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Phys. Rev. Lett. **121**, 026403 — Published 11 July 2018

DOI: 10.1103/PhysRevLett.121.026403

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Motivated by recent experiments on Kondo insulators, we theoretically study quantum oscillations from disorder-induced in-gap states in small-gap insulators. By solving a non-Hermitian Landau level problem that incorporates the imaginary part of electron's self-energy, we show that the oscillation period is determined by the Fermi surface area in the absence of the hybridization gap, and derive an analytical formula for the oscillation amplitude as a function of the indirect band gap, scattering rates, and temperature. Over a wide parameter range, we find that the effective mass is controlled by scattering rates, while the Dingle factor is controlled by the indirect band gap. We also show the important effect of scattering rates in reshaping the quasiparticle dispersion in connection with angle-resolved photoemission measurements on heavy fermion materials.

Quasiparticles in interacting/disordered systems generally have a finite lifetime due to the presence of electron-electron, electron-phonon or electron-impurity scattering. The decay of quasiparticles is formally described by the imaginary part of electron's self-energy. In small-gap systems, the decay of a quasiparticle can alter its energy-momentum dispersion significantly, for example, transform two-dimensional Dirac points into "bulk Fermi arcs" [1, 2].

In this work, we study the effect of quasiparticle lifetime on the quantum oscillation in small-gap insulators. The oscillation of various physical quantities, such as the magnetic susceptibility and resistivity with respect to the magnetic field is usually regarded as a key characteristics of metals with a Fermi surface [3]. The period of the oscillation is determined by the Fermi surface area, and the amplitude decay with the temperature is determined by electron's effective mass. Intriguingly, recent experiments found quantum oscillations in heavy fermion materials SmB_6 [4, 5] and YbB_{12} [6, 7], which are Kondo insulators with a small energy gap. The physical origin of these quantum oscillations in insulators is hotly debated [8–19].

Motivated by, but not limited to, these experiments on Kondo insulators, we theoretically study quantum oscillations from disorder-induced in-gap states in small-gap insulators. In a generic two-band model with a hybridization gap, disorder leads to finite quasiparticle lifetime and in-gap states. The spectrum and width of Landau levels in a magnetic field is calculated by solving a *non-Hermitian* Landau quantization problem that incorporates the imaginary part of electron's self-energy. The density of states inside the gap, which comes from the tails of broadened Landau levels, is found to exhibit oscillations periodic in $1/B$. The period is given by the Fermi surface in the absence of hybridization. An analytical formula is derived for the oscillation amplitude as a function of the indirect band gap, scattering rates and the temperature. For a wide range of parameters, the temperature dependence of the quantum oscillation is qualitatively similar to Lifshitz-Kosevich (LK) theory of normal metals [3, 20, 21]. A key difference, however, is that the cyclotron mass in the LK factor is not the band mass, but depends on the scattering rate. Moreover, the oscillation amplitude at a fixed temperature, i.e., the Dingle factor, is controlled by the indirect band gap, when the scattering rate is small.

The peculiarity of quantum oscillation amplitude we found in small-gap insulators, where the scattering rate controls LK factor instead of Dingle factor, is quite the opposite to the case of normal metals, where the scattering rate controls Dingle factor instead of LK factor. This result is an important prediction of our theory. It contrasts clearly with quantum oscillations in clean insulators that lack in-gap states, where the amplitude of magnetization oscillation exhibits non-monotonous temperature dependence [8] or deviates from LK factors [22], and the oscillation of thermally averaged density of states exhibits thermal activation behavior and drops to zero, instead of saturates, in the zero temperature limit [9, 11, 22].

