Critical examination of quantum oscillations in SmB_6

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We critically review the results of magnetic torque measurements on SmB_6 that show quantum oscillations. Similar studies have been given two different interpretations. One interpretation is based on the existence of metallic surface states, while the second interpretation is in terms of a three-dimensional Fermi surface involving neutral fermionic excitations. We suggest that the low-field oscillations that are seen by both groups for B fields as small as 6 T might be due to metallic surface states. The high-field three-dimensional oscillations are only seen by one group for fields $B > 18$ T. The phenomenon of magnetic breakthrough occurs at high fields and involves the formation of Landau orbits that produces a directional-dependent suppression of Bragg scattering. We argue that the measurements performed under higher-field conditions are fully consistent with expectations based on a three-dimensional semiconducting state with magnetic breakthrough.

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I. INTRODUCTION

SmB_6 is a narrow-gap mixed-valent semiconductor [1,2], with a gap of the order of 20 meV. The gap is considered to be caused by the hybridization of the $4f$ levels with a conduction band, but is renormalized to the small value by strong electronic correlations [3,4]. Transport measurements indicate that the material is a bulk semiconductor [2], but has metallic surface states [5–7] which give rise to a plateau in the resistivity for temperatures below 4 K. It has been proposed that SmB_6 is a strongly correlated topological insulator [8], which gives rise to topologically protected metallic surface states. The existence of metallic surface states is consistent with angle-resolved photoemission spectroscopy (ARPES) measurements [9–11] that indicate the presence of a Weyl cone of surface electron states with the Weyl point located inside the valence band.

Magnetic torque measurements on flux-grown SmB_6 samples have revealed quantum oscillations. Li *et al.* [12] have reported oscillations that show a $1/\cos\theta$ dependence of the amplitudes, where θ is the angle between the field and the normal to the surface. This angular variation is characteristic of (two-dimensional) surface states. The inferred small area enclosed by the surface Fermi-surface orbits is consistent with the small Γ pocket observed in ARPES measurements [13]. However, a second set of measurements [14] on floating-zone-grown samples have been interpreted in terms of a bulk (three-dimensional) metallic Fermi surface, enclosing areas similar to those of metallic LaB_6 [15]. The observation of the insulating nature of bulk SmB_6 and the interpretation of a Fermi surface of neutral fermions responding to a magnetic field pose a serious challenge to the Lorentz invariant descriptions based on quantum electrodynamics (QED). In QED the coupling to charged particles is described by the minimal coupling transformation, whereby $p^\mu \to p^\mu - \frac{e}{c}A^\mu$, which suggests that only charged particles couple to magnetic and electric fields. It is important to note that the analysis of Li *et al.* [12] focused on the metallic surface states found for fields around 10 T, whereas the anomalous oscillations found in the measurements of Tan *et al.* [14] were observed in the field range of 18 to 40 T. Since the data are similar (to within the noise) for fields below 10 T [13], the difference in interpretation seems to be related to the high-field regime.

II. MAGNETIC BREAKTHROUGH

Here we point out that the two sets of measurements may be reconciled by using the well-established concept of magnetic breakthrough [16,17]. At low fields, quantum oscillations in a metal are usually interpreted in terms of Onsager's quasiclassical picture [18]. In Onsager's picture, the magnetic field causes electrons to move in orbits around planar cuts of equi-energy surfaces. This implies that the energy splitting of the Landau levels $\hbar\omega_c$, where the cyclotron frequency is defined by

$$\omega_c = \frac{eB}{mc}, \tag{1}$$

is a small perturbation to the zero-field Hamiltonian of the periodic lattice. In terms of the Fourier components of the lattice potential $V(\underline{Q})$, this requires

$$\hbar\omega_c \ll |V(\underline{Q})|. \tag{2}$$

Therefore, in this limit, the orbiting electrons do not to jump over band gaps. On the other hand, for

