Quantum Oscillations in (Topological) Insulators

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Johannes Knolle & NRC, Phys. Rev. Lett. **115**, 146401 (2015)

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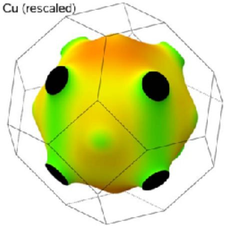
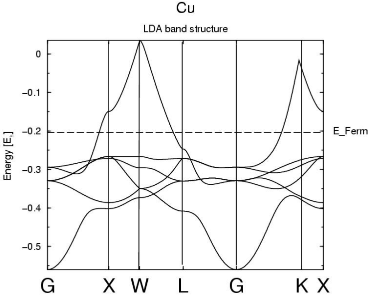
Band Theory

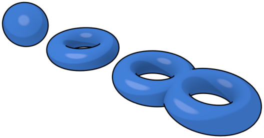
- Metal vs. Insulators from band theory
  → Bloch states + Pauli exclusion principle





Bands gaps, Fermi surface geometry, effective masses...

Topological Invariants

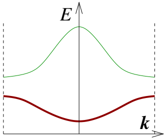


genus $g = 0, 1, 2, \ldots$

$$\frac{1}{2\pi}\int_{\text{closed surface}} \kappa \, dA \quad = \; (2-2g)$$

Gaussian curvature $\kappa = \dfrac{1}{R_1 R_2}$

2D Bloch bands [Thouless, Kohmoto, Nightingale & den Nijs (1982)]



Chern number $\mathcal{C} = \dfrac{1}{2\pi}\displaystyle\int_{\text{BZ}} d^2k\, \Omega_{\boldsymbol{k}}$

Berry curvature $\Omega_{\boldsymbol{k}} = -i\nabla_{\boldsymbol{k}} \times \langle u_{\boldsymbol{k}} | \nabla_{\boldsymbol{k}} u_{\boldsymbol{k}} \rangle \cdot \hat{\boldsymbol{z}}$

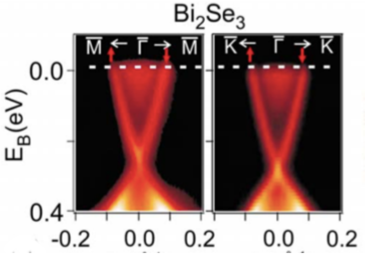
$\Rightarrow$ bulk insulator with $\mathcal{C}$ (chiral) metallic surface states

Topological Insulators

- Many generalizations when *symmetries* included:
topological insulators/superconductors in all d... [Hasan & Kane, RMP 2010]

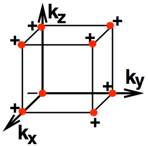
e.g. time-reversal symmetry
(non-magnetic material in $B = 0$)

⇒3D bulk insulator
with metallic 2D surfaces



[ARPES: Xia *et al.*, 2008]

Crossing of bands with
differing inversion symmetries



Topological Semimetals

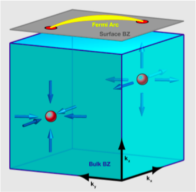
Topologically protected band touching points (topological defects)

[Armitage, Mele & Vishwanath, RMP **90**, 15001 (2018)]

e.g. 3D material with monopole of Berry flux

“Weyl node” $H_{\pm} = \mp \boldsymbol{p} \cdot \boldsymbol{\sigma}$

$\Rightarrow$surface metal with open “Fermi arcs”



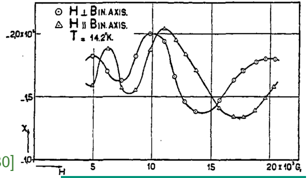
Re-emergence of exploration of band theory for novel settings

$+$ symmetry & topology in *strongly correlated* systems

Outline

de Haas – van Alphen Effect

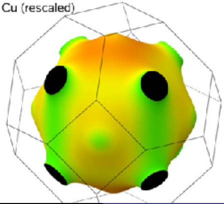
- Oscillation of the magnetization with applied magnetic field [dHvA, 1930]

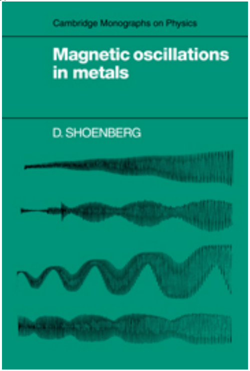


⇒quantization of cyclotron orbits [Landau, 1930]

