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Diagnosing a strong topological insulator by quantum oscillations

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Abstract. We show how quantum oscillation measurements of surface states in an insulator may allow to diagnose a strong topological insulator and distinguish it from its weak or topologically trivial counterpart. The criterion is defined by the parity of the number of fundamental frequencies in the surface-state quantum oscillation spectrum: an even number of frequencies implies a weak or a topologically trivial insulator, whereas an odd number points to a strong topological insulator. We also discuss various aspects and issues related to applying this criterion in practice.

1. Introduction

Study of topological properties of matter has become a frontier of condensed matter physics. Materials new and old are studied with respect to their topology, experimentally and theoretically alike. In particular, due to great interest in topological insulators, surface states in various insulating materials are being actively sought and studied. Whenever such states are experimentally detected, one would like to find out whether they are of topological or of an accidental origin.

For some materials such as Bi_2Te_3 , $\text{Bi}_{2-\delta}\text{Ca}_\delta\text{Te}_3$ and $\text{Bi}_{1-x}\text{Sb}_x$, this question, to a great extent, has been answered by spin-resolved angle-resolved photoemission (ARPES) measurements [1,2], that were able to detect non-degenerate helical surface bands with topologically non-trivial spin texture, a key signature of a topological insulator. On other occasions, the results have been less definitive. Indeed, in some materials spin-resolved ARPES experiments turn out to be extremely difficult because of peculiarities of their surface structure. In other compounds, a significant bulk conductivity [3,4] does not allow transport measurements to diagnose the topological nature of the material.

An interesting case has recently emerged in the class of the so-called “Kondo insulators” [5,6], where a gap in the electron spectrum opens due to coupling between conduction electrons and local magnetic moments. After it was pointed out that Kondo insulators may be topologically non-trivial [7] while being truly insulating in the bulk [3], experiments on SmB_6 , a mixed-valence semiconductor [8], have indeed detected surface states, and more theoretical contributions followed [9,10]. However, even after transport [11–14], point contact [15], ARPES [16–19] and scanning tunneling spectroscopy (STS) [20,21] experiments, the available evidence for topological origin of the surface states in SmB_6 remained circumstantial – until very recent spin-resolved ARPES experiment [22] on the (001) surface of the material.

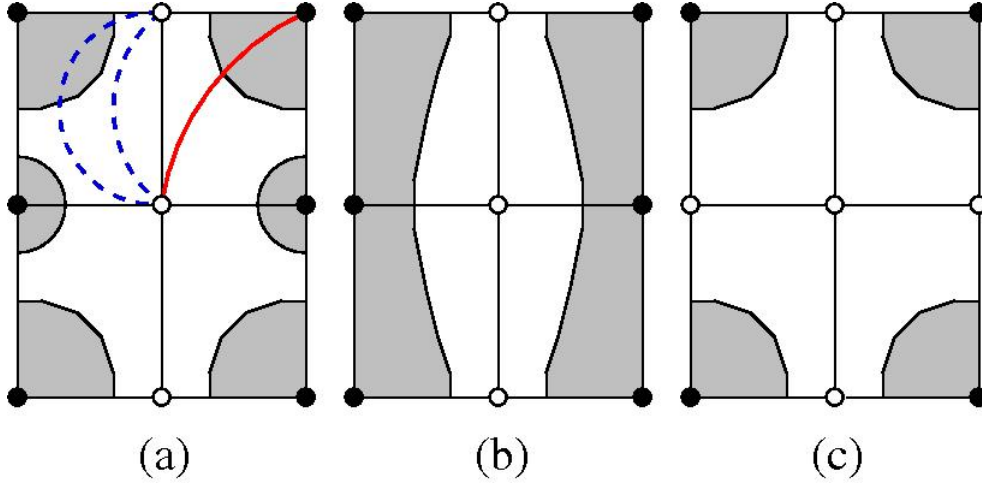


Figure 1. The first Brillouin zone for the (1 0 1) surface. The small empty and full circles correspond to the time reversal polarization values $\pi = 1$ and $\pi = -1$, respectively. The panels (a) and (b) show the two generic Fermi surface configurations, allowed in the same case of a weak topological insulator. The (a) panel corresponds to two closed Fermi surfaces, and hence two different fundamental frequencies. The dashed (blue) arcs are examples of paths connecting two time reversal invariant momenta with the same values of time reversal polarization. They cross the Fermi surface an even number of times – or not at all. The solid (red) arc is a path connecting two time reversal invariant momenta with the opposite values of time reversal polarization. It crosses the Fermi surface an odd number of times. The (b) panel involves a single open Fermi surface, and thus no quantum oscillations at all. The case (c) is the generic Fermi surface configuration in the case of a strong topological insulator, it produces a single fundamental frequency.

Here, we show how a *strong* topological insulator may be identified via a relatively simple analysis of quantum oscillations due to surface bands. In SmB_6 , surface-state quantum oscillations have already been observed [23]. We hope that an analysis of the data [23] using the approach that we propose here may confirm the strong topological insulator nature of this material. We also hope that this approach can be used to diagnose other potential topological insulators, where spin-resolved ARPES experiments have not yet been available.

