Quantum Oscillation in Narrow-Gap Topological Insulators

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The canonical understanding of quantum oscillation in metals is challenged by the observation of the de Haas–van Alphen effect in an insulator, SmB_6 [Tan *et al*, Science 349, 287 (2015)]. Based on a two-band model with inverted band structure, we show that the periodically narrowing hybridization gap in magnetic fields can induce the oscillation of low-energy density of states in the bulk, which is observable provided that the activation energy is small and comparable to the Landau level spacing. Its temperature dependence strongly deviates from the Lifshitz-Kosevich theory. The nontrivial band topology manifests itself as a nonzero Berry phase in the oscillation pattern, which crosses over to a trivial Berry phase by increasing the temperature or the magnetic field. Further predictions to experiments are also proposed.

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Introduction.—Quantum oscillation is a nontrivial manifestation of Landau quantization in metals [1]. In a uniform magnetic field, an electron makes a cyclotron motion with a conserved energy. If a constant energy surface forms a closed orbit in the reciprocal space, the quantization condition dictates that the area A enclosed by the orbit satisfies,

$$\frac{A\hbar}{e}\frac{1}{B} = 2\pi(n+\gamma), \qquad n \in \mathbb{N}. \tag{1}$$

So the single-particle eigenstates form Landau levels (LLs). In metals, the chemical potential intersects an energy band, so the density of states (DOS) near the chemical potential peaks periodically as LLs cross the chemical potential with the variation of $1/B$ with the frequency given by $F = A_F\hbar/(2\pi e)$, in which A_F is the area of the Fermi surface [see Fig. 1(a)] [2]. The DOS oscillation results in the oscillation of various physical quantities, e.g., the magnetic susceptibility (de Haas–van Alphen effect) and the resistivity (Shubnikov–de Haas effect).

The constant γ in Eq. (1) is directly related to the Berry phase ϕ_B the electron accumulates during a cyclotron period, $2\pi(\gamma - 1/2) = -\phi_B$ [3]. γ determines the positions of peaks and dips in the oscillation and can be extracted with the Landau level index analysis [4–7].

This canonical understanding of quantum oscillation is challenged by the recent observation of the de Haas–van Alphen effect in an insulator, SmB_6 [8]. SmB_6 has a narrow thermal activation gap in its bulk states, $\Delta \simeq 40$ K, even in strong magnetic fields [8,9]. It is argued that the high-frequency quantum oscillation originates in the bulk states, as opposed to the topologically protected metallic surface states [7] (however, cf. Ref. [10] for a different interpretation), which is a consequence of the proposal of SmB_6 as a topological Kondo insulator [11–14]. The temperature dependence deviates from the Lifshitz-Kosevich (LK) theory [8]. So it is interesting to check the possibility of the insulating bulk states displaying quantum oscillation. Furthermore, it is desirable to find if any signature of the nontrivial band topology arises in the quantum oscillation.

Before proceeding to a detailed study model, we first present an intuitive argument based on the semiclassical treatment of the Landau quantization as illustrated in Fig. 1. In contrast to the metals, in an insulator with parabolic bands either filled or empty, all LLs flow away from the chemical potential as the magnetic field increases, so the low-energy DOS [defined in Eq. (4)] decreases monotonically and does not oscillate at all. However, if the insulator has an inverted band structure as shown in Fig. 1(c), which is modeled by the two-band Hamiltonian in Eq. (3), as the magnetic field increases, LLs periodically approach the band edges, i.e., the bottom of the conduction band and the top of the valence band, resulting in periodic narrowing

