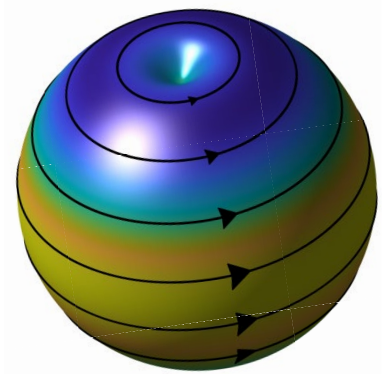
New twists in the research of strongly correlated electronic systems

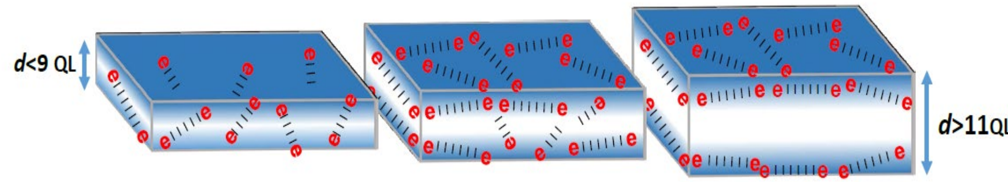
Chung-Yu Mou

National Tsing Hua University

Taiwan

Outline:





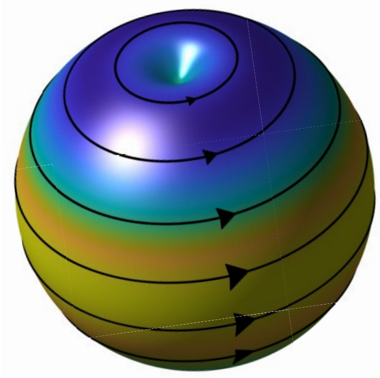
- A recent puzzle from quantum oscillation experiment (Phys. Rev. B 101, 115102, 2020; Phys. Rev. B, 106, 195107, 2022)
- Exotic superconductivity that can arise in topological materials
  - ➢ Topological Kondo superconductivity (Communication Physics 7, 253, 2024)
  - ➢ Geometry induced topological superconductivity (Phys. Rev. B 103, 014508,2021)
  - ➢ Flat band superconductivity, charge density wave and superconducting pair density wave state (Phys. Rev. B 98, 205103, 2018, Phys. Rev. X 11, 041038,2021)
- Conclusion and summary

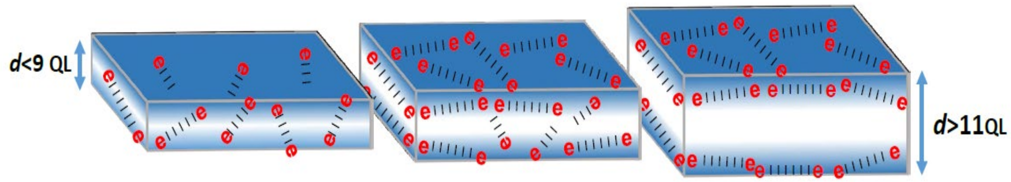
Collaborators:

Theory: Chia-Hsin Chen (NTHU, Taiwan)
Po-Hao Chou (NCTS, Taiwan)
Yung-Yeh Chang (NYCTU, Taiwan)
Chung-Hou Chung (NYCTU, Taiwan)
T. K. Lee (Academia Sinica, Taiwan)
Feng Xu (Shaanxi Univ. of technology, China)

Experiment:
M.N. Ou, Yang-Yuan Chen (Academia Sinica, Taiwan)
Sergey R. Harutyunyan (Institute for Physical Research, NASRA, Armenia)
W.H. Tsai, F.Y. Chiu C.H. Chien, P.C. Lee, Y.C. Chang (Academia Sinica, Taiwan)
Di-Jing Huang (NSRRC), Atsushi Fujimori (U. of Tokyo)

Outline:





•A recent puzzle from quantum oscillation experiment (Phys. Rev. B 101, 115102, 2020; Phys. Rev. B, 106, 195107, 2022)

Outline:

- A recent puzzle: quantum oscillation experiment

PHYSICS TODAY

DOI:10.1063/PT.5.7188

20 Jul 2015 in Research & Technology

An insulator with conducting electrons?

Quantum oscillation

-- has long been known as an experimental technique to map out the Fermi surface in metals.