- Landau, 1930: "unobservably small"

- Most precise method for determining Fermi surfaces of metals





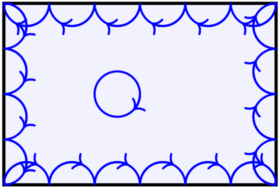
Peierls: Surprises in Theoretical Physics

Classical cyclotron orbit

$v = \omega_c r \qquad \omega_c = \frac{eB}{m}$

$$M = \pi r^2 \left(e \frac{v}{2\pi r} \right) = \frac{mv^2}{2B} \to \infty \text{ for } B \to 0 \text{ !?}$$

$\Rightarrow$surface currents



cancel the bulk moments exactly!

1) Use the free energy, $M = -\frac{\partial F}{\partial B}$

Classical partition function: $[F = -k_B T \ln Z, \beta = 1/k_B T]$

$$Z = \int e^{-\beta H(\boldsymbol{p} - e\boldsymbol{A}, \boldsymbol{r})} d^3\boldsymbol{p} d^3\boldsymbol{r}$$

vector potential, $\boldsymbol{A}$

$$= \int e^{-\beta H(\boldsymbol{p}', \boldsymbol{r})} d^3\boldsymbol{p}' d^3\boldsymbol{r}$$

Independent of vector potential $\Rightarrow$ $M = 0$

[Bohr – van Leeuwen theorem]

Classical cyclotron orbit  $v = \omega_c r \qquad \omega_c = \frac{eB}{m}$

Landau quantization: $E_n = (n + 1/2)\hbar\omega_c$

$$Z \sim \sum_{n=0}^{\infty} e^{-(n+1/2)\hbar\omega_c/k_B T} = \frac{1}{\sinh(\hbar\omega_c/2k_B T)}$$

Taylor expansion for small $z \equiv \frac{\hbar\omega_c}{k_B T}$

$$\Rightarrow M = -\frac{\mu_B^2 B}{3k_B T} + \ldots \qquad [\mu_B = \frac{e\hbar}{2m}]$$

No oscillatory component... ....even for FD statistics...

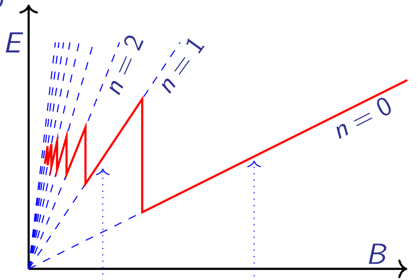
Surprise: $M_{\rm osc}(z) \sim \exp(-1/z)$ has no useful Taylor expansion in z

2) Consider extreme limit, $T = 0$

$$E_n = (n + 1/2)\hbar\omega_c$$

$$N_\phi = \frac{eB}{h} \times \mathcal{A}$$

fixed particle number N



$N_\phi > N \Rightarrow E_{tot} = N\frac{1}{2}\hbar\omega_c$

$2N_\phi > N > N_\phi \Rightarrow E_{tot} = N_\phi\frac{1}{2}\hbar\omega_c + (N - N_\phi)\frac{3}{2}\hbar\omega_c$

$E_{\rm tot}$ has cusps at $i \times \frac{eB}{h}\mathcal{A} = N$

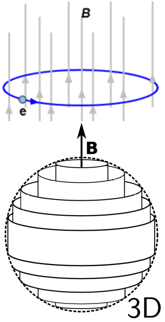
$\Rightarrow$ M oscillates with $\Delta\left(\frac{1}{B}\right) = \frac{\mathcal{A}}{N}\frac{e}{h}$

Lifshitz-Kosevich Theory [1954]

- Fermi liquid (non-interacting quasiparticles)
- Semiclassical quantization $[\ell_B = \sqrt{\frac{\hbar}{eB}} \gg \lambda_F]$

k-space area: $S_k \frac{\ell_B^2}{2\pi} = (n + 1/2)$

$$\text{Period: } \Delta\left(\frac{1}{B}\right) = \frac{1}{B_{n+1}} - \frac{1}{B_n} = \frac{2\pi e}{\hbar S_k}$$



