Chemical potential asymmetry and quantum oscillations in insulators

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(Received 14 April 2016; revised manuscript received 24 July 2016; published 21 September 2016)

We present a theory of quantum oscillations in insulators that are particle-hole symmetric and nontopological but with arbitrary band dispersion, at both zero and nonzero temperature. At temperatures T less than or comparable to the gap, the dependence of oscillations on T is markedly different from that in metals and depends crucially on the position of the chemical potential μ in the gap. If μ is in the middle of the gap, oscillations do not change with T; however, if μ is asymmetrically positioned in the gap, surprisingly, oscillations go to zero at a critical value of the inverse field determined by T and μ and then change their phase by π and grow again. Additionally, the temperature dependence is different for quantities derived from the grand canonical potential, such as magnetization and susceptibility, and those derived from the density of states, such as resistivity. However, the nontrivial features arising from asymmetric μ are present in both.

DOI: 10.1103/PhysRevB.94.125140

I. INTRODUCTION

Quantum oscillations provide one of the most commonly used experimental tools to study metallic band structures, in both weakly and strongly correlated systems [1–5]. They arise from Landau levels (LLs) crossing the Fermi level periodically as a function of the magnetic field. Such oscillations, therefore, are expected only in metallic systems with a Fermi surface.

Recently, this canonical understanding has been challenged by the observation [6] of quantum oscillations in SmB_6, which is believed to be a topological Kondo insulator [7–11]. While the exact origin of the oscillations is still being debated [12,13], it raises the questions: can quantum oscillations arise in insulators? If yes, how are they different from oscillations in metals? Two recent works have addressed these questions for specific models. Reference [14] considered a model—inspired by the experiment in Ref. [6]—of a flat band hybridized with a dispersive band leading to a gap, and found oscillations in the magnetization with a temperature dependence that is nonmonotonic. However, it is not clear to what extent such findings depend on the enhanced density of states due to the flat band and the resulting strong particle-hole asymmetry. In contrast, Ref. [15] considered a model of a topological insulator and found multiple phase changes in oscillations in density of states (DOS) accompanied by a nonmonotonic temperature dependence. These features, however, are entirely a consequence of the topological properties of the model and are not expected in an ordinary insulator. A theory—and general understanding—of oscillations in insulators is missing.

In this paper, we present a theory of quantum oscillations in insulators, at both zero and nonzero temperature. We construct our theory for a class of systems that are particle-hole symmetric and nontopological, but with arbitrary band dispersion. The motivation for adopting such a model is not to simply contrast our results with those of Refs. [14] and [15]: realistic systems with narrow gap and inverted bands where oscillations could be observed (reasons for such requirements are discussed later), such as bilayer graphene at certain rotation angles [16–18], materials at the onset of spin/charge density wave [19,20], gapped nodal-line semimetals [21,22], etc., are, in fact, well described by the above model. In spite of the simplicity of our model, we find oscillations that do not follow the Lifshitz-Kosevich (LK) formula valid for metals, with features different from those reported in previous works [14,15]. The gap provides a new scale in the problem leading to new features when the temperature T is less than or comparable to this scale. Our main finding is that, in addition, the gap also provides a new degree of freedom not found in metals: the position of the chemical potential μ inside the gap. If μ is in the middle of the gap, i.e., $\mu = 0$, oscillations do not change with temperature leading to a plateau in the temperature dependence; however, if it is asymmetrically positioned in the gap, i.e., $\mu \neq 0$ (but still in the gap), surprisingly, oscillations go to zero at a critical value of the inverse field determined by T and μ and then change their phase by π and grow again, mimicking properties of a topological insulator in an ordinary insulator! Additionally, oscillations behave differently for physical observables that are derived from the grand canonical potential and those that are related to the DOS; however, the nontrivial features arising from $\mu \neq 0$ are present in both families of observables.

