fermi surface evolution of CsV_3Sb_5 under pressure.

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I. INTRODUCTION

AV_3Sb_5 ($A = \text{K}, \text{Cs}, \text{and Rb}$) is a representative kagome family material [1], where vanadium atoms form a perfect kagome lattice. All members of this family host a three-dimensional (3D) charge density wave (CDW) coexisting with the superconductivity [2–9]. The CDW manifests as a 2×2 superlattice in the kagome ab plane [8–11] with c -axis modulations [7,9,12], reducing the in-plane rotational symmetry from sixfold to twofold, and the electronic nematicity was discovered below 40 K [6]. In addition, evidence of time-reversal symmetry breaking (TRSB) below the CDW transition has been observed, including a giant anomalous Hall effect [13,14], chirality tunable by an external magnetic field [7], and the emergence of spontaneous internal magnetic fields [5,15]. As the temperature decreases, superconductivity emerges inside the CDW order with a critical temperature 0.9–2.5 K. Rotation symmetry breaking and TRSB are also

observed to persist into the superconducting state [3,5,6,8,16], which is believed to be related to a series of unconventional features, such as a pair-density wave [8] and twofold rotational symmetry [16], indicating that the CDW is intertwined with superconductivity in an intriguing way.

While AV_3Sb_5 materials share 3D CDW and low-temperature superconductivity (SC), their CDW structures and SC states vary significantly. $(\text{K}, \text{Rb})\text{V}_3\text{Sb}_5$ shares a common CDW structure characterized by trihexagonal (TrH) in-plane distortions that stack along the c axis, forming a $2 \times 2 \times 2$ supercell [17–19]. In contrast, the CDW state of CsV_3Sb_5 is more complex and controversial. Many x-ray diffraction (XRD) studies have reported $2 \times 2 \times 2$ supercells, $2 \times 2 \times 4$ supercells, and the coexistence of these structures [10,17,20–23], suggesting that the CDW structure is sample dependent. These structures are close in energy and compete with each other, so that external perturbations such as chemical disorder [24], thermal history [21,22], and mechanical deformation [25] can effectively modulate the CDW patterns.

In terms of superconducting properties, CsV_3Sb_5 has the highest superconducting transition temperature ($T_c \sim 2.5$ K) among the AV_3Sb_5 materials at ambient pressure, which is much higher than the $T_c \sim 0.9$ K for $(\text{K}, \text{Rb})\text{V}_3\text{Sb}_5$ [1]. By increasing pressure, its CDW is rapidly suppressed and completely disappears at 2 GPa, while its SC exhibits a double-dome behavior with maxima at $P_1 \sim 0.7$ GPa ($T_c \sim 7$ K) and $P_2 \sim 2$ GPa ($T_c \sim 8$ K) [26,27]. The suppression of the CDW order by applying pressure is a

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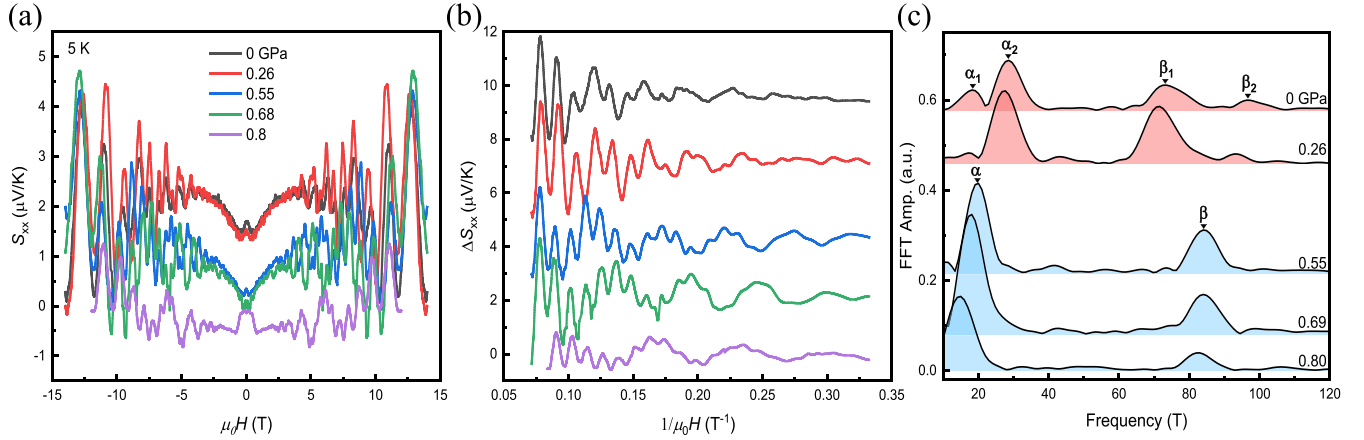