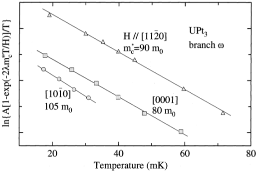
- Poisson summation formula (2D)

$$M_{\rm osc} \propto \sin\left(\frac{\hbar S_k}{e}\frac{1}{B}\right)\frac{\chi}{\sinh\chi} \qquad [\chi = \frac{2\pi^2 k_B T}{\hbar\omega_c}]$$

Lifshitz-Kosevich formula ⇒universal temperature dependence

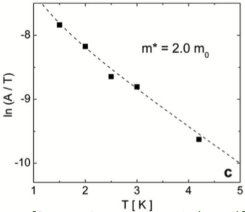
$$R(T) = \frac{\chi}{\sinh \chi} \qquad [\chi = \frac{2\pi^2 k_B T}{\hbar \omega_c}]$$

heavy fermions



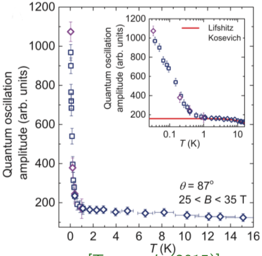
[Kimura *et al.* (2000)]

cuprates [YBCO]



[Doiron-Leyraud *et al.* (2007)]

SmB_6



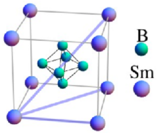
[Tan *et al.* (2015)]

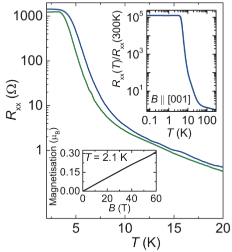
....a triumph of Fermi liquid theory... but... not always...

widespread assumption that QO implies FL theory is incorrect

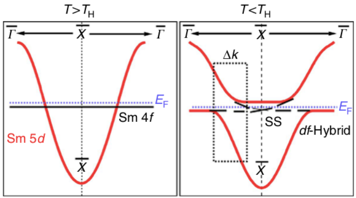
Samarium Hexaboride

- First "Kondo insulator" [Geballe 1969, Vainshtein 1964]
  - itinerant d electrons + localized f spins
  - insulating gap develops below $\sim$ 50K
  - mean-field description: interaction-induced d-f hybridization





[Tan et al., Science (2015)]

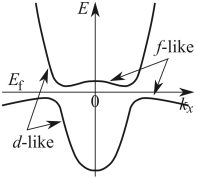


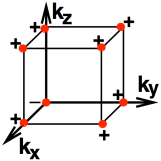
  - resistivity saturates at low temperatures!?

Samarium Hexaboride

⇒ *topological* Kondo insulator

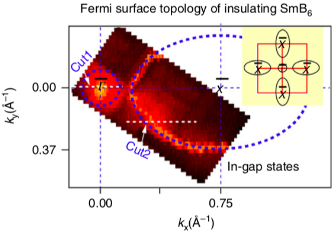
[Dzero, Coleman & Galitskii, 2010]





Saturation of resistance due to surface conduction

[Kim *et al.*, Sci. Rep. 2013]

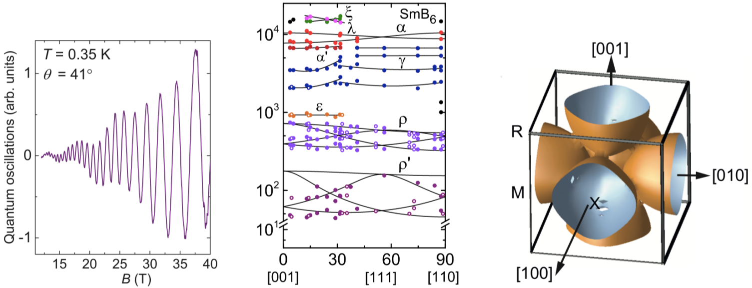


[Neupane *et al.*, Nat. Commun. 2013]

Unconventional Fermi surface in an insulating state

[Science **349**, 287-290 (2015)]

B. S. Tan,[1] Y.-T. Hsu,[1] B. Zeng,[2] M. Ciomaga Hatnean,[3] N. Harrison,[4] Z. Zhu,[4] M. Hartstein,[1] M. Kiourlappou,[1] A. Srivastava,[1] M. D. Johannes,[5] T. P. Murphy,[2] J.-H. Park,[2] L. Balicas,[2] G. G. Lonzarich,[1] G. Balakrishnan,[3] Suchitra E. Sebastian[1]*



Do you always measure what you think you measure?