II. MODEL

Consider two identical overlapping bands with opposite curvature hybridized by some parameter. In band space, the Hamiltonian can be written as ($\hbar = k_B = 1$)

$$H_{\mathbf{k}} = \begin{pmatrix} \varepsilon_{\mathbf{k}} - \Delta & \zeta \\ \zeta & -\varepsilon_{\mathbf{k}} + \Delta \end{pmatrix}, \tag{1}$$

where $\varepsilon_{\mathbf{k}}$ and 2Δ denote the band dispersion (assumed nontopological) and band overlap in the absence of the gap, respectively, and $\zeta > 0$ is a parameter that opens a gap (we assume $\varepsilon_{k=0} = 0$ is an extremum and Δ has the appropriate sign to ensure band overlap at $\zeta = 0$). The LLs for the Hamiltonian in Eq. (1) are given by

$$E_n^{\pm} = \pm\sqrt{(\varepsilon_n - \Delta)^2 + \zeta^2}, \tag{2}$$

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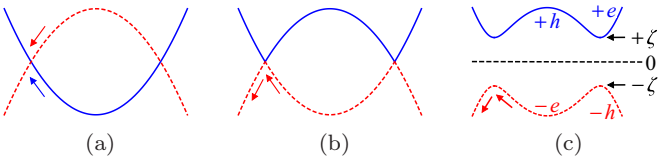

FIG. 1. Alternative ways of viewing overlapping bands: in terms of (a) electron (blue, solid) and hole (red, dashed) levels and (b) occupied (red, dashed) and unoccupied (blue, solid) levels. (c) The latter picture easily extends to the case when a gap opens (gap exaggerated for clarity): ± are band indices and e/h refer to electron/holelike parts. In the presence of a magnetic field, LLs are formed. The arrows show the direction in which they move as field is increased.

where ε_n denotes the LLs corresponding to $\varepsilon_{\mathbf{k}}$. In the ungapped case, the customary way to understand quantum oscillations is in terms of electron and hole levels in the two bands crossing the Fermi level μ at the intersection of the bands in opposite directions as a function of the magnetic field [Fig. 1(a)]. An alternative way is to think only in terms of occupied levels in the two bands. The LLs from the electron band, on reaching the Fermi level, just "rolls over" to the hole band [arrows in Fig. 1(b)]. As seen in Fig. 1(c), even when the system is gapped, one can still separate the lower filled band into electronlike and holelike parts. The band edge $E_v = -\zeta$ now plays a role similar to the Fermi level in the ungapped case, giving rise to oscillations [15].

III. ZERO TEMPERATURE

Consider a 2D system described by the Hamiltonian in (1). In the presence of a magnetic field B, the grand canonical potential at $T = 0$ reads $\Omega = D\sum_{E_n^- \leqslant E_v}[E_n^- - E_v]$, where $D = geB/2\pi$ is the degeneracy factor in 2D (g denotes any extra degeneracy from internal degrees of freedom) [1]. Following our previous discussion, we decompose the sum into two parts:

$$\frac{\Omega(B)}{D} = \sum_{n=0}^{N_v}\left(E_n^{-,e} - E_v\right) + \sum_{N_v+1}^{\Lambda}\left(E_n^{-,h} - E_v\right) = \frac{\Omega^{-,e}}{D} + \frac{\Omega^{-,h}}{D}, \tag{3}$$

where $E_n^{-,e/h}$ denote the electronlike and holelike parts of the lower filled band, respectively, N_v is the highest LL with energy smaller than E_v in the electronlike part of the spectrum, and Λ is a cutoff for the holelike part of the band ($E_\Lambda^- \sim$ bandwidth).[1]

[1]One can argue that the presence of the artificial cutoff Λ can give rise to spurious oscillations [15]. However, as mentioned before, the decomposition in Eq. (3) can as well be applied to the ungapped case when $\zeta = 0$, where we are guaranteed to have no oscillations other than the ones arising from the Fermi level, i.e., the results do not depend on the cutoff. In the case of $\zeta \neq 0$, we formally choose the same cutoff, and avoid the problem of spurious oscillations.

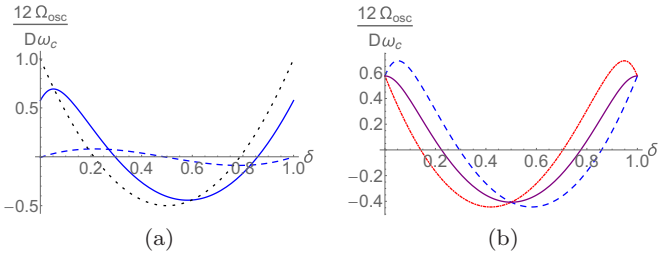

FIG. 2. (a) $\Omega_{\rm osc}^{-,e}$ for $\zeta/\omega_c = 0.1$ (blue, solid) and $\zeta/\omega_c = 1.2$ (blue, dashed) compared with the case of $\zeta = 0$ (black, dotted). (b) $\Omega_{\rm osc}^{-,e}$ (blue, dashed), $\Omega_{\rm osc}^{-,h}$ (red, dot-dashed), and $(\Omega_{\rm osc}^{-,e} + \Omega_{\rm osc}^{-,h})/2$ (purple, solid) for $\zeta/\omega_c = 0.1$. Here, δ is a quantity that measures how far the last LL N_v is from the lower edge of the gap in $-,e$ band (for an exact definition refer to the text); thus, $\delta = 0$ and $\delta = 1$ signify the crossing of two consecutive LLs across the gap edge, and corresponds to one period of oscillation. The pattern is repeated giving rise to quantum oscillations.