FIG. 1. (a) The thermoelectric power S_{xx} of CsV_3Sb_5 measured under external magnetic field applied along c axis at $T=5$ K and at different pressures. (b) The oscillatory component ΔS_{xx} as a function of $1/\mu_0 H$ at $T=5$ K and at different pressures. The ΔS_{xx} data are extracted by subtracting a polynomial background from the S_{xx} results shown in panel (a). (c) The FFT spectra in the range of 10–120 T extracted from the oscillation data in panel (b). At pressures below 0.4 GPa, the FFT spectra reveal four distinct frequencies, represented by Greek letters α_1 , α_2 , β_1 , and β_2 , respectively. These four frequencies evolve into two frequencies at pressures above 0.4 GPa, which are assigned by the Greek letters α and β , respectively. The data in panels (b) and (c) have been shifted vertically for clarity.

common feature of all AV_3Sb_5 materials [28,29], whereas the double-dome SC behavior is unique to CsV_3Sb_5 . The rich pressure-superconducting phase diagram of CsV_3Sb_5 is closely related to its unique CDW order evolution and corresponding Fermi surface reconstruction. The emergence of a stripelike or incommensurate CDW was believed to be related to the suppression of superconductivity and the appearance of the first superconducting maximum. Previous high-pressure single-crystal XRD study reveals that the CDW phase undergoes a transformation around $p \sim 0.7$ GPa from a 2×2 pattern to a long-range ordered modulation characterized by the commensurate modulation vector $\mathbf{q} = (0, 3/8, 1/2)$, which is aligned with inferred changes in the CDW pattern from high-pressure nuclear magnetic resonance spectroscopy studies [30–32]. The pressure-induced CDW structure modulations correlate with two peaks in the superconducting transition temperature as pressure changes, suggesting that the rich pressure-superconducting phase diagram of CsV_3Sb_5 is closely related to its unique CDW order evolution.

Understanding these phenomena requires experimental insight into the Fermi surface evolution under pressure. Traditional surface-sensitive methods such as angle-resolved photoemission spectroscopy (ARPES) and scanning tunneling microscopy (STM) are incapable for the high-pressure experiments. Fortunately, quantum oscillation measurements, which can be used to extract information such as the extremal area of Fermi surfaces, quasiparticle effective mass, and topological properties of the band structure, are an effective means to infer the Fermi surface of CsV_3Sb_5 under high pressure. In this work, we investigate the quantum oscillation signals in in-plane resistivity (ρ_{xx}) and the thermoelectric effect (Seebeck coefficient S_{xx} and Nernst S_{xy}) of CsV_3Sb_5 under various pressures, accompanied by density functional theory (DFT) calculations. Our results show for the first time that frequency spectra of CsV_3Sb_5 obtained by fast Fourier transform (FFT)

analysis change significantly above 0.4 GPa, which may be related to the change of interlayer modulation in the CDW state. Additionally, we observe a Dirac band that moves away from the Fermi surface with increasing pressure, which may be related to the rapidly increment of T_c with pressure below P_1 . These findings provide direct experimental evidence for understanding the evolution of electronic structure under pressure, fill the gap that conventional surface-sensitive techniques such as ARPES and STM cannot be used for high-pressure studies, and provide experimental support for theoretical computational models of kagome superconductors under high pressure.

II. RESULTS AND DISCUSSION

Figure 1(a) shows the thermoelectric power S_{xx} of CsV_3Sb_5 measured under a magnetic field applied along c axis at $T=5$ K, with pressures ranging from 0.1 to 0.8 GPa. Pronounced quantum oscillations can be observed in all data. The S_{xx} curve exhibits a distinct mustache-shaped profile near zero field, which is consistent with previous reports and can be explained by a multiband model [33]. As pressure increases, the superconducting transition temperature of CsV_3Sb_5 increases, causing the thermoelectric power to drop to zero near zero field, which obscures the mustache-shaped feature. Since thermoelectric power and Nernst are determined by the energy derivative of the electrical conductivity tensor in the vicinity of the Fermi energy, it is highly sensitive to changes in the Fermi surface. Notably, a large difference in the zero field S_{xx} value is observed as the pressure increases from 0.26 to 0.55 GPa, and there is also an obvious change in the high-field slope of the Nernst signals (see Fig. S1(a) of the Supplemental Material [34]), which potentially indicates a change in the band structure within this pressure range.