We start by considering a generic two-band model with a hybridization gap:

$$H_0(\mathbf{k}) = \begin{pmatrix} \epsilon_1(k) & \Delta(\mathbf{k}) \\ \Delta(\mathbf{k}) & -\epsilon_2(k) \end{pmatrix}, \tag{1}$$

with $k \equiv |\mathbf{k}|$. Diagonal terms $\epsilon_1(k)$ and $-\epsilon_2(k)$ describe the dispersion of an electron-type and a hole-type band respectively, and $\Delta(\mathbf{k})$ describes their hybridization. This Hamiltonian in the inverted regime is widely used as a minimal model for the electronic structure of Kondo insulators at low temperatures [23]. In this context, the two bands come from d- and f-orbitals, and exhibit an avoided crossing on a circle or a sphere in k space $k = k_F$, which is set by the condition $\epsilon_1(k_F)+\epsilon_2(k_F) = 0$. Note that the hybridization gap $\delta(k_F) \equiv |\Delta(k_F)|$ is (much) larger than the indirect band gap δ, when the two bands are (highly) asymmetric, as shown in Fig. 1.

Disorder introduces in-gap states in the above model. The disordered Hamiltonian we shall study is $H = \sum_{\mathbf{k}} c^\dagger_{\mathbf{k}} H_0(\mathbf{k}) c_{\mathbf{k}} + \int d\mathbf{r} U(\mathbf{r}) c^\dagger_{\mathbf{r}} \Lambda c_{\mathbf{r}}$, where $c^\dagger \equiv (d^\dagger, f^\dagger)$ is the electron creation operator for the two orbitals. $U(\mathbf{r})$ is the impurity potential, which is assumed to be characterized by $\langle U(\mathbf{r})\rangle = 0$ and $\langle U(\mathbf{r})U(\mathbf{r}')\rangle = n_{\rm imp} U_0^2 \delta(\mathbf{r}-\mathbf{r}')$

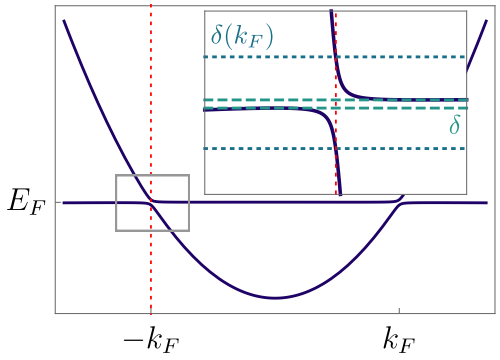

FIG. 1. Schematic band structure of a Kondo insulator. Inset: Zoom of the hybridization gap near $k = k_F$. $\delta(k_F)$ is the hybridization gap defined as the energy difference of the two bands at $k = k_F$. δ is the indirect band gap.

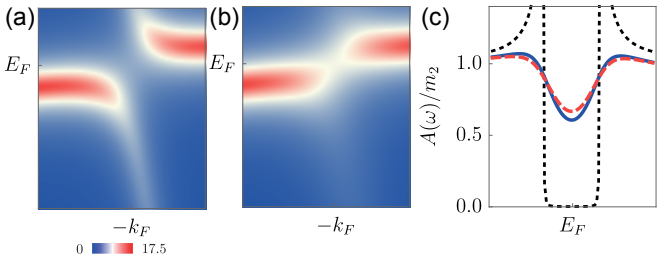

FIG. 2. (a) Spectral function $A(k,\omega)$ for model $\epsilon_i = k^2/(2m_i) - \mu_i$ $(i = 1, 2)$, $m_2/m_1 = 50$, $\delta(k_F)/(\mu_2 - \mu_1) = 0.02$, $\Gamma_2/\delta(k_F) = 0.1$, $\Gamma_1/\delta(k_F) = 0.7$, where the electron is spinless. The unit for colorbar is $1/\delta(k_F)$. (b) Same as (a) but with $\Gamma_1/\delta(k_F) = 1.7$. (c) Momentum-integrated spectral function $A(\omega)$ for model in (a) (blue, solid) and (b) (red, dashed) and in the clean limit $\Gamma_1 = \Gamma_2 = 0$ (black, dotted). The unit for $A(\omega)$ is m_2.

under disorder average. $n_{\rm imp}$ is the impurity density. The electron-impurity scattering is allowed to be orbital dependent, so the scattering vertex takes the form $\Lambda = \alpha I + \beta\sigma_z$. In heavy fermion systems, f-orbitals are tightly bound to the nucleus and scatter much less with impurities than d-orbitals do.