To compute the discrete sums in Eq. (3), we use the Euler-MacLaurin formula. This gives for each of the terms $\Omega^{-,e/h}$ a part that varies smoothly with the field and a part that oscillates with the inverse of the field. The behavior is decided by two energy scales: the gap parameter ζ and the cyclotron frequency of the unhybridized bands, $\omega_c = eB/m$, where m is the cyclotron mass of the unhybridized bands. In the limits $\zeta/\omega_c \ll 1$ and $\zeta/\omega_c \gg 1$, the oscillating terms $\Omega_{\rm osc}^{-,e/h}$ can be calculated exactly, but they are cumbersome—see Ref. [23]. Instead, in Fig. 2(a), we plot $\Omega_{\rm osc}^{-,e}$ as a function of δ in the two limits. Here, $\delta = (l_B^2/2\pi)[S(E_v) - S(E_{N_v})]$, where $l_B = 1/\sqrt{eB}$ is the magnetic length and $S(E)$ is the $\mathbf{k}$-space area occupied at energy E by an orbit, governing the semiclassical quantization condition $S(E_n)l_B^2 = 2\pi(n+\gamma)$, with γ being a phase [1]. To understand the meaning of δ, consider the simple case of parabolic bands: δ reduces to $\Delta/\omega_c - (N_v + 1/2)$; thus, it is a measure of how far the last LL is from E_v in the $-,e$ band. Clearly, $0 \leqslant \delta < 1$, with the limits denoting the crossing of two consecutive LLs across E_v, and a plot of $\Omega_{\rm osc}^{-,e}$ versus δ gives one period of oscillations—the pattern must be repeated. Compared to the ungapped case, we find two features as a result of the gap: a reduction in amplitude and a phase offset, with both becoming more pronounced as ζ/ω_c increases. Also, in Fig. 2(b), we compare $\Omega_{\rm osc}^{-,e}$ with $\Omega_{\rm osc}^{-,h}$ along with the total, $\Omega_{\rm osc} = \Omega_{\rm osc}^{-,e} + \Omega_{\rm osc}^{-,h}$. The phases in $\Omega_{\rm osc}^{-,e}$ and $\Omega_{\rm osc}^{-,h}$ differ by a sign, resulting in a further reduction in amplitude in the total. With this insight, we approximate the curves by their leading Fourier components,

$$\frac{\Omega_{\rm osc}^{-,e/h}(B)}{D} \sim \omega_c f\left(\frac{\zeta}{\omega_c}\right)\cos\left[S(E_v)l_B^2 - 2\pi\gamma \pm \phi\left(\frac{\zeta}{\omega_c}\right)\right], \tag{4}$$

with ± referring to e/h parts, respectively, and $f = 1$ and $\phi = 0$ at $\zeta = 0$. Note that the area at the band edge in the gapped case is same as the area at the intersection of the two bands in the ungapped case, i.e., $S(E_v) = S(0)|_{\zeta=0}$. Denoting this area by S_0 and adding the e/h contributions in Eq. (4), we get

$$\frac{\Omega_{\rm osc}(B)}{D} \sim \omega_c f\left(\frac{\zeta}{\omega_c}\right)\cos\left[\phi\left(\frac{\zeta}{\omega_c}\right)\right]\cos\left[S_0 l_B^2 - 2\pi\gamma\right]. \tag{5}$$