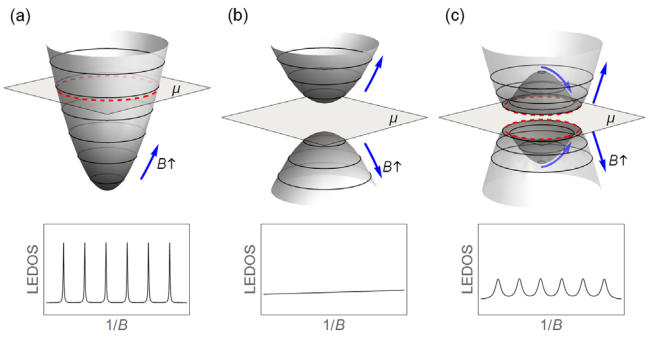

FIG. 1. Illustration of LLs and possible low-energy DOS oscillation in (a) metals, (b) parabolic band insulators, and (c) insulators with an inverted band structure. The planes and the thin circles denote the chemical potential and LL orbits, respectively. The blue arrows indicate the flow of LLs with increasing magnetic fields. The red dashed circles denote the Fermi surface in (a) and the band edges in (c).

of the hybridization gap and low-energy DOS oscillation. Therefore, the band edges play a similar role as the Fermi surface in metals and the oscillation frequency is proportional to the enclosed area A_{edge},

$$F = \frac{\hbar}{2\pi e} A_{\text{edge}}. \tag{2}$$

The oscillation is observable only if the amplitude of gap narrowing, which is related to the LL spacing near the band edge, is comparable to the activation gap itself. For a narrow hybridization gap, A_{edge} roughly equals the Fermi pocket area of the metal in the absence of hybridization. This semiclassical picture will be adopted again to show that there is a nontrivial Berry phase in the quantum oscillation pattern as a consequence of the nontrivial band topology. The temperature dependence of the oscillation amplitude is found to strongly deviate from the LK theory. Further predictions to experiments will also be discussed.

Model.—We shall study the following two-band model in the continuum,

$$H = \sum_k \begin{pmatrix} d_k^\dagger & f_k^\dagger \end{pmatrix} \begin{pmatrix} \frac{k^2}{2m_d} - \mu_d & V\vec{k}\cdot\vec{\sigma} \\ V\vec{k}\cdot\vec{\sigma} & -\frac{k^2}{2m_f} - \mu_f \end{pmatrix} \begin{pmatrix} d_k \\ f_k \end{pmatrix}, \tag{3}$$

in which $d_k = (d_{k\uparrow}, d_{k\downarrow})^T$ and $f_k = (f_{k\uparrow}, f_{k\downarrow})^T$ are d- and f-band electrons with pseudospin $1/2$. $\vec{\sigma}$ are the Pauli matrices acting on the pseudospin space. If $\delta\mu \equiv \mu_d - \mu_f > 0$, the model has an inverted band structure. The electronlike d band and the holelike f band are hybridized by the parity-odd $V\vec{k}\cdot\vec{\sigma}$ term and open a finite gap. If the chemical potential lies within the gap, this model describes topological insulators in two and three dimensions [15–20].

There are four bands in SmB_6 with pseudospin- $1/2$ near the chemical potential and the band inversion happens around the three X points [13,14,21]. Equation (3) can be taken as a simplified two-band $k\cdot p$ model expanded around one X point [21,22]. We adopt the following band parameters derived from a tight-binding model [23] throughout this work unless specified otherwise, $m_d = \hbar^2/2ta_0^2$, $\alpha \equiv m_d/m_f = 0.1$, $\delta\mu = 0.5t$. The d-band hopping amplitude t is set to be unity. A weak hybridization $V/a_0 = 0.015t$ leads to a narrow gap $\Delta_g = 0.012t$. Substituting $t \simeq 640$ meV estimated from the calculated SmB_6 band structure [21], one finds $\Delta_g = 7.7$ meV, which roughly equals two times of the 40 K activation energy. Therefore, our model captures the main features of the SmB_6 band structure. The strongest magnetic field in experiments $\sim$50 T corresponding to $1/500$ flux quanta per unit cell is covered in our calculations. The Zeemann effect estimated in experiments is quite weak [8,9] and does not qualitatively change our results, so will be neglected in our presentation.