Using self-consistent Born and T-matrix approximation, we compute disorder-induced electron self-energy operator $\Sigma(\omega)$, which is a 2×2 matrix. In systems with p-wave hybridization, the self-energy is guaranteed to be diagonal [24]. The real part of $\Sigma(\omega)$ renormalizes the chemical potential and the inverted gap at $k = 0$, and for convenience, will be absorbed into H_0 in the following. The imaginary part of the self-energy becomes a nonzero diagonal matrix when the disorder strength $n_{\rm imp}U_0$ exceeds a critical value on the order of hybridization gap $\delta(k_F)$. At low energy $|\omega| \lesssim \delta(k_F)$, $\mathrm{Im}\,\Sigma(\omega)$ is weakly dependent on ω, hence can be approximated by

$$\Sigma(\omega) \simeq \begin{pmatrix} -i\Gamma_1 & 0 \\ 0 & -i\Gamma_2 \end{pmatrix} \equiv \frac{-i}{2}(\Gamma I + \gamma\sigma_z). \qquad (2)$$

$\Gamma_1, \Gamma_2 > 0$ are the inverse lifetimes of quasiparticles on the d- and f-band respectively, and we have defined $\Gamma \equiv \Gamma_1 + \Gamma_2$ and $\gamma \equiv \Gamma_1 - \Gamma_2$. Generally, $\Gamma_1 \neq \Gamma_2$ or $\gamma \neq 0$, as the two bands have different masses and disorder potentials.

The imaginary part of electron's self-energy modifies and broadens the quasiparticle dispersion, and creates in-gap states. To see this, we compute the spectral function $A(\mathbf{k},\omega) = -2\mathrm{Im}\left[1/(w - H_0(\mathbf{k}) - \Sigma)\right]$. For a given $\mathbf{k}$, $A(\mathbf{k},\omega)$ is a sum of Lorentzians associated with the poles of the Green's function $\mathcal{E}_\pm(\mathbf{k})$, which are complex eigenvalues of the non-Hermitian quasiparticle Hamiltonian $H(\mathbf{k}) \equiv H_0(\mathbf{k}) + \Sigma$. For our two-band model and self-energy defined by Eq. (1) and (2), the two eigenvalues $\mathcal{E}_\pm(\mathbf{k})$ are [1]

$$\mathcal{E}_\pm(\mathbf{k}) = \frac{1}{2}\Big(\epsilon_1(k) - \epsilon_2(k) - i\Gamma \pm \sqrt{(\epsilon_1(k) + \epsilon_2(k) - i\gamma)^2 + \Delta^2(\mathbf{k})}\Big) \qquad (3)$$

The real part of $\mathcal{E}_\pm(\mathbf{k})$, denoted as $\epsilon_\pm(\mathbf{k})$, is the dispersion of quasiparticle conduction and valence band, while its imaginary part determines the width of the broadened spectral function. In the special case of a single scattering rate $\Gamma_1 = \Gamma_2$ or $\gamma = 0$, the imaginary part is a constant so that the original band dispersion of $H_0(\mathbf{k})$ is broadened uniformly.

In the general case of two distinct scattering rates $\Gamma_1 \neq \Gamma_2$, $H_0(\mathbf{k})$ and Σ do not commute. Then $\gamma \neq 0$ has the nontrivial effect of altering the quasiparticle band dispersion $\epsilon_\pm(\mathbf{k})$, namely, damping reshapes dispersion. In particular, the quasiparticle hybridization gap at $k = k_F$ becomes reduced, given by

$$\epsilon_+(k_F) - \epsilon_-(k_F) = \begin{cases} \sqrt{\delta^2(k_F) - \gamma^2}, & \text{when } |\gamma| < \delta(k_F), \\ 0, & \text{when } |\gamma| \geq \delta(k_F). \end{cases} \qquad (4)$$