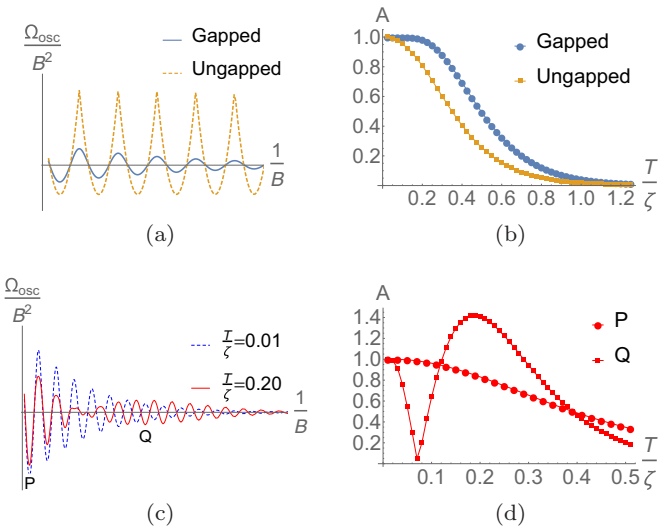

FIG. 3. Numerical calculations on a lattice model mimicking (1) with two square lattices hybridized to open a gap at quarter filling (see Ref. [23] for details). Here, $\zeta = 0.1t$, where t is the hopping parameter. (a) Oscillations at $T = 0$: frequency of oscillations does not change with the introduction of the gap; (b) Dependence of amplitude A on T for $\mu = 0$: a plateau appears at $T < \zeta$ in the gapped case (both curves are normalized with their respective $T = 0$ values); (c) Oscillations at two different temperatures for $\mu = -0.09t$ (i.e., $|\mu|/\zeta = 0.9$). The beatlike pattern with change of phase by π accompanied by an increase in amplitude emerges when temperature is increased. (d) Dependence of oscillations on T at two different field values marked P and Q in (c), normalized with their respective $T = 0$ values.

In the limit $\zeta/\omega_c \gg 1$, we find $f(\zeta/\omega_c) \propto 1/(\zeta/\omega_c)$ and $\phi(\zeta/\omega_c) \to \pi/2$. Thus, on opening a gap, the system shows quantum oscillations with a frequency equal to that in the ungapped case, but with an amplitude that decays as the product of the functions f and $\cos[\phi]$. This is verified by numerical calculations on a lattice—see Fig. 3(a). Numerically, we find that the oscillations decay rapidly, becoming inappreciable at $\zeta \gtrsim \omega_c$. As an estimate, at field ~10 T, and mass equal to 0.01 time the bare electronic mass, gaps <100 meV are expected to show oscillations; thus, bands with light masses and narrow gap are required. The main result of the $T = 0$ study is the factorization of the amplitude into two terms, and in particular the appearance of the term $\cos[\phi]$. This is unanticipated, and leads to novel effects at nonzero temperature, as shown below. All quantities derived from Ω by taking appropriate derivatives with respect to the field (magnetization, susceptibility), will inherit oscillations with the same characteristics as well.

IV. NONZERO TEMPERATURE

We now consider the effects of temperature which is included by averaging $\Omega_{\rm osc}$ at different energies at zero temperature, appropriately weighted by the derivative of the Fermi-Dirac function f_0:

$$\Omega_{\rm osc}(\mu,T) = \int_{-\infty}^{\infty} \frac{-\partial f_0(E-\mu)}{\partial E}\Omega_{\rm osc}(E,0)dE. \qquad (6)$$

Although oscillations at $T = 0$ do not depend on the exact value of μ as long as μ lies in the gap, the behavior at $T \neq 0$ is dependent on the position of μ inside the gap (via f_0). This extra degree of freedom is a unique feature of insulators not found in metallic systems.

Consider first the case when μ is exactly in the middle of the gap, i.e., $\mu = 0$. It is important to note that, while $\Omega_{\rm osc}(E,0)$ varies with energy inside the bands, inside the gap it is independent of energy and *nonzero*—it is simply equal to the value at the gap edge, i.e., $\Omega_{\rm osc}^{\rm gap}$ is given by Eq. (5). At low temperatures, $T/\zeta \ll 1$, since the integral in Eq. (6) gets its dominant contribution from the gap, it implies $\Omega_{\rm osc}$ is independent of T resulting in a plateau–a departure from conventional behavior and supported by numerical calculations [Fig. 3(b)]. This should be compared to the behavior found in Ref. [14] in the same regime: instead of a plateau the dependence was found to be nonmonotonic with a maximum. This implies that the behavior found in Ref. [14] is a result of the extreme particle-hole asymmetry arising from the flat band in their model and is not a generic feature of an insulator. In the other limit, $T/\zeta \gg 1$, the dominant contribution to the integral comes from the two bands and the gap can be neglected. One then recovers the exponential decay due to dephasing typical of metals, provided by LK formalism.