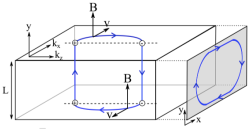
The dHvA effect widely assumed to be a signature of a metal

Quantum Oscillations in Insulators

1) Use free energy, $M = -\frac{\partial \Omega}{\partial B}$ [here GCE, $\Omega(\mu, T)$]

Surface states (topological or not) play no special role.

cf. QOs in Weyl semimetals
require phase coherence over width L
[mesoscopic effect]

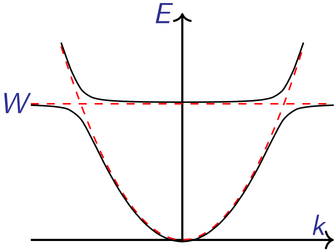


[Potter, Kimchi & Vishwanath, Nat. Comm. (2014)]

[J. Knolle & NRC, PRL **115**, 146401 (2015)]

Toy model of Kondo insulator (2D)

$$H_k = \begin{pmatrix} \epsilon_k & \gamma \\ \gamma & W \end{pmatrix} \qquad \epsilon_k = \hbar^2 k^2/2m$$



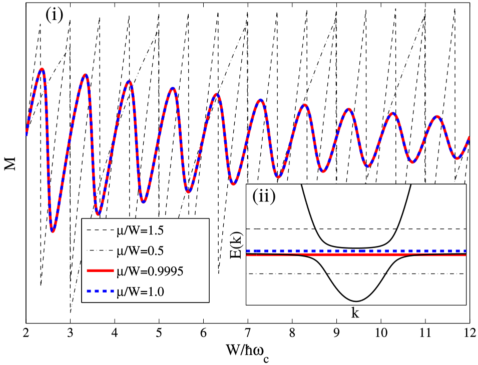
$$E_\pm = \frac{1}{2}\left[\epsilon_k + W \pm \sqrt{(\epsilon_k - W)^2 + \gamma^2}\right]$$

+ magnetic field (no spin) $\epsilon_k \to (n + 1/2)\hbar\omega_c$

Exact spectrum (no semiclassical approx.)
⇒use to calculate grand canonical potential

$$\Omega(\mu, T) = -k_B T N_\phi \sum_{n,\pm} \ln\left[1 + e^{[\mu - E_\pm(n)]/k_B T}\right]$$

Exact evaluation of $M = -\dfrac{\partial \Omega}{\partial B}$ for $T = 0$

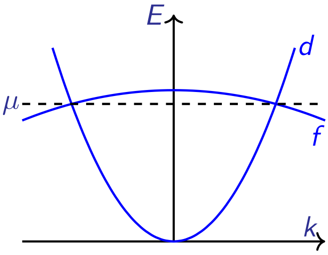


Quantum oscillations without a Fermi surface! ...why?

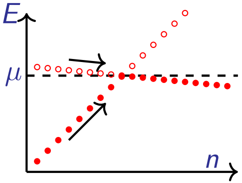
$M_{\rm osc}(\zeta \equiv \frac{\hbar\omega_c}{\gamma})$ has no useful Taylor expansion in ζ

2) Consider extreme limit, $\gamma = 0$

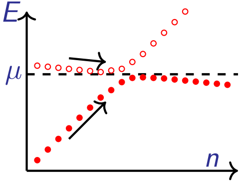
$\gamma = 0 \Rightarrow$ metallic $\Rightarrow$ conventional QOs



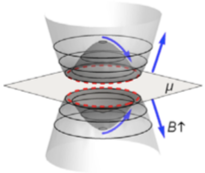
$$\Omega(\mu, T=0) = N_\phi \sum_{n,\pm;E_\pm<\mu} [E_\pm(n) - \mu]$$



$\gamma = 0$



$\gamma \lesssim \hbar\omega_c$



Minimal gap defines closed surface in reciprocal space

Anomalous Temperature Dependence

- Starting point: $M = -\frac{\partial \Omega}{\partial B} = k_B T \frac{\partial}{\partial B} \sum_\lambda \ln \left[1 + e^{(\mu - E_\lambda)/k_B T} \right]$