$$\hbar\omega_c \gg |V(\underline{Q})|, \tag{3}$$

the effectiveness of a band gap [caused by $V(\underline{Q})$] in interrupting the performance of field-induced Landau orbits is greatly reduced. As we describe later, the inequality shown in Eq. (3) is too restrictive and should be replaced by a less stringent inequality. In the high-field regime, the electronic states are localized. The electronic motion in the plane perpendicular to the applied field can be described by Landau orbits localized around fixed centers in the x-y plane. The motion parallel to the field is not perturbed by the Lorentz force or, equivalently, scattering by $V(\underline{Q}_z)$ is not affected by the in-plane Landau orbits. Hence, for the k_z motion, Bragg scattering is fully in effect. When applied to a semiconductor, the k_z motion of electrons is prohibited by the band gap at the k_z boundaries of the Brillouin zone. Despite the localized nature of the electronic wave functions, due to the ineffectiveness of Bragg scattering through either Q_x or Q_y, the Landau levels are split according to

$$E_n(k_z) = \hbar\omega_c(n+\gamma) + \epsilon(k_z) \tag{4}$$

and can still lead to de Hass–van Alphen (dHvA) oscillations. The phenomenon whereby an applied magnetic field drives the electrons between different cross-sectional areas of the zero-field Fermi surface is known as magnetic breakthrough. This phenomenon was noticed in experiments on Mg [19] and was explained by Cohen and Falicov [16], who proposed the criterion for breakdown given in Eq. (3) which is too restrictive. A criterion that is more favorable for the occurence of breakdown was subsequently derived by Blount [17]. Coincidentally, two branches of the dHvA oscillations observed in metallic LaB_6 were attributed to magnetic breakthrough on neck orbits of the Fermi surface [15].

Here, in order to emphasize the important factor that was absent in the original work of Cohen and Falicov [16], we present a simplified derivation of the criterion for magnetic breakdown. The critical value of the magnetic field is that which separates the regions where magnetic breakthrough does and does not occur. This criterion can be stated in terms of the lifetime of the nth Landau orbit τ_n due to scattering by the potential of the crystal lattice and the cyclotron frequency of the orbits ω_c. The critical field is determined to be such that

$$\left(\frac{\omega_c\tau_n}{2\pi}\right) \sim 1. \tag{5}$$

For $\frac{\omega_c\tau_n}{2\pi} > 1$, the electrons are able to complete multiple Landau orbits before being scattered by the lattice potential. This is the region where magnetic breakthrough can occur. On the other hand, for $\frac{\omega_c\tau_n}{2\pi} < 1$, a complete orbit cannot be traversed before the electron is Bragg scattered. The resulting orbits are strongly restricted to those allowed by the zero-field band structure. In the Landau gauge, the vector potential caused by applying a uniform B field in the z direction is given by

$$\underline{A} = xB_z\hat{e}_y. \tag{6}$$

In this gauge, the Landau orbits are described by the wave functions

$$\frac{1}{L}\exp[i(k_y y + k_z z)]\phi_n\left(x - \frac{\hbar k_y}{m\omega_c}\right), \tag{7}$$

where $\phi_n(x)$ are one-dimensional harmonic oscillator wave functions. These unconstrained Landau orbits will acquire a width due to scattering by the periodic potential. For scattering through Q_y, one sees that the scattering can only occur between Landau orbits that are centered at differ x positions, namely at $x_0 = \frac{\hbar k_y}{m\omega_c}$ and at $x_{Q_y} = \frac{\hbar(k_y \pm Q_y)}{m\omega_c}$. The Fermi-Golden rule expression for the lifetime of the nth Landau orbit is given by

$$\frac{1}{\tau_n} = \left(\frac{2\pi}{\hbar}\right)\sum_{n'} |<\phi_n(x_0)|V(Q_y)|\phi_{n'}(x_{Q_y})$$
$$>|^2\delta[E_n(k_z) - E_{n'}(k_z)]$$
$$\sim \left(\frac{2\pi}{\hbar}\right)\frac{|<\phi_n(x_0)|V(Q_y)|\phi_n(x_{Q_y})>|^2}{\hbar\omega_c}, \tag{8}$$