With increasing disorder, the scattering rates $\Gamma_{1,2}$ and hence $|\gamma|$ increases. Above a critical amount of disorder $|\gamma| > \delta(k_F)$, the quasiparticle gap completely vanishes, leading to a disorder-induced semimetal. In the semimetallic phase, the quasiparticle conduction and valence bands stick together on the Fermi surface $k = k_F$, despite that the hybridization term is present. Such band sticking without fine-tuning is a remarkable and topologically robust feature which is unique to non-Hermitian band theory of finite-lifetime quasiparticles [25], but forbidden by level repulsion in Hermitian band theory. As we shall show later, quantum oscillation appears in both insulator and semimetal phases.

In Fig. 2, we plot the spectral function $A(\mathbf{k},\omega)$ and the density of states $A(\omega) \equiv \int \frac{d\mathbf{k}}{(2\pi)^2} A(\mathbf{k},\omega)$ for different scattering rates $\Gamma_{1,2}$. Due to its localized nature, the

f-orbital has a smaller disorder-induced scattering rate $\Gamma_2 < \Gamma_1$. Panel (a) and (b) correspond to $|\gamma| < \delta(k_F)$ and $|\gamma| > \delta(k_F)$ respectively. We emphasize that the presence of two distinct scattering rates is necessary to reproduce many important features of the angle-resolved photoemission spectroscopy (ARPES) data on heavy fermion materials, which cannot be captured using $\Gamma_1 = \Gamma_2$ [24]. We note a systematic temperature-dependent ARPES study of the Kondo insulator SmB_6 showing that f-state spectra peak grows in height and narrows at low temperatures [26]. This observation is consistent with the existence of well-defined electron quasiparticles in the zero temperature limit, but does not favor the scenario of fractional excitations.

Due to the disorder scattering, the hybridization gap is partially filled, as shown by the density of states $A(\omega)$ in Fig. 2(c). Assuming the hybridization gap and scattering rates are small compared to the d-state band width, the density of states at low energy can be computed analytically [24]

$$A(\omega) = D_0 \mathrm{Im}\left[\frac{1}{\sqrt{\delta^2/\left[4(\omega + i\Gamma_A)^2\right] - 1}}\right]. \qquad (5)$$

with

$$\Gamma_A = \frac{m_1\Gamma_1 + m_2\Gamma_2}{m_1 + m_2},\ \delta \equiv \frac{2\sqrt{m_1 m_2}}{m_1 + m_2}\delta(k_F). \qquad (6)$$

Here $m_{1,2} > 0$ are effective masses for d- and f-band respectively, $D_0 = D_1 + D_2$ is the total density of states from both the d- and f-bands at the Fermi energy $\omega = 0$ in the absence of hybridization gap, and δ is the indirect band gap in the clean limit. The imaginary part Γ_A, a weighted sum of the two scattering rates, leads to disorder-induced broadening of density of states. Since the f band has a much larger mass $m_2 \gg m_1$, the indirect gap δ is much smaller than the hybridization $\delta(k_F)$, and even a small scattering rate Γ_2 is sufficient to generate considerable density of states within the gap, which is consistent with previous theoretical studies [27, 28] and experimental findings [29]. In-gap states in SmB_6 were also reported in numerous experiments, although its origin remains an open question. For example, the low temperature electronic specific heat grows linearly with temperature $C \sim \gamma T$ instead of exponentially. Our theory is consistent with recent experiments where a variation of γ from sample to sample is found [5, 30–32]. The large bulk AC conduction recently found in SmB_6 [33] also supports the existence of localized in-gap states.