The possible quantum oscillation from the bulk states is characterized by the low-energy DOS (LEDOS) *near* the chemical potential, defined as the broadened DOS at temperature T,

$$D_T = \int_{-\infty}^{+\infty} d\xi \frac{\partial n_F(\xi-\mu,T)}{\partial\mu} D(\xi) = \sum_i \frac{\partial n_F(\epsilon_i-\mu,T)}{\partial\mu}, \tag{4}$$

in which $D(\xi)$ is the single-particle DOS. The summation on the right-hand side of Eq. (4) is taken over the single-particle energy spectrum. LEDOS is related to various physical quantities at finite temperature, e.g., the Pauli susceptibility, the compressibility and the resistivity, and its oscillation necessarily results in the oscillation of these quantities. Besides, an advantage in calculating LEDOS is that it does not require any regularization procedure. In contrast, the free energy is (formally) divergent due to the holelike f band. Upon regularization, a cutoff at some negative energy may play a similar role as the Fermi surface in metals and result in artificial oscillation, which is avoided in the LEDOS calculations.

2D semimetal.—If the hybridization is turned off, $V = 0$, the chemical potential lies exactly where the d and f bands intersect, forming electronlike and holelike Fermi pockets with equal size [Fig. 2(a)]. In magnetic fields, these bands form two sets of LLs,

$$\epsilon_n^d = \frac{eB\hbar}{m_d}\left(n+\frac{1}{2}\right) - \mu_d, \qquad \epsilon_n^f = -\frac{eB\hbar}{m_f}\left(n+\frac{1}{2}\right) - \mu_f, \quad n \in \mathbb{N}. \tag{5}$$

LLs cross the Fermi surface periodically and result in the LEDOS oscillation as shown in Figs. 2(b) and 2(c).

The temperature dependence of the oscillation amplitude has an unusual two-plateau feature [Fig. 2(d)], which resembles that found in SmB_6 [8]. The reason is that both Fermi pockets contribute to the LEDOS oscillation with equal frequency. At finite temperature, the contribution from each band is captured by the LK theory, so the total oscillation amplitude is described by the *two-component* LK formula,

$$R_T = c_d \frac{\chi_d}{\sinh\chi_d} + c_f \frac{\chi_f}{\sinh\chi_f}, \tag{6}$$

in which $\chi_{d,f} = 2\pi^2 m_{d,f} T/eB\hbar$, $c_{d,f} \propto m_{d,f}$. The oscillation amplitudes are extracted as the heights of the dominant Fourier peaks, which are fitted perfectly by Eq. (6) [23].

2D topological insulator.—In a magnetic field, the $Vk\cdot\vec{\sigma}$ term is replaced by $V(\vec{k} - e\vec{A}/\hbar)\cdot\vec{\sigma}$, which hybridizes different LLs. In two dimensions, the Hamiltonian is decoupled into two sectors, the $d_\uparrow - f_\downarrow$ ($\uparrow\downarrow$) sector and the $d_\downarrow - f_\uparrow$ ($\downarrow\uparrow$) sector. Within each sector, the LLs are

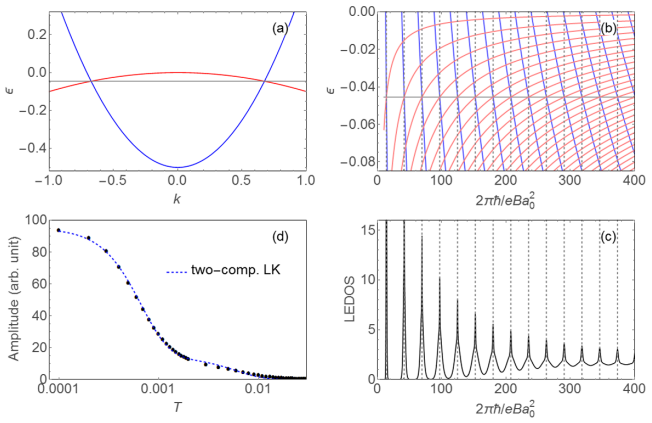

FIG. 2. (a) Band structure, (b) LL spectrum, and (c) LEDOS oscillation of the semimetal in two dimensions. The dashed gray lines in (b) and (c) indicate whenever Eq. (1) is satisfied at the chemical potential with $\gamma = 1/2$. (d) The temperature dependence of the oscillation amplitude (black dots) and the fitting by the two-component LK formula (dashed blue curve). Band structure parameters are specified in the main text with t set to be unity. The abscissas in (b) and (c) are labeled with the inverse number of flux quanta per unit cell.