which involves the overlap of shifted harmonic oscillators. According to the aufbau principle, Landau levels are successively filled according to their energies and the Pauli exclusion principle. For metals and semiconductors, typical values of n at the chemical potential are given by

$$n\hbar\omega_c = W, \tag{9}$$

where W is the width of the occupied portion of the (free-electron or unhybridized) conduction band. For large values of n, one may use the asymptotic expressions for the overlap of the displaced oscillator wave functions and arrive at the expression

$$\frac{\hbar}{\tau_n} = \frac{|V(Q_y)|^2}{n\,\hbar\omega_c}. \tag{10}$$

Hence, the relative time spent in the Landau orbital before Bragg scattering occurs is given by

$$\left(\frac{\omega_c\tau_n}{2\pi}\right) = \frac{W\,\hbar\omega_c}{|V(Q_y)|^2}. \tag{11}$$

The criterion for magnetic breakthrough is that the broadening of the Landau levels due to Bragg scattering should be smaller than the spacing of the Landau levels

$$\frac{W\,\hbar\omega_c}{|V(Q_y)|^2} > 1, \tag{12}$$

which is same criterion arrived at by Blount [17], Pippard [20,21], and Reitz [22]. Although the above derivation assumes that the lattice potential is weak, as shown by Chambers [23], the same criterion can be found by considering the case where the crystalline potential is strong. The criterion can also be applied to real metals [24]. The above expression for the criterion carries an extra factor of $n \sim \frac{W}{\hbar\omega_c}$ compared to the criterion shown in Eq. (3) that was originally proposed by Cohen and Falicov [16]. The factor of n is not inconsequential for most metals, since for Cu with $B = 10$ T, $n \sim 6000$. The correct criterion is much more favorable for the occurrence of magnetic breakthrough. The amplitude of the oscillations is affected by the smearing of the Landau levels, which results in the amplitudes being suppressed by an exponential factor:

$$\exp\left[-\frac{2\pi}{\omega_c\tau_n}\right] = \exp\left[-\frac{|V(Q_y)|^2}{W\hbar\omega_c}\right]. \tag{13}$$

The above exponential factor is similar to the Dingle factor incorporated into the standard Lifshitz-Kosevich formulation of dHvA oscillations. The Dingle factor represents the disruption of Fermi-surface orbits caused by scattering off impurities [25] or off collective electronic fluctuations [26]. However, it should be stressed that the above exponential factor does not represent scattering by spatial or temporal fluctuations (collisions) but, instead, is due to the static periodic crystalline potential. The exponential factor only produces a small effect on the anomalous orbits in the breakthrough regime, but produces a large suppression of the anomalous oscillations in the low-field regime.

III. DISCUSSION

The above analysis can be applied to the hybridization gap model of SmB_6 [4], in which case the hybridization matrix element V that produces the avoided band crossings should be identified with $V(\underline{Q})$. With this identification, the direct gap is given by $2V$ and the indirect gap is given by 2Δ, where

$$\Delta = \frac{V^2}{W}. \tag{14}$$

One finds that the magnetic breakthrough should occur whenever

$$\hbar\omega_c > \Delta \tag{15}$$

and that the amplitude of the anomalous oscillations are suppressed by a factor of