We now show that in-gap density of states in our model exhibits quantum oscillation under magnetic field. To the leading order approximation, the scattering rates are taken to be field-independent. The density of states is then given by $A(\omega) = -(B/\pi)\mathrm{Im}\sum_j [1/(\omega - \mathcal{E}_j)]$, where $\mathcal{E}_j$ denotes the complete set of complex eigenvalues of the non-Hermitian Hamiltonian with Pierels substitution $\mathbf{k} \to \mathbf{k} - \mathbf{A}$ ($e = \hbar = 1$), i.e., $H(B) = H_0(\mathbf{k} - \mathbf{A}) + \Sigma$.

For concreteness, we consider two bands with quadratic dispersion in two dimensions: $\epsilon_i = k^2/(2m_i) - \mu_i$ ($i = 1, 2$), where $m_{1,2} > 0$ are the effective masses for d- and f-bands respectively. We take an isotropic p-wave hybridization gap: $\Delta(\mathbf{k}) = v(k_x s_x + k_y s_y)$. Its band structure is schematically shown in Fig. 1.

The exact non-Hermitian Landau level spectrum of $H(B)$ is derived analytically [24]. Each Landau level $n \geq 1$ consists of two sets of complex eigenvalues in each spin sector denoted by $s = \uparrow, \downarrow$:

$$\mathcal{E}^s_{n\geq 1,\pm} = \frac{1}{2}\Big(\epsilon^s_{1,n} - \epsilon^s_{2,n} - i\Gamma \pm \sqrt{\left[\left(\epsilon^s_{1,n} + \epsilon^s_{2,n}\right) - i\gamma\right]^2 + v^2(8nB)}\Big), \qquad (7)$$

where $\epsilon^s_{1,n} = B(n \pm 1/2)/m_1 + \mu_1$ and $\epsilon^s_{2,n} = B(n \mp 1/2)/m_2 + \mu_2$ (with upper/lower sign for $s = \uparrow, \downarrow$). For high Landau level $n \gg 1$, the exact result Eq. (7) is identical to the one obtained by simply replacing $k \to \sqrt{2nB}$ in the zero-field dispersion (Eq. (3)), and is thus also identical for both spin sectors. This agreement shows that semi-classical approximation remains valid for Landau quantization of finite-lifetime quasiparticles whose self-energy has an imaginary part.

Typical Landau level energy spectrum is plotted as a function of the magnetic field in Fig. 3(a) for the insulator phase, and (b) for the disorder-induced metal phase. Band edge oscillation can be seen clearly in both cases. For a given Landau level n, the hybridization gap is minimized when $B = k_F^2/(2n)$. In this way, the band edges of Landau levels oscillate with period $\Delta(1/B) = 2/k_F^2 = 2\pi/S_F$, where $S_F \equiv \pi k_F^2$ is the Fermi surface area in the absence of the hybridization. The oscillation of Landau level band edges leads to the oscillation of spectral function inside the gap, as the spectral weights inside the gap come from the tail of the broadened Landau levels. This effect, originated from the lifetime effect, persists even at zero temperature and in the limit of small (but nonzero) scattering rates.

We now turn to the field-dependent and thermally averaged density of states inside the gap, defined as $D(\omega, T) \equiv -\int_{-\infty}^{+\infty} dE \frac{\partial n_F(E-\omega,T)}{\partial E} A(E)$, where $n_F(\mu, T) = (e^{(E-\mu)/T} + 1)^{-1}$ is the Fermi-Dirac distribution function. Under the assumption of small hybridization gap $\delta(k_F) \ll k_F^2/\sqrt{m_1 m_2}$, weak magnetic field $B \ll k_F^2$ and low temperature $T \ll \delta(k_F), B/m_{1,2}$, the density of states can be analytically computed as [24]

$$D(\omega = 0, T) = -4\cos\left(\frac{\pi k_F^2}{B}\right)\sum_{i=\pm}\frac{M_i\frac{\pi^2 T}{\omega_{c,i}}}{\sinh\left(\frac{2\pi^2 T}{\omega_{c,i}}\right)}\exp\left(-\frac{\mathcal{D}_i}{B}\right), \qquad (8)$$