Next, we consider $\mu \neq 0$ with $|\mu| < \zeta$, i.e., the system remains an insulator but μ lies asymmetrically in the gap. Such a situation can arise due to impurities (extrinsic semiconductors) or can be imposed by an external gate in experiments. The behavior for $T \ll \zeta - |\mu|$ and $T \gg \zeta$ is similar to that in the case $\mu = 0$. However, in the intermediate regime, $\zeta - |\mu| \lesssim T \lesssim \zeta$, the new scale $|\mu|$ introduces surprising new features. The effect of temperature is no longer restricted to the overall amplitude. Instead, as seen in Fig. 3(c) obtained numerically, oscillations go to zero at a critical value of the inverse field, $1/\omega_c^*$, and then change their phase by π and grow again. With increase in temperature, $1/\omega_c^*$ moves to the left with increase in amplitude to its right and decrease in amplitude to its left [Fig. 3(d)]. In the limit of strong asymmetry in μ, i.e, $\zeta - |\mu| \ll \zeta$, such a behavior can be explained analytically. When $\mu = 0$, oscillations arising from $+E$ and $-E$ get equal thermal weight while computing the average in Eq. (6). This particle-hole symmetry in the averaging is lost when $\mu \neq 0$, even though the bands are still particle-hole symmetric. One can show that (see Ref. [23]) this leads to an extra phase in Eq. (4) on top of the overall prefactor: the zero temperature result is modified into $\Omega_{\rm osc}^{e/h}(T)/D \sim \omega_c A(T) f(\zeta/\omega_c)\cos[S_0 l_B^2 - 2\pi\gamma \pm \phi(\zeta/\omega_c) \pm \psi(T)]$. Adding the two contributions, we have

$$\frac{\Omega_{\rm osc}(T)}{D} \sim \omega_c A\left(\frac{T}{\omega_c},\frac{T}{\zeta},\frac{|\mu|}{\zeta}\right) f\left(\frac{\zeta}{\omega_c}\right)\cos\left(S_0 l_B^2 - 2\pi\gamma\right) \times \cos\left[\phi\left(\frac{\zeta}{\omega_c}\right) + \psi\left(\frac{T}{\omega_c},\frac{T}{\zeta},\frac{|\mu|}{\zeta}\right)\right]. \qquad (7)$$

Whereas $A(T)$ is a decreasing function as in the case of $\mu = 0, \psi(T)$ increases with T and reaches a maximum determined by $|\mu|$, before going to zero. Equation (7) leads to an unusual beatlike (but not exactly a beat) pattern driven by temperature that matches Fig. 3(c). This arises from a competition between ϕ and ψ in the second cosine function in Eq. (7). Recall, $\phi \to \pi/2$ as $1/\omega_c \to \infty$. In the presence of ψ, $\phi + \psi$ reaches $\pi/2$ at a finite value of $1/\omega_c$. This is where oscillations go to

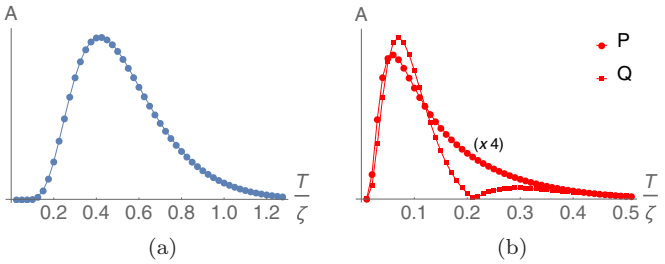

FIG. 4. Amplitude of oscillations A (arbitrary units) vs T for the density of states in the gapped case obtained from numerical calculations on a lattice (same as in Fig. 3) with $\zeta = 0.1t$ for (a) $\mu = 0$ and (b) $\mu = -0.09t$ [P and Q correspond to two field values given in Fig. 3(c)]. The figures should be compared to Figs. 3(b) and 3(d), respectively. The behavior for $T \ll \zeta$ is clearly different. Note, however, the extra nontrivial features in the case $\mu \neq 0$ found in Fig. 3(d) persist in Fig. 4(b) as well.

zero and is the origin of the critical field. The sign of the cosine function is opposite on either side of $1/\omega_c^*$ leading to a phase change by π. Note the crucial role ϕ, arising in the $T = 0$ theory, plays here: it forces the effect of $T \neq 0$ to be no longer separable from the $T = 0$ contribution, and is at the heart of the unusual behavior. The π phase shift here is temperature driven and not topological in origin, unlike in metals where it originates due to Berry phase [15,24]. Also, without proper insight, the pattern could easily be misconstrued as resulting from two Fermi surface pockets in metallic systems.