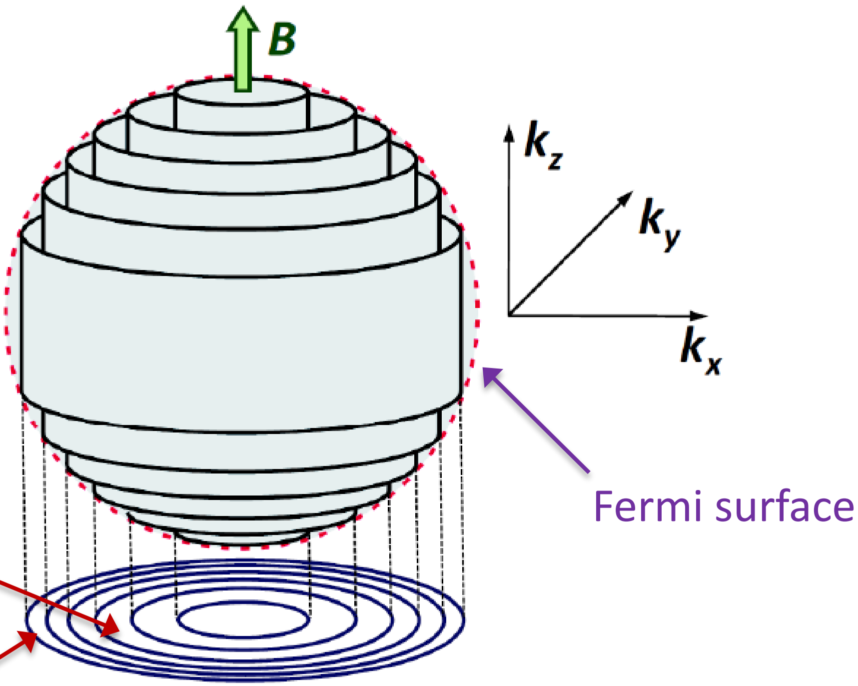
$$\epsilon_n = \left(n + \frac{1}{2}\right)\hbar\omega_c + \frac{\hbar^2}{2m_e}\mathbf{k}_\parallel^2$$

$$\frac{\hbar^2}{2m_e}(k_x^2 + k_y^2)$$

$$S_n = (n + \gamma)\frac{2\pi e}{\hbar}B$$

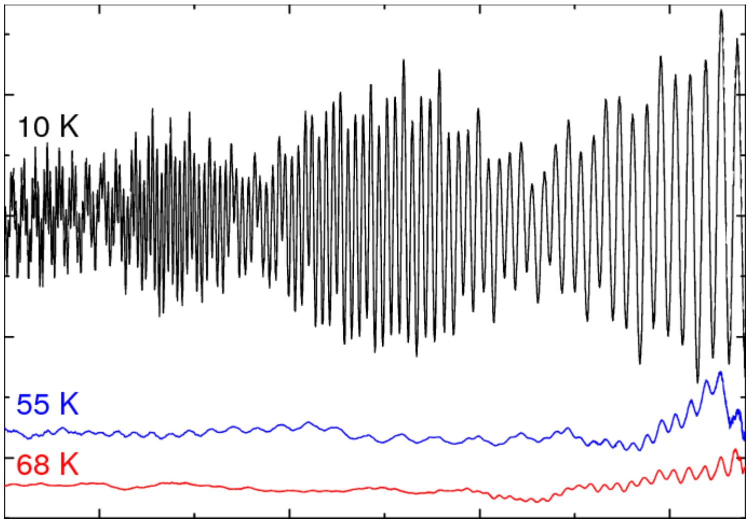
$$S_{n+1}(B) = S_n(B') = S_F$$

$$\longrightarrow \Delta\frac{1}{B} = \frac{1}{B} - \frac{1}{B'} = \frac{2\pi e}{hS_F}$$



de Haas–van Alphen oscillation

$\frac{dM}{dB}$



shape-memory alloy AuZn
PRL **94,** 116401 (2005)