where $\omega_{c,i} \equiv B/M_i$ are the cyclotron frequencies associ-

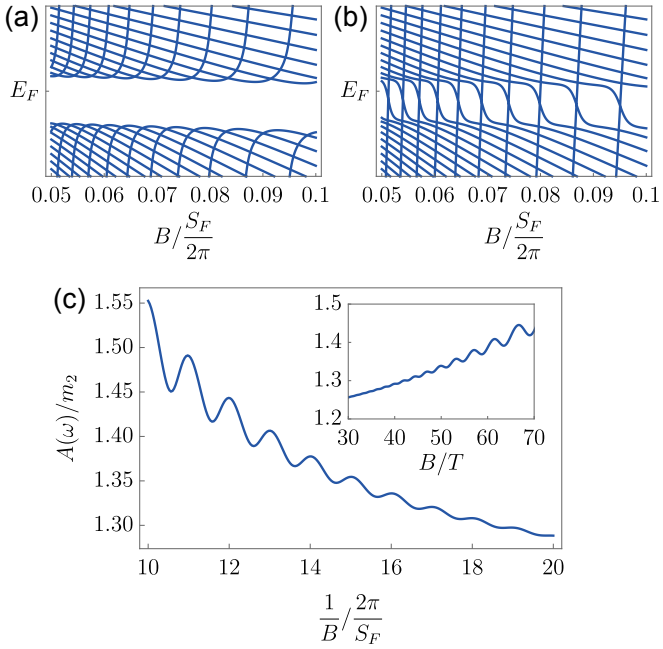

FIG. 3. (a) Real part of the Landau level spectrum $\mathrm{Re}[\mathcal{E}^{\downarrow}_{n,\pm}]$ as function of magnetic field, with the same model in Fig. 2(a). $s=\uparrow$ sector is similar. (b) Same as (a) but with the same model in Fig. 2(b). (c) Exact numerics of spectral function $A(\omega=0)$ as function of $1/B$ and B (inset) with the model in (a). Here both spin sectors are taken into account. The unit for $A(\omega)$ is m_2. $m_1=m_e$ is the free electron mass, hybridization gap is $\delta(k_F)=2$meV. The resulting indirect band gap is $\delta=0.56$meV and the oscillation frequency is $F=800$T.

ated with following effective masses

$$M_\pm=\frac{(m_1+m_2)}{2}\left[\frac{1}{\sqrt{1+\delta^2/(4\Gamma_A^2)}}\pm\frac{m_1-m_2}{m_1+m_2}\right], \quad (9)$$

and $\mathcal{D}_\pm$ are renormalized Dingle exponents

$$\mathcal{D}_\pm=\pi(m_1+m_2)\left(\Gamma_A\sqrt{1+\delta^2/(4\Gamma_A^2)}\pm\Gamma_D\right), \quad (10)$$

where $\Gamma_D\equiv(m_1\Gamma_1-m_2\Gamma_2)/(m_1+m_2)$.

The analytical formula for quantum oscillation amplitude, Eq. (8), is one of our main results, whose form is similar to that in free electron models [21] but with renormalized LK and Dingle factors. It is a sum of two oscillating components that share the same period $\Delta(1/B)=2\pi/S_F$. This periodicity is consistent with our expectation from the Landau level spectrum shown in Fig. 3, and has also been reported in previous works without including lifetime effects [8, 11, 14]. Note that this result is not completely obvious, as the conduction band minimum and valence band maximum are located at two different momenta $k_\pm\equiv\sqrt{k_F^2\pm(m_1-m_2)\delta}$, rather than at k_F [24]. Instead of having two periods given by $k_\pm^2$, the oscillation has a single period given by k_F^2, the Fermi surface area of the two bands in the absence of hybridization. We also note the phase of the oscillation is zero in Eq. (8), which is different from the π phase shift in a free electron model. Under strong magnetic field $B\sim k_F^2$, there will be a field-dependent phase shift [24] as has been reported recently [34–37].