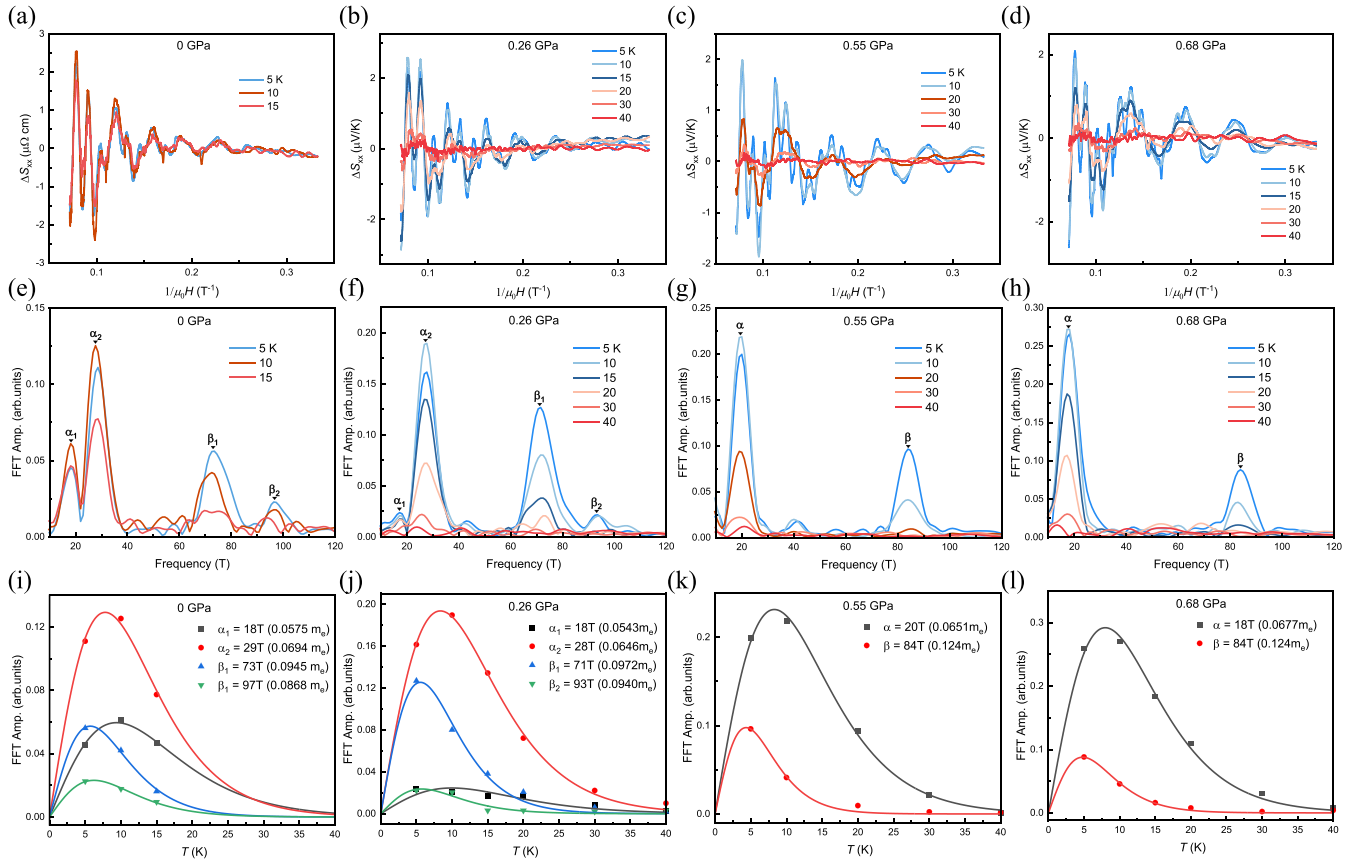


FIG. 2. (a)–(d) The oscillatory component ΔS_{xx} as a function of $1/\mu_0 H$ at different temperatures and pressures. (e)–(h) The FFT spectra in the range of 10–120 T extracted from the oscillation data in panels (a)–(d). The dominant frequencies are labeled with Greek letters, and the amplitudes extracted from these frequencies are plotted in panels (i)–(l) as a function of temperature. The solid curves represent the best fit to the data using the derivative of the LK formula. The quasiparticle effective masses estimated using the derivative of the LK formula are shown in the upper right corner of panels (i)–(l), respectively.