hybridized *obliquely*; i.e., the nth $d_\uparrow$ LL is hybridized with the $(n-1)$th $f_\downarrow$ LL, while the $(n-1)$th $d_\downarrow$ LL with the nth $f_\uparrow$ LL, forming the following spectrum,

$$\epsilon^{\uparrow\downarrow}_{n\pm} = \frac{1}{2}\left(\epsilon^d_n + \epsilon^f_{n-1} \pm \sqrt{(\epsilon^d_n - \epsilon^f_{n-1})^2 + 8nV^2eB/\hbar}\right), \quad (7)$$

$$\epsilon^{\downarrow\uparrow}_{n\pm} = \frac{1}{2}\left(\epsilon^d_{n-1} + \epsilon^f_n \pm \sqrt{(\epsilon^d_{n-1} - \epsilon^f_n)^2 + 8nV^2eB/\hbar}\right), \quad (8)$$

for $n \geq 1$. The $d_\uparrow$ and $f_\uparrow$ LLs with index $n = 0$ are unaffected.

Let us start from the semimetal without hybridization and dub the highest occupied d-LL index N, $N = \lfloor \delta\mu/\hbar\omega_c^* - 1/2 \rfloor$, with $\omega_c^* \equiv eB\hbar(m_d + m_f)/m_d m_f$. The highest unoccupied f-LL index is also N. As the hybridization is turned on, all LLs are pushed away from the chemical potential, except one pair in each sector, the $(N+1)$th $d_\uparrow$ LL and the Nth $f_\downarrow$ LL, and the Nth $d_\downarrow$ LL and the $(N+1)$th $f_\uparrow$ LL, as illustrated in Fig. 3. One LL out of each pair is pushed *toward* the chemical potential. In weak magnetic fields, the level repulsion overcomes the small LL spacing and these two LLs pass each other, leaving a hybridization gap. If the hybridization is perturbatively small in strong magnetic fields, the LLs do not pass each other, so the spectrum near the chemical potential is largely unaffected and remains metallic. Therefore, the magnetic field induces a gap-closing transition from a topological insulator to a metal [23].

The energy spectrum in magnetic fields is plotted in Fig. 4(a). The hybridization gap is closed above a critical field B_c. For $B > B_c$, the low energy spectrum is nearly the same as the unhybridized case, resulting in similar LEDOS oscillation. The temperature dependence is captured by the two-component LK formula, as shown in Fig. 4(c).

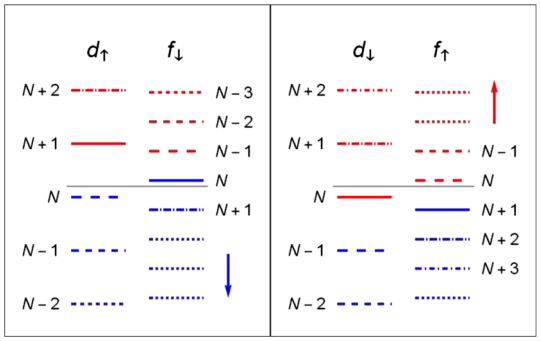

FIG. 3. Illustration of the LL hybridization in two dimensions. In each sector, each d LL hybridizes with an f LL drawn in the same dashing style. LLs in red are pushed upward while the blue downward. The long gray bars denote the chemical potential. All LLs shift away from it except that in the $\{N, N+1\}$ LL pairs (solid bars), one LL out of each pair shifts toward it and may pass each other.

For $B < B_c$, a close inspection on the LL spectrum finds periodic gap narrowing as expected from the semiclassical argument, which leads to the smooth oscillation of LEDOS. However, we find various peculiarities detailed below.