$$\exp\left[-\frac{\Delta}{\hbar\omega_c}\right]. \tag{16}$$

These estimates are consistent with the results for the hybridization gap model found numerically by Knolle and Cooper [27]. However, Knolle and Cooper did not identify the origin of their results as being due to magnetic breakthrough. On using an effective mass of 0.23 m_e [15] and an indirect hybridization gap, 2Δ, of the order of 20 meV [28], one finds a critical field of 20 T. For fields of the order of 40 T, it is estimated that the amplitude of the anomalous oscillations is suppressed by a factor of the order of 0.6 that should render them observable with amplitudes similar to usual oscillations in a bulk metal. On the other hand, for fields in the range between 5 and 10 T, the anomalous amplitudes are suppressed to between 2% and 14% of their high-field values and so should be difficult to observe. This is consistent with the three-dimensional oscillation that were observed by Tan *et al.* [14] and their absence in the analysis of Li *et al.* [12] which focused on the small area oscillations of the metallic surface states found in the lower-field regime. The magnetic breakthrough of the hybridization gap in SmB_6 should lead to the anomalous orbits enclosing areas similar to the Fermi-surface areas found for LaB_6 [15], since the $4f$ levels in La are above the Fermi energy and, therefore, do not produce hybridization gaps. This assertion is supported by the estimates of the Fermi surface from magnetoresistance measurements [29] on the metallic state of SmB_6, produced by the application of high fields and pressure. The hypothesis of magnetic breakthrough is also supported by the similarity of the small effective masses of $m^* \sim 0.18\, m_e$ found by Tan *et al.* [14] to the smallest effective masses ($m^* \sim 0.23\, m_e$) inferred from dHvA measurements on LaB_6 [15]. Since larger masses are also found in LaB_6, they could be expected to be observed in SmB_6; however, larger masses are harder to see in dHvA experiments.

A related explanation of the high-field oscillations in SmB_6 has recently been proposed [31] which is based on a model that consists of a pair of hybridized bands. The model was constructed to accommodate parity inversion as required for a topological insulator. Crucially, the authors use a spin-orbit-coupling hybridization matrix element V which, due to the factor of $\underline{k}$, mixes states with opposite parity. The two bands are modeled by inverted parabolic bands with different effective masses, in which the Fermi-level lies within the hybridization gap. The assumed dispersion of the bands is not crucial since, by adiabatically continuing the $4f$ mass upwards, the model reduces to a (spin-orbit) hybridized band model with an almost flat $4f$ band. To be sure, the topological invariants are independent of the dispersion relation and, as long as there is no band-crossing, can be calculated by using the flat-band approximation. Since the adiabatic continuation does not produce degeneracy [32], the topological character of the model remains invariant but remains inequivalent to the hybridization band model in which the hybridization matrix element is assumed to be k independent. The inequivalence occurs since a k-independent hybridization matrix element only mixes states with the same parity. Since the spin-orbit-induced hybridization is associated with the potential of the crystalline lattice, the oscillations are classifiable as being due to magnetic breakthrough. The criterion at which the breakthrough occurs is different from that of the hybridized band model, in that the W in the factor of $\frac{W}{\hbar\omega_c}$ is replaced by the small energy-separation $\sim$300 meV between the top and the bottom of the electron and hole pockets.

IV. CONCLUSION

While the above analysis does not rule out more exotic scenarios, such as a Fermi sea of Majorana fermions [33] or the description of SmB_6 as a failed superconductor [34], it does offer an explanation in terms of the well-known and well-tested mechanism of magnetic breakthrough. It remains to be shown whether the field and temperature dependencies of the experimentally observed high-field three-dimensional oscillations have an amplitude and field dependence consistent with the breakthrough formula that includes the field [29,30] and temperature [3] dependencies of the hybridization gap. Likewise, the small values of the effective masses extracted from the surface oscillations ($m^* \sim 0.1-0.2\, m_e$) need to be reconciled with the larger quasiparticle masses ($m^* \sim m_e$) inferred from the Weyl cone dispersion relations found in ARPES [9–11] and the heavy quasiparticle masses ($m^* \sim 10-100\, m_e$) inferred from magnetothermoelectric measurements [35]. A second crucial question that needs to be answered is the following: Why are Shubnikov–de Haas oscillations not seen in the surface resistivity? Another interesting and possibly related question is whether bulk spin-excitons in SmB_6 [36–38], due to the long decay lengths of the surface state (estimated from $\xi \sim \frac{\hbar v_F}{\Delta}$, with $v_F \sim 6.5 \times 10^5$ m/s [12] as $\xi \sim 430$ Å), couple to the metallic surface states [39], and if so, is the resonant interaction [40] responsible for the observed decrease in magnetic activity within 400–900 Å of the surface [41]?

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