Lifshitz-Kosevich (LK) theory

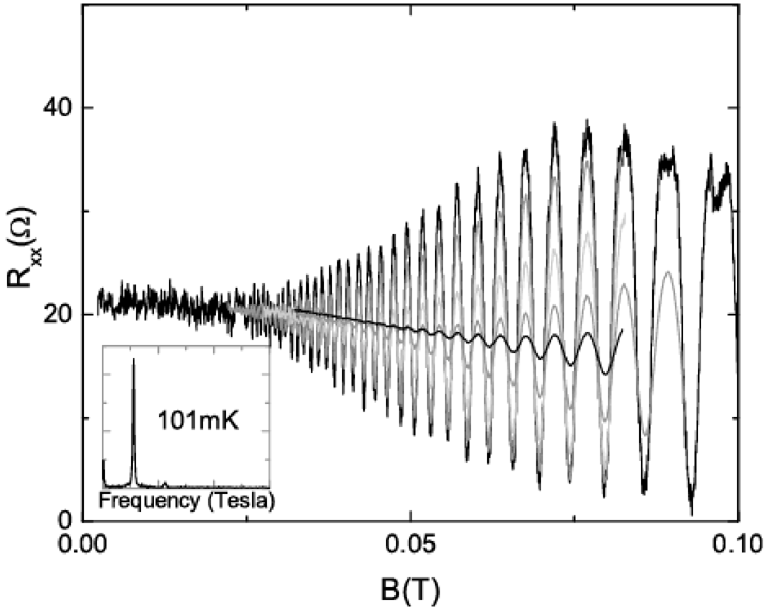
$$M \propto \frac{eFk_BTV}{\sqrt{2\pi H A"}} \sum_{p=1}^{\infty} p^{\frac{-3}{2}} R_T(p)\, R_D(p)\, R_s(p) \times$$

$$\times \sin\left[2\pi p\left(\frac{F}{H}-\frac{1}{2}\right) \pm \frac{\pi}{4}\right]$$

$$A" = \left|\frac{\partial^2 A}{\partial k_z^2}\right|_{k_z=k_{extr}}$$

$$R_T(p) = \frac{\pi\kappa}{\sinh \pi\kappa} = \frac{2\pi^2 p k_B T/\beta^* H}{\sinh\left(2\pi^2 p k_B T/\beta^* H\right)}$$

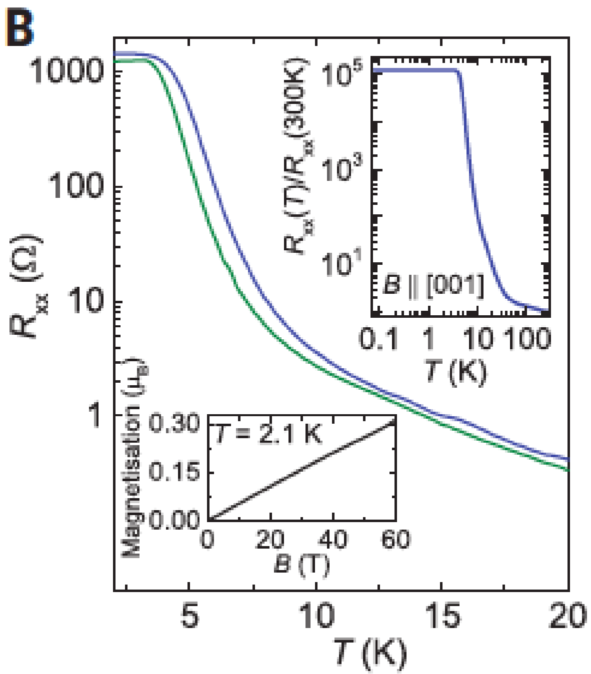
Shubnikov-de Haas oscillation

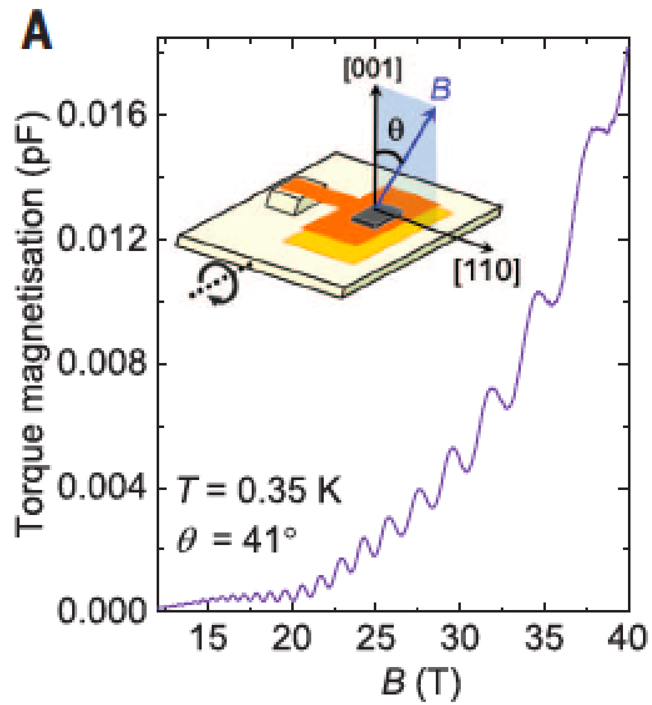


2DEG in GaAs/AlGaAs at different T (101mK, 180mK…)
PRL **94,** 016405 (2005)

Quantum Oscillations in Kondo insulator SmB_6

They were, however, observed in Kondo insulators. This poses as a great challenge to explain it.