V. GRAND CANONICAL POTENTIAL VERSUS DENSITY OF STATES

It is usually thought that quantum oscillations in all physical observables have the same temperature dependence [1,25]. In an insulator, however, this is no longer true. Unlike quantities that are derived from the grand canonical potential, such as magnetization and susceptibility, quantities that depend on the DOS, such as resistivity and quantum capacitance, will obviously vanish in the gap at $T = 0$. This implies that the averaging in Eq. (6) at $T \neq 0$ is different: it is still governed by an equation similar to Eq. (6) (with Ω replaced by DOS ρ), except that now the integral gets no contribution from the gap. This results in a temperature dependence that is nonmonotonic, arising from a competition between thermal activation and dephasing. Numerical calculations on the lattice also confirm this behavior—see Fig. 4. Note, however, that the nontrivial features for $\mu \neq 0$ survive: oscillations show a similar pattern as in Fig. 3(c) changing their phase by π at a critical field with an unusual temperature dependence as shown in Fig. 4(b).

It is a remarkable coincidence that the nontirival features in the case of $\mu \neq 0$ discussed above also arise from a different physical mechanism, viz., nontrivial topology in topological insulators [15]. The question then arises, how to distinguish in an experiment which physical mechanism is at play. We point out two key differences between the two scenarios: first, in a topological insulator the gap is a function of the field, and the critical field marks the point when the Landau levels overlap in the gap making the system metallic. Thus, at $T = 0$, the DOS is zero on the insulating side but nonzero on the metallic side. In the case considered here, the system stays gapped at all

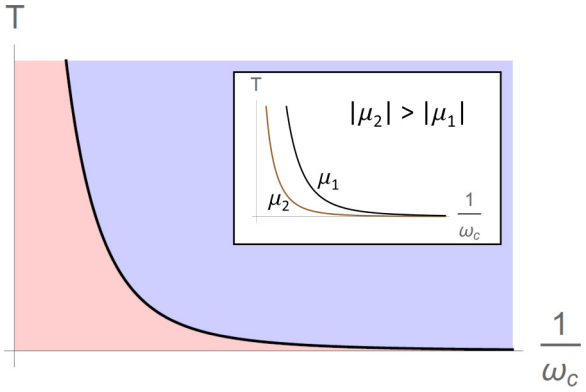

FIG. 5. The two shaded regions differ by a phase π in oscillations. The separatrix is a schematic variation of the critical field with temperature. (Inset) The separatrix moves to the left as $|\mu|$ increases. Numerical calculations on a lattice confirm this behavior—see Ref. [23].

fields; therefore, the DOS is zero at $T = 0$ on both sides of the critical field. Consequently, while both curves in Fig. 4(b) in our case start from zero at $T = 0$, one of the curves start from a nonzero value at $T = 0$ in the case of topological insulators (cf. Figs. 4(c) and 5(c) in Ref. [15]). Second and more importantly, the critical field in a topological insulator is a function of the band parameters only, and is independent of temperature. In our case, it is a function of both T and $|\mu|$. Thus, with increase in temperature, not only will oscillations behave differently on either sides of the critical field, the critical point itself will move to the left on $1/\omega_c$ axis—see Fig. 5. This should be compared with Figs. 4(d) and 5(d) in Ref. [15].

VI. CONCLUDING REMARKS

To summarize, we have presented a theory of quantum oscillations in insulators that are particle-hole symmetric and nontopological, but with arbitrary band dispersion, at both zero and nonzero temperature. The dependence of oscillations on temperature is found to be surprisingly rich, depending crucially on the position of the chemical potential in the gap. It is important to note that not all types of insulators will show quantum oscillations. If we change the sign of Δ in Eq. (1) so that there is no band inversion, it is obvious that such a model will show no oscillations. Thus, in addition to having a narrow gap, band inversion, which leads to a closed loop at the band edge, is needed. Although our results are derived for a 2D system, they apply as well to 3D systems, as long as the system is described by Eq. (1): as in metals, oscillations will arise from extremal orbits, but with properties modified due to the gap in a manner described above. Quantum oscillations, traditionally used to study metallic systems, could soon become a useful experimental tool to study narrow-gap systems with inverted bands.

ACKNOWLEDGMENTS

This work has been supported by the French program ANR DIRACFORMAG (ANR-14-CE32-0003) and LabEx PALM Investissement d'Avenir (ANR-10-LABX-0039-PALM).

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