2. Characterizing a strong topological insulator

Following the Refs. [24, 25], consider the time reversal polarization $\pi = \pm 1$ at the four time reversal invariant momenta of the surface Brillouin zone. Both a weak topological insulator and a trivial one will have an even number of time reversal invariant surface momenta with polarization $\pi = +1$, while for a strong topological insulator this number must be odd. A surface state is labeled by its momentum in the surface Brillouin zone and by a surface band index. Now, in the surface Brillouin zone, consider a path connecting two time reversal invariant momenta with the same (different) values of time reversal polarization. Any such path must contain an even (odd) number of surface states at the Fermi energy, as shown in the Fig. 1(a).

Thus we are lead to conclude that both a weak topological insulator and a trivial one may have either an even non-zero number of different *closed* Fermi surfaces at the sample boundary, as shown in the Fig. 1(a) – or none at all. The latter case also allows for a surface band with an *open* Fermi surface, as shown in the Fig. 1(b). However, an open Fermi surface does not contribute to quantum oscillations, a point which is important for the arguments to follow.

By contrast, as illustrated in the Fig. 1(c), a topologically protected surface band in a *strong* topological insulator has an odd number of closed Fermi surfaces producing quantum oscillations.

Each closed Fermi surface contributes a fundamental frequency to the spectrum of quantum oscillations. Thus, barring special cases to be discussed below, the spectrum of quantum oscillations due to surface states in a *strong* topological insulator contains an odd number of fundamental frequencies. By contrast, for the quantum oscillation spectrum due to surface bands in a trivial or a weak topological insulator the number of fundamental frequencies is even.

In other words, the distinction is not in the number parity of non-degenerate surface bands: as one can see in the Figs. 1 (b) and (c), this number may be odd both in a weak and a strong topological insulator. Rather, it is the odd number of surface bands with a *closed* Fermi surface (that is, an odd number of fundamental frequencies) that distinguishes a strong topological insulator from its weak or topologically trivial counterpart.

The arguments above assume that the physical picture of a non-interacting topological insulator, developed in the Refs. [24, 25], holds for the materials in question, in spite of the presence of electron correlations.

In practice, one should first determine the bulk or surface nature of the studied pocket of carriers by examining the dependence of the quantum oscillations on the direction of the applied magnetic field [26]. Next, one shall find out whether the observed surface band is degenerate or not. This amounts to checking whether it produces one or two fundamental frequencies. If two fundamental frequencies F_1 and F_2 were to be resolved, they would be seen as two separate peaks in the Fourier transform of the quantum oscillation data. However, if the F_1 and F_2 were too close to be resolved as separate peaks, they could still be detected via the emerging modulation factor (beats) [26]:

$$\mathcal{R} = \cos \left[\pi \frac{\delta F}{H} \right], \quad (1)$$

where $\delta F = F_1 - F_2$. For this, there are two distinct possibilities.

The first one corresponds to the Zeeman splitting, where the Eq. (1) reduces to

$$\mathcal{R} = \cos \left[\pi \frac{\delta \mathcal{E}_Z}{\Omega_0} \right]. \quad (2)$$

Here, $\delta \mathcal{E}_Z$ is the Zeeman splitting, Ω_0 the cyclotron frequency, and the \mathcal{R} is usually referred to as the spin reduction factor. Since both the $\delta \mathcal{E}_Z$ and the Ω_0 are proportional to the field strength, the \mathcal{R} depends only on the field orientation with respect to the surface, and vanishes for particular orientations known as "spin zeros" [26].

The second possibility corresponds to an intrinsic spin-orbit coupling, where the splitting δF in the Eq. (1) does not vanish in the $H \rightarrow 0$ limit. By contrast with the case of Zeeman splitting, here the amplitude modulation is a function of both the field strength and its orientation.

One may argue that in certain special cases two non-degenerate surface bands may give rise to a single fundamental frequency, and thus a trivial insulator would look like a topological one. Indeed, this could happen in a system with an anomalously weak Zeeman effect, that would not allow for the separation of spin degenerate surface states, even in the presence of a magnetic field. The same problem may arise if two non-coincident Fermi surfaces can be mapped on each other by a symmetry transformation: in this case, the two fundamental frequencies coincide. In the former case, a simple estimation of the Zeeman splitting and of the cyclotron frequency would allow one to determine the intensity of the magnetic field needed to resolve two distinct frequencies. By contrast, the latter case is more delicate: here, the degeneracy of the two fundamental frequencies is protected by symmetry.

3. An example: the case of SmB₆

An interesting candidate topological material, SmB₆, appeared recently in the class of the so-called “Kondo Insulators”. A beautiful transport experiment [11] successfully distinguished bulk-dominated from surface-dominated conduction: it was found that, as the material is cooled below 4 K, it exhibits a crossover from bulk to surface conduction. Soon, a quantum oscillation experiment [23] probed the electron states, bound to the (101) surface. The reported torque data exhibit two fundamental frequencies, attributed to the two pockets, named α and β . The two frequencies are shown in the Fig. 2 (b) of the Ref. [23]: only the β -frequency depends on the magnetic field orientation in a way consistent with a (101) surface state behavior (see the Fig. 3 (a) of the Ref. [23]).