By subtracting a polynomial background, we can extract the oscillatory component ΔS_{xx} as a function of $1/\mu_0 H$ at $T = 5$ K under varying pressures, as shown in Fig. 1(b). The oscillation pattern presents periodic characteristics but exhibit complex periodic behavior, indicating the contributions of several frequency components. We used the FFT to separate these frequencies in the range of 10–120 T, and the results are displayed in Fig. 1(c). At pressures below 0.4 GPa, the FFT spectra reveal four distinct frequencies, represented by Greek letters α_1 , α_2 , β_1 , and β_2 , respectively. At ambient pressure, these four frequencies are located at 18, 29, 73, and 97 T, respectively, which is similar to the previous studies [10,26,40]. According to the Onsager relation $F = (\hbar/2\pi e)A_F$ [41], we can estimate the extremal orbits area A_F of the Fermi surfaces. The obtained values are very small, which only occupy 0.11%, 0.18%, 0.46%, and 0.61% of the whole area of the first Brillouin Zone in the k_x – k_y plane (taking $a = 5.4949$ Å [1,2]), respectively. As the pressure increases above 0.4 GPa, these four frequencies evolve into two frequencies, which are assigned by the Greek letters α and β , respectively. This phenomenon is also observed in the Nernst signals, as shown in Fig. S1(c) of the Supplemental Material [34], hinting for a Lifshitz transition under pressure.

Figures 2(a)–2(d) show the temperature-dependent oscillatory components ΔS_{xx} at different pressures, and the raw S_{xx} data without subtracting a polynomial background are shown in Fig. S2 of the Supplemental Material [34]. Figures 2(e)–2(h) display the corresponding FFT spectra. The temperature dependence of the amplitudes extracted from the dominant frequencies labeled by Greek letters is plotted in Figs. 2(i)–2(k). The oscillation of ΔS_{xx} can be described by the derivative of Lifshitz-Kosevich (LK) formula [42,43]. R_T is the only temperature-dependent damping factor in the amplitude term of the derivative of LK formula. By utilizing R_T to fit the temperature dependence of the FFT peak amplitudes of ΔS_{xx} , we can extract the effective mass. The expression for R_T is

$$R_T = \frac{(\alpha X) \coth(\alpha X) - 1}{\sinh(\alpha X)}, \quad (1)$$

where $\alpha = 2\pi^2 k_B / e\hbar \approx 14.69$ T/K and $X = m^* T / B_{\text{eff}}$. Here, m^* represents the quasiparticle effective mass in unit of free electron mass m_e and B_{eff} is the magnetic flux density. In the nonmagnetic material CsV₃Sb₅, $B_{\text{eff}} \approx \mu_0 H_{\text{eff}}$. The effective field over the field window of the FFT is given by $\frac{1}{\mu_0 H_{\text{eff}}} = \frac{1}{2} \left(\frac{1}{\mu_0 H_{\text{min}}} + \frac{1}{\mu_0 H_{\text{max}}} \right)$. The solid curves in Figs. 2(h)–2(k) show