The oscillation amplitude in Eq. (8) is determined by two scattering rates Γ_A and Γ_D, the indirect band gap δ and the temperature T. It reduces to familiar results in various limits. In the gapless limit $\delta(k_F)=0$, we reproduce the LK factors and Dingle factors for two metals. In the clean limit $\Gamma_1=\Gamma_2=0$, there is no density of state within the gap to the leading order of temperature and we find $D(\omega=0,T)=0$.

Although Eq. (8) is valid both in the insulating phase $\Gamma_{1,2}\ll\delta(k_F)$ and in the semimetallic phase $|\gamma|>\delta(k_F)$, in the following we focus on the insulating phase, which applies to Kondo insulators. A detailed study of the disorder-induced semimetallic phase will be presented elsewhere.

We first analyze the simplest particle-hole symmetric model when $m_1=m_2=m$ and $\Gamma_1=\Gamma_2=\Gamma$. In this case, $\Gamma_A=\Gamma$, $\Gamma_D=0$, and the LK effective mass and the Dingle exponent are

$$M=\frac{m}{\sqrt{1+\delta^2/(4\Gamma^2)}},\ \mathcal{D}=2m\pi\sqrt{\Gamma^2+\delta^2/4}. \quad (11)$$

For small scattering rate $\Gamma\ll\delta$, they reduce to $M\sim 2m\Gamma/\delta$ and $\mathcal{D}\sim m\pi\delta$. Decreasing the damping rate Γ leads to a smaller LK effective mass, and the Dingle exponent remains a constant controlled by the band gap.

The LK effective mass reflects the density of states inside the gap, since finite temperature effect is a thermal sampling of the spectral function through the convolution. Therefore, it is not a coincidence that Eq. (5) and Eq. (9) look similar. Indeed, the zero field density of states inside the gap is $A(\omega=0)=2m\Gamma/\delta=M$, which is exactly the LK effective mass.

In the general asymmetric cases $m_1\neq m_2$ and $\Gamma_1\neq\Gamma_2\ll\delta(k_F)$, the LK effective mass can vary in a wide range between m_1 and m_2 with proper choices of δ and Γ_A. The Dingle exponent remains a constant controlled by the band gap. This is opposite to that in normals metals when the scattering rate does not affect the LK effective mass but the Dingle factor.

As a concrete example, we present the quantum oscillation of the same model in Fig. 2(a). The density of states as function of $1/B$ is shown in Fig. 3(c). Since $\Gamma_D\neq 0$, the oscillation component associated with the larger Dingle factor becomes dominant [38], whose LK effective mass is $M=8.5m_e$, in between m_1 and m_2.

We note that the band edge oscillation in the absence of the scattering rate is also reported in Ref. [11]. Contrary to our theory, in that case, the quantum oscillation comes from thermally excited occupation of Landau levels above the gap, hence the oscillation amplitude vanishes at zero

temperature. Similar LK behavior of oscillation of thermodynamic observables in an insulator is also reported in a recent numerical study [14], which is consistent with our result.

Both the LK effective mass and the Dingle factor provide testable predictions of our theory. The parameters in our analysis—the two scattering rates—can be extracted from other measurements on in-gap density of states and ARPES spectral function. The oscillation of density of states inside the gap naturally leads to magnetic susceptibility oscillation, i.e., de Haas-van Alphen effect. The in-gap states may also contribute to the quantum oscillation in resistivity, and we leave a detailed study for future work. We hope the results of this work can help understand quantum oscillations in Kondo insulators, and motivate further study of quantum oscillations from in-gap states in small-gap insulators.

We thank Patrick Lee for insightful discussions and suggestions, Michal Papaj for collaboration on a related project, Lu Li and Yuji Matsuda for sharing their unpublished experimental results, and T. Senthil for interesting remarks. We also thank the anonymous referee who brings our attention to the enlightening experimental works. This work is supported by DOE Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-SC0010526. L.F. is partly supported by the David and Lucile Packard Foundation.

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