The oscillation amplitude has a nonmonotonic temperature dependence in sharp contrast to the LK theory. At low temperature, the amplitude has a broad hump, which is a consequence of the activation gap Δ. For $T \ll \Delta$, the oscillation amplitude is captured by the asymptotic formula [23],

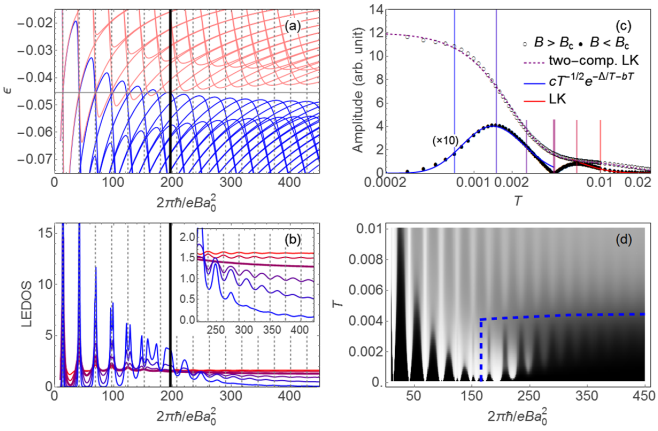

FIG. 4. (a) LL spectrum and (b) LEDOS oscillation of the 2D model with a hybridization gap. The thick vertical lines indicate B_c, the critical field of gap closing. The inset of (b) highlights the phase jump at finite temperature. The LEDOS are plotted at temperatures indicated by the vertical lines in (c). (c) Temperature dependence of the oscillation amplitudes extracted in $B > B_c$ (open circles) and $B < B_c$ (closed circles, multiplied by 10 for clarity). (d) Intensity plot of LEDOS, highlighting the π phase jump around $B \simeq B_c$ and $T \simeq \Delta$, which are indicated by the dashed curves.

$$R_T \sim T^{-1/2} e^{-\Delta/T - bT}, \tag{9}$$

in which the $e^{-\Delta/T}$ factor comes from the thermal activation while the e^{-bT} factor reflects the thermal smearing similar to the LK theory.

Around $T \simeq \Delta$, the amplitude dips to zero, which coincides with a π phase jump in the oscillation pattern, as highlighted in the inset of Fig. 4(b). Furthermore, at low temperature, there is another (approximate to) π phase jump around B_c, while the high-temperature oscillation varies smoothly across B_c without any phase change as shown in Fig. 4(d). Therefore, the Berry phase changes by π in both circumstances.

The phase jump across B_c is actually implied by the LL spectrum, in which the periodic gap narrowing for $B < B_c$ is replaced by periodic widening for $B > B_c$ due to the gap closing, and the LEDOS peaks are replaced by dips correspondingly. Moreover, the nonzero Berry phase for $B < B_c$ turns out to be a manifestation of the oblique hybridization. Let us turn back to the semiclassical picture and focus on one LL in the $d_\downarrow - f_\uparrow$ sector with energy $\epsilon_{n+}^{\downarrow\uparrow}$, which comes from the hybridization between the $(n-1)$th $d_\downarrow$ LL and the nth $f_\uparrow$ LL. As it flows from the f-band top downward to the conduction band bottom and upward again along the d band with increasing B, the total phase in Eq. (1) changes by -2π, implying that the Berry phase near the band bottom is approximate to π, consistent with the LEDOS oscillation pattern at low temperature. At high temperature, $T > \Delta$, LLs with trivial Berry phase dominate over those near the band edges, leading to the crossover of the oscillation phase.

Quantum oscillation in three dimensions.—The two-band model Eq. (3) is easily generalized to three dimensions with the z components included in $\vec{k}$ and $\vec{\sigma}$. The LEDOS oscillation shown in Fig. 5 is qualitatively similar to the 2D case with minor modifications.

First, in the oscillation frequency formula Eq. (2), A_{edge} should be understood as the area enclosed by the extremum orbit on the band edges. For weak hybridization, it roughly equals that of the Fermi surface in the absence of hybridization.