On the other hand, the α -pocket has been argued to arise from the less clean and polar (001) surface [19, 23, 27]. Another explanation would be that this pocket is of a bulk origin, as the α -frequency depends on the field orientation very weakly if at all, which is hardly consistent with surface character of the carrier states, but rather suggestive of the said pocket being three-dimensional. As we wish to concentrate on the (101) surface, we disregard the α -pocket as extrinsic to the physics at hand.

Our task is thus to find out whether the β oscillations represent one or two fundamental frequencies. Unfortunately, the Ref. [23] presents no explicit analysis of amplitude modulations or spin zeros as a function of field orientation and magnitude, and thus we do not know whether these are actually present in the data. However, the analysis we propose offers a direct and robust test of whether a material (in the present case, SmB₆) is a strong topological insulator. We argue here, that, to be consistent with spin-resolved ARPES measurement, an analysis of the data should point out that the β oscillations represent a unique fundamental frequency.

It is important to note that if a quantum oscillation experiment were done on the (001) surface, the results would probably be less definitive than on the (101) surface. Indeed, it has been shown by ARPES experiments [16–18, 22], that on this surface, there are three closed Fermi surfaces, shown in the Fig. 2. According to [10], the two Fermi pockets centered at the point X of the surface Brillouin zone and its image upon rotation by $\pi/2$ around Γ produce identical fundamental frequencies. The counting of fundamental frequencies (two) would thus point to a weak topological insulator, while the number of closed Fermi surfaces is odd and, in fact, the model describes a strong topological insulator. This spurious degeneracy can be removed by subjecting the sample to an uniaxial pressure. However, this reduces the practical simplicity of the criterion we propose.

4. Conclusion

To summarize, we proposed a method of diagnosing a strong topological insulator by counting the number of fundamental frequencies, observed in magnetic quantum oscillations due to surface states. We expect the method to work well except for cases of surface-state Fermi surfaces that are degenerate by symmetry. How does the method we proposed compare with its counterparts?

Recently, quantum oscillation data have been used to verify the Dirac dispersion of carriers via analysis of the Berry phase γ of the oscillations as in $\cos \left[2\pi \frac{F_i}{H} + \pi + \gamma \right]$ – both in graphene [28] and in topological insulators [29]. However, such an analysis comes with its own challenges, described in the Section 8.3 of the Ref. [3], and in the Ref. [4]. By contrast, counting the fundamental frequencies of surface-state quantum oscillations, as we propose, appears to present a much simpler task.

The Berry phase analysis and the counting of fundamental frequencies may be viewed as complementary to each other, in the following sense. The $\gamma = \pi$ does not, by itself, prove the topological nature of the surface states, to which the Dirac spectrum in single-layer graphene is an example. Another example is the Rashba Hamiltonian $\mathcal{H}_R = \alpha(\mathbf{n} \cdot \mathbf{p} \times \sigma) + \mathbf{p}^2/2m$ of surface states in an inversion layer [30]: it is not related to non-trivial band topology in the

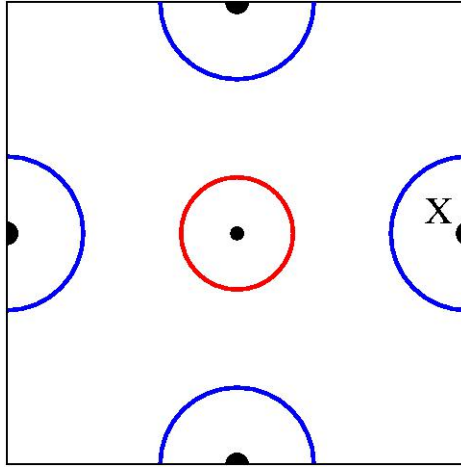


Figure 2. The first Brillouin zone for the (1 0 0) surface of SmB_6 . As shown by [10], the surface pockets centered at the point X and its $\pi/2$ rotation counterpart yield degenerate fundamental frequencies. The pocket centered at the point Γ of the surface Brillouin zone yields a different fundamental frequency. By the fundamental frequency count, the model would thus mimic as a weak topological insulator while in fact corresponding to a strong one.

bulk, yet in the vicinity of zero momentum it is equivalent to the Hamiltonian of a surface Dirac branch in a topological insulator. However, once a material has been independently shown to be a topological insulator, finding $\gamma = \pi$ serves as a confirmation of the Dirac character of the surface state spectrum.

Note that, compared with ARPES, the present approach allows to routinely resolve the Zeeman-split quantum oscillation frequencies, whereas even for the state-of-the-art ARPES with its current energy resolution of several meV [1, 2, 31] this remains a challenge.

To summarize, we pointed out how quantum oscillation experiments may allow to distinguish surface states in a strong topological insulator from those in its weak or topologically trivial counterpart. As an illustration, we discussed recent experiments [23] on SmB_6 .

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