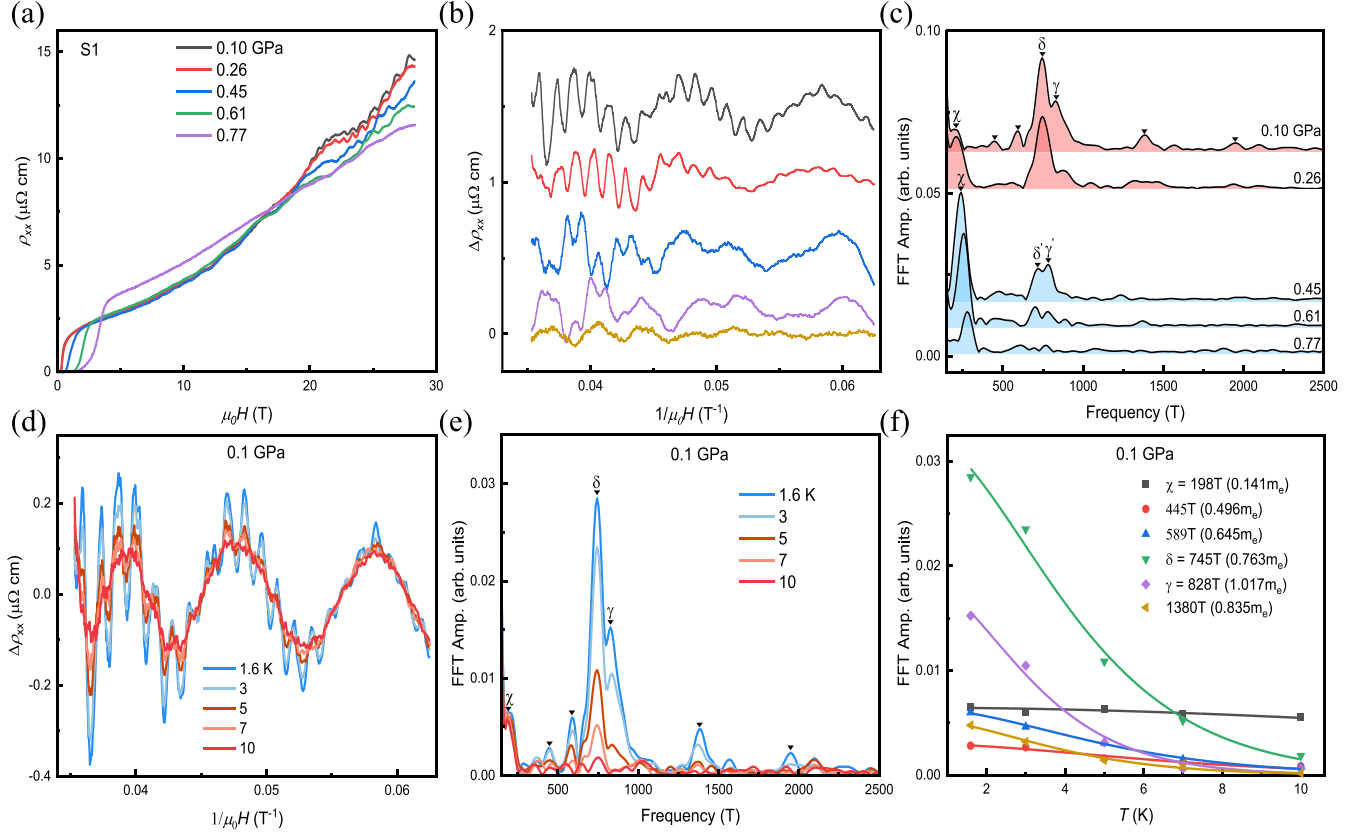


FIG. 3. (a) The resistivity ρ_{xx} of CsV_3Sb_5 measured under high magnetic field applied up to 28 T along c axis at $T = 1.6$ K and at different pressures. (b) The oscillation parts of resistivity $\Delta\rho_{xx}$ as a function of $1/\mu_0 H$ at various pressures. The $\Delta\rho_{xx}$ data are extracted by subtracting a polynomial background from the ρ_{xx} results shown in panel (a). (c) The FFT spectra in the range of 150–2500 T extracted from the oscillation data in panel (b). The data in panels (b) and (c) have been shifted vertically for clarity. (d) The oscillatory component $\Delta\rho_{xx}$ as a function of $1/\mu_0 H$ at different temperatures and selected pressure of 0.1 GPa. (e) The FFT spectra in the range of 150–2500 T extracted from the oscillation data in panel (d). There are seven well-defined frequencies, which are identified by inverted triangles. The extracted amplitudes from these frequencies are plotted in panel (f) as a function of temperature. The solid curves represent the best fit to the data using the LK formula. The quasiparticle effective masses estimated using the LK formula are shown in the upper right corner of panel (f).

the best fit to the data using the derivative of the LK formula, and the estimated quasiparticle effective masses are shown in the upper right corner of Figs. 2(h)–2(k), respectively. The resulting m^* values are not more than 1/10 of the free electron and are comparable to those reported in previous quantum oscillation studies [10,40] on CsV_3Sb_5 , confirming the robustness of the measurements.

In order to further explore how the higher frequencies in CsV_3Sb_5 evolve under pressures, we have carried out longitudinal resistivity measurements in high magnetic fields up to 28 T. The field dependence of resistivity ρ_{xx} of CsV_3Sb_5 measured at $T = 1.6$ K and at different pressures is shown in Fig. 3(a). Clear Shubnikov-de Haas (SdH) quantum oscillations are observed at selected pressures from 0.1 to 0.77 GPa. After subtracting a slowly changed polynomial background, the oscillation parts of resistivity $\Delta\rho_{xx}$ as a function of $1/(\mu_0 H)$ at various pressures are shown in Fig. 3(b). The FFT spectra in the range of 150–2500 T extracted from the oscillation data in Fig. 3(b) are displayed in Fig. 3(c), which change significantly around 0.4 GPa. We selected three representative frequencies in different frequency bands to describe this change. These three frequencies are assigned by