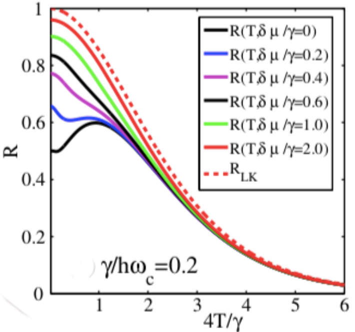
- Analytical formula : $\Omega_{\mathrm{osc}} = k_B T N_\phi \sum_{k=1}^{\infty} \frac{1}{k} \mathrm{Re} \sum_{m=0}^{\infty} e^{i 2\pi k\, n^*(m)}$

[Hartnoll & Hofman, PRB 2010]

- Exact spectrum ⇒ pole $n^*(m)$

$$M_{\mathrm{osc}} \simeq -\frac{\mathcal{A} W e}{2\pi^2 \hbar} \sin \frac{2\pi W}{\hbar \omega_c} R(T, \mu, \gamma)$$

⇒new exact T-dependence

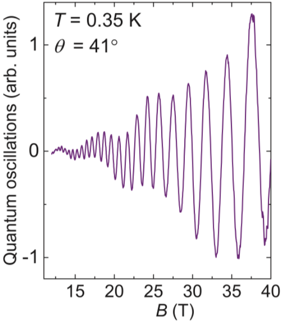


Relevance for SmB_6?

- Requires $\hbar\omega_c \gtrsim \gamma$

- Transport and ARPES suggest $\gamma \sim 5 - 10\text{meV}$

  [ARPES: Frantzeskakis *et al.*, PRX 2013]



[Tan et al., Science (2015)]

- Light mass of unhybridised bands $m \simeq 0.44 m_e$ [Feng, Lu PRL 2013]

$\rightarrow$ cyclotron freq. at 15T is $\hbar\omega_c \simeq 4\text{meV}$

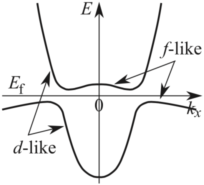
$\rightarrow$ marginal?

- Fermi surface for neutral particles?

[Baskaran (2015); Sodemann, Chowdhury & Senthil (2017); Ertan, Chang, Coleman & Tsvelik (2017)]

Role of topology?

- Crossed bands of differing symmetry:
  ideal scenario for required band structure



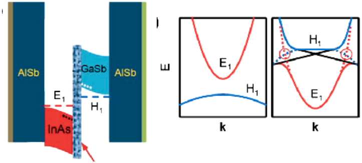
- Realistic topological model has important quantitative effects:
  - Quantum Oscillations for $\hbar\omega_c \gtrsim \frac{\gamma}{3}$
  - Can even fit anomalous T-dependence of QOs in SmB_6...

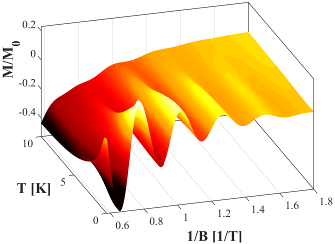
    ...but strong correlations + other anomalous features...

InAs/GaSb Quantum Wells

[J. Knolle & NRC, PRL **118**, 176801 (2017)]

- simple 2DEG model system
- tuneable crossed bands
- model 2D Topological Insulator





Theoretical predictions (gap $\simeq 1.3$meV)

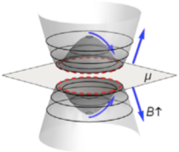
oscillating magnetization (dHvA)
without oscillating conductivity (SdH)

$\Rightarrow$sensitive tool to measure band gap and chemical potential

Summary

- Topological insulators and semimetals call for a re-examination of band theory & transport in novel settings

- Quantum oscillations appear in certain narrow gap insulators
  - unusual non-LK temperature dependence
  - relation to recent experiments in SmB_6
  - general relevance (InAs/GaSb quantum wells)
  - re-examine QOs with poor LK fits?



- Excitons in ring-like minima [J. Knolle & NRC, PRL (2017)]
  - Thermodynamic/transport anomalies
  - Excitonic dHvA effect (QO in thermal conductivity)