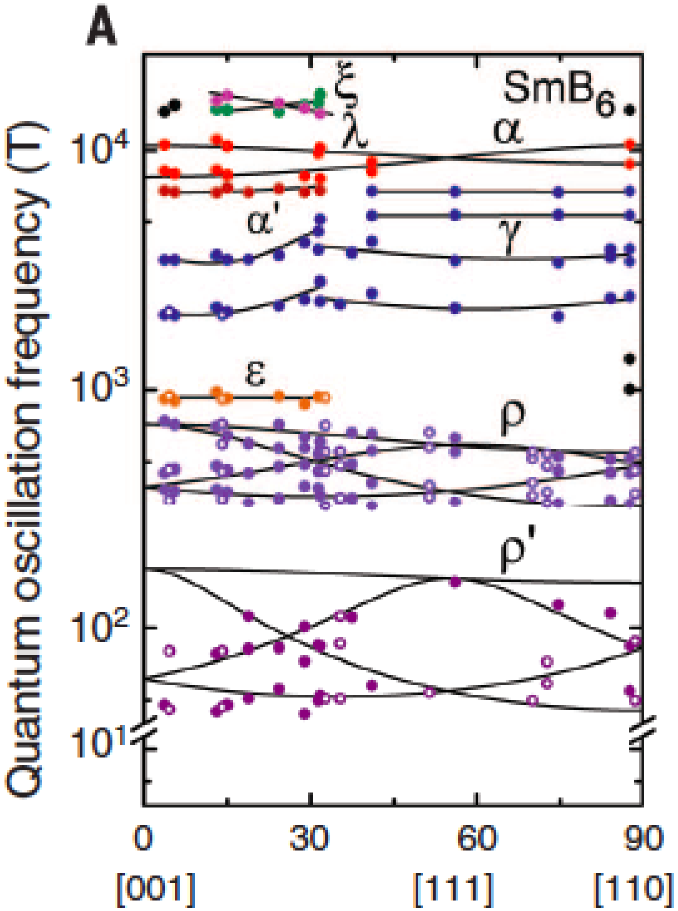




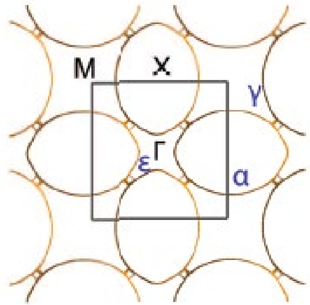
Insulator!

S. E. Sebastian et al, Science 349, 287(2015)

Fermi Surface and unconventional temperature dependence

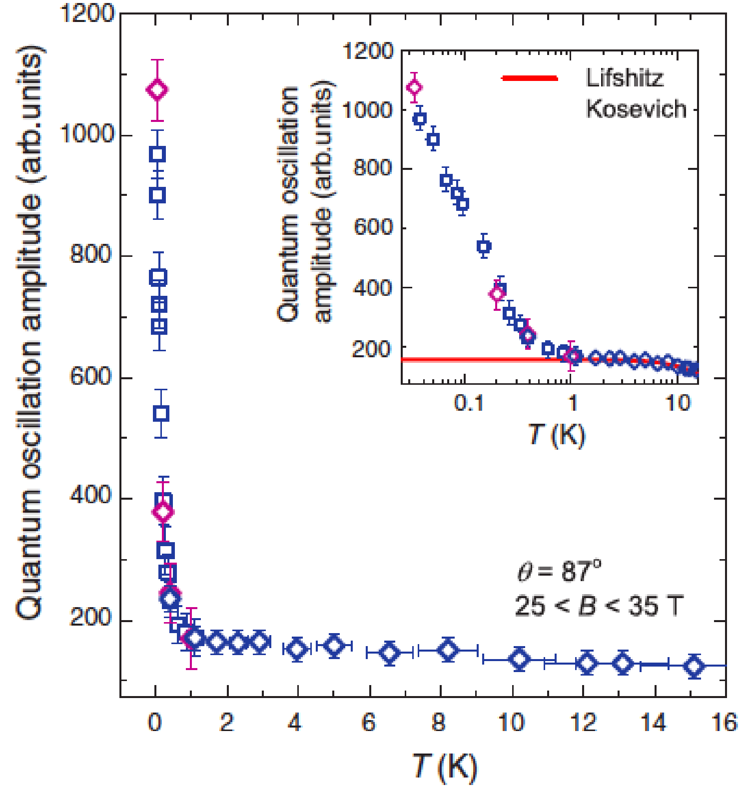


Observed Fermi Surface