the Greek letters χ (200–300 T), δ , and γ (700–900 T), respectively. It is clear that the peak χ moves continuously toward higher frequencies as the pressure increases, while the peaks δ and γ change discontinuously to δ' and γ' at pressure greater than 0.4 GPa. However, we cannot judge whether the δ' and γ' peaks evolved from the splitting of the δ peak or from the gradual approach of the δ and γ peaks. Figure 3(d) shows the oscillatory component $\Delta\rho_{xx}$ as a function of $1/\mu_0 H$ at different temperatures and selected pressure of 0.1 GPa, and the corresponding FFT spectra in the range of 150–2500 T extracted from the oscillation data are shown in Fig. 3(e). There are seven well-defined frequencies, which are identified by inverted triangles. The extracted amplitudes from these frequencies are plotted in Fig. 3(f) as a function of temperature. The amplitude of the oscillations monotonically enhances with decreasing temperature, which can be well described by LK formula [41]. The oscillation amplitude at a fixed magnetic field is proportional to the thermal damping factor R_T :

$$R_T = \frac{\alpha X}{\sinh(\alpha X)}. \quad (2)$$

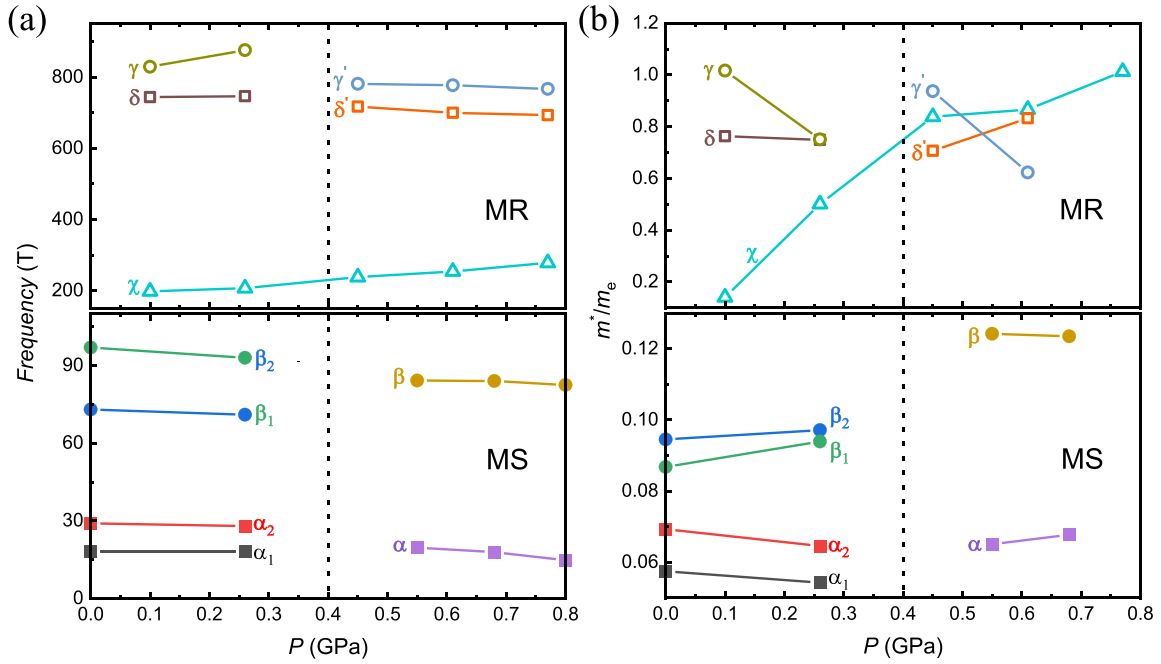


FIG. 4. Pressure evolution of (a) quantum oscillation frequencies and (b) quasiparticle effective masses for CsV_3Sb_5 . The data points in the lower half of panels (a) and (b) are extracted from the field dependence of thermoelectric power S_{xx} data, and the upper half the data points are extracted from the field dependence of resistivity ρ_{xx} data.

The solid curves in Fig. 3(f) represent the best fit to the data. The quasiparticle effective masses estimated using the LK formula are shown in the upper right corner of Fig. 3(f).

We summarize the extracted pressure evolution of quantum oscillation frequencies and quasiparticle effective masses in Fig. 4. It can be seen that most of the frequencies and the corresponding m^* do not change much with pressure, even if they have discontinuous changes around 0.4 GPa. Notably, the peak χ shifts steadily toward higher frequencies, from 198 to 278 T, as increasing pressure. This trend suggests an expansion in the extremal orbital area of the corresponding energy bands. Previous DFT calculations [44] have also identified a concave Fermi surface at the Brillouin zone boundary in the TrH CDW phase and named it band 265. Band 265 contributes a quantum oscillation frequency of approximately 220 T. With increasing pressure, the concave structure of band 265 undergoes slight expansion, which shows excellent agreement with both the frequency of the χ band and its high-pressure evolutionary behavior. In addition, the m^* of χ also increases from a small value of 0.141 to a value close to that of free electron mass (1.013). The simultaneous increase of orbital area and effective mass is consistent with the behavior of the Dirac band moving away from Fermi energy. Previously studies of de Haas-van Alphen oscillations [45] have also reported that the Berry phase determined from the χ band is close to the theoretical topologically nontrivial value, which is also in line with the characteristics of Dirac band. The T_c exhibits a notable increase from 2.5 K at ambient pressure to approximately 7 K at P_1 . This value significantly surpasses the maximum T_c observed in the pressurized (Rb, K) V_3Sb_5 , close to the maximum T_c at P_2 , where T_{CDW} is entirely suppressed. Concurrently, the T_{CDW} declines from 94 K to around 65 K. As

we know, the formation of a CDW order introduces a gap in the electronic structure at the Fermi level, which diminishes the density of states (DOS) available for Cooper pair. Conversely, the suppression of the CDW restores the original DOS at the Fermi surface, thereby enhancing the electron pairing interactions that are crucial for superconductivity. However, in the case of compressed CsV_3Sb_5 , the nearly threefold increase in T_c occurs alongside a reduction in T_{CDW} of less than one third, a phenomenon that cannot be solely attributed to DOS recovery. From our quantum oscillation measurements, most of the frequency and effect mass does not change much with pressure, while the χ band continually changes under pressure, which might be linked to the notable enhancement of the T_c and deserves further investigations, particularly in conjunction with computational studies.

The origin of the Lifshitz transition in compressed CsV_3Sb_5 at approximately 0.4 GPa warrants further exploration. The abrupt alteration in frequencies suggests a transformation in the supercells within the CDW states. While most frequencies remain relatively stable, indicating that the in-plane 2×2 superlattice is likely unchanged, the sudden modification of the Fermi surface can be attributed to changes in the interlayer modulation of the supercell. As reported in previous research, mechanical deformation can quench the $2 \times 2 \times 4$ supercell in CsV_3Sb_5 [25], leading to the hypothesis that the $2 \times 2 \times 4$ supercells in CsV_3Sb_5 may transfer to a pure $2 \times 2 \times 2$ supercell under hydrostatic pressure, resulting in abrupt changes of the Fermi surface. For CsV_3Sb_5 , its low frequency FFT spectra (10–150 T) evolve from four dominant frequencies to two under pressures. In contrast, (Rb,K) V_3Sb_5 , which possesses only a pure $2 \times 2 \times 2$ supercell, also exhibits low frequency FFT spectra with only two dominant frequencies. This observation supports

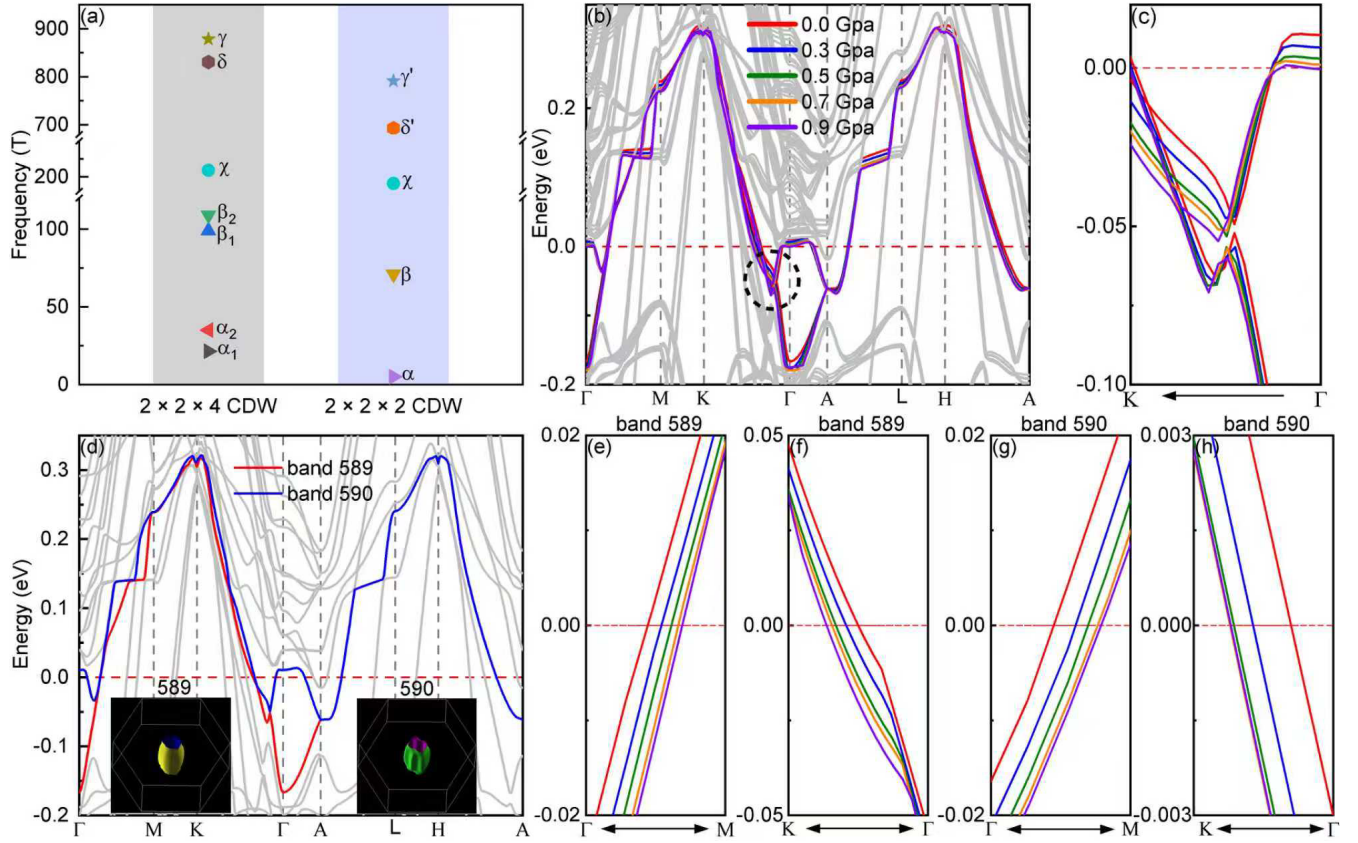


FIG. 5. (a) The calculated SdH oscillation frequencies of the $2 \times 2 \times 4$ supercell and the $2 \times 2 \times 2$ supercell at ambient pressure, respectively. (b) The calculated band structures of the $2 \times 2 \times 2$ supercell under different pressures. The Dirac bands near the Fermi level are circled by the black dotted circle. (c) Close-up of the Dirac bands. (d) The bands 589 and 590 corresponding to χ branch are highlighted by red and blue lines. The Fermi surfaces are inserted. (e)–(h) The evolution of bands 589 and 590 with the increase of pressure.

the speculation that the supercell may change to a $2 \times 2 \times 2$ configuration above 0.4 GPa in compressed CsV_3Sb_5 . To further verify our hypothesis, the DFT calculations are performed [34]. Figure 5(a) depicts the calculated SdH oscillation frequencies of the $2 \times 2 \times 4$ supercell and the $2 \times 2 \times 2$ supercell. Both the low- and high-frequency branches align well with the results obtained from experimental measurements. And the abrupt alteration in frequencies is also observed, which illustrates the quenching of the $2 \times 2 \times 4$ supercell into the $2 \times 2 \times 2$ supercell as pressure increases. Furthermore, it is found that the Dirac bands move away from the Fermi level as pressure increases in the $2 \times 2 \times 2$ supercell [see Figs. 5(b)–5(c)]. Notably, the χ branch emerges in both the $2 \times 2 \times 4$ supercell and the $2 \times 2 \times 2$ supercell. For the $2 \times 2 \times 2$ supercell, the χ branch is formed by bands 589 or 590, which cross the Fermi level nearly at the same positions, resulting in an almost identical Fermi surface. With the increase of pressure, the crossing points with the Fermi level gradually migrate to M or K points, respectively, as shown in Figs. 5(e)–5(h), implying the expansion of the Fermi surface. Thus, the frequency of the χ branch increases as well. For the $2 \times 2 \times 4$ supercell (see Fig. S5), the χ branch is formed by bands 1179 or 1180, which also cross the Fermi level nearly at the same positions. And their trend of evolution under pressure is similar to the $2 \times 2 \times 2$ supercell.

III. SUMMARY

In summary, by measuring the quantum oscillation signals of in-plane resistivity, thermoelectric effect, and theoretical calculations of CsV_3Sb_5 under different pressures, we reveal for the first time that the Fermi surface of CsV_3Sb_5 undergoes an abrupt change above 0.4 GPa. This transformation may be linked to changes in interlayer modulation within the CDW state. Furthermore, we have identified the potential presence of a Dirac band that shifts away from the Fermi surface as pressure increases. These findings provide valuable data for studying the Fermi surface evolution of CsV_3Sb_5 under pressure.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

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