Second, the $k_z\sigma_z$ term introduces further hybridization between the nth $d_\uparrow$ ($d_\downarrow$) LL and the nth $f_\uparrow$ ($f_\downarrow$) LL and opens a gap in the $B > B_c$ regime for nonzero k_z (B_c is defined as the gap-closing field for $k_z = 0$), resulting in a persistent gap in DOS as shown in Fig. 5(a). As a result, the LEDOS oscillation in the $B > B_c$ regime also shows thermal activation behavior at low temperature, which is captured by an asymptotic formula similar to Eq. (9), $R_T \sim e^{-\Delta'/T - bT}$. Because of the gap nodes at $k_z = 0$ at particular field strengths, Δ' is much smaller than the gap away from these fields. So the temperature with the maximum oscillation amplitude $T_{\max}$ should be much lower than the activation energy measured with resistivity.

Otherwise the LEDOS oscillation in three dimensions carries all essential features as in the 2D case. For $B > B_c$,

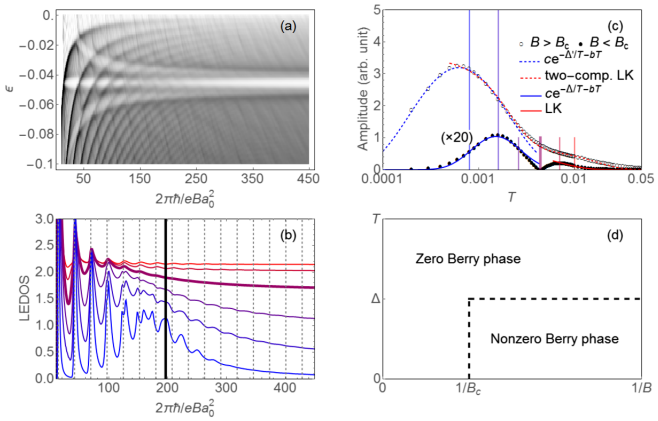

FIG. 5. (a) Single-particle DOS of the 3D model and (b) LEDOS oscillation. The thick vertical line indicates B_c. The LEDOS are plotted at temperatures indicated by the vertical lines in (c). (c) Temperature dependence of the oscillation amplitudes for $B > B_c$ (open circles) and $B < B_c$ (closed circles, multiplied by 20 for clarity). (d) Schematic illustration of Berry phases in different regimes.

the temperature dependence is captured by the two-component LK formula for $T > T_{\max}$. For $B < B_c$, the nontrivial Berry phase shows up, which crosses over to the trivial Berry phase at high temperature or high magnetic fields.

Summary and discussion.—To summarize, we find that an insulator with inverted bands can show quantum oscillation in its bulk low-energy DOS due to the periodic gap narrowing in magnetic fields. The oscillation frequency is proportional to the area enclosed by the extremum orbit on the band edge. For a topological insulator, the nontrivial band topology manifests itself as a nonzero Berry phase in the oscillation. The temperature dependence deviates from the LK theory and shows thermal activation behavior at low temperature in particular. These features are also reproduced by a tight-binding model on the lattice [23].

In a recent publication [27], the authors found quantum oscillation in a similar two-band model. The oscillation frequency is consistent with our result. However, the hybridization term in their work is parity even, so the hybridization gap is topologically trivial. The nonzero Berry phase and the bulk gap closing at B_c found in our work are missing.

Several features can be tested in experiments. First is the sizable periodic gap narrowing in magnetic fields that causes the LEDOS oscillation, which can be extracted from the resistivity or with infrared spectroscopy. Second is the thermal activation behavior, i.e., the decreasing oscillation amplitude at temperatures much lower than the activation energy. Third is the nonzero Berry phase. Even if it is difficult to extract the Berry phase directly [6], it is possible to observe a π phase jump at the boundaries sketched in Fig. 5(d).

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Note added.—Upon completion of this work, we became aware of Ref. [10], in which a different scenario for the quantum oscillation in SmB_6 was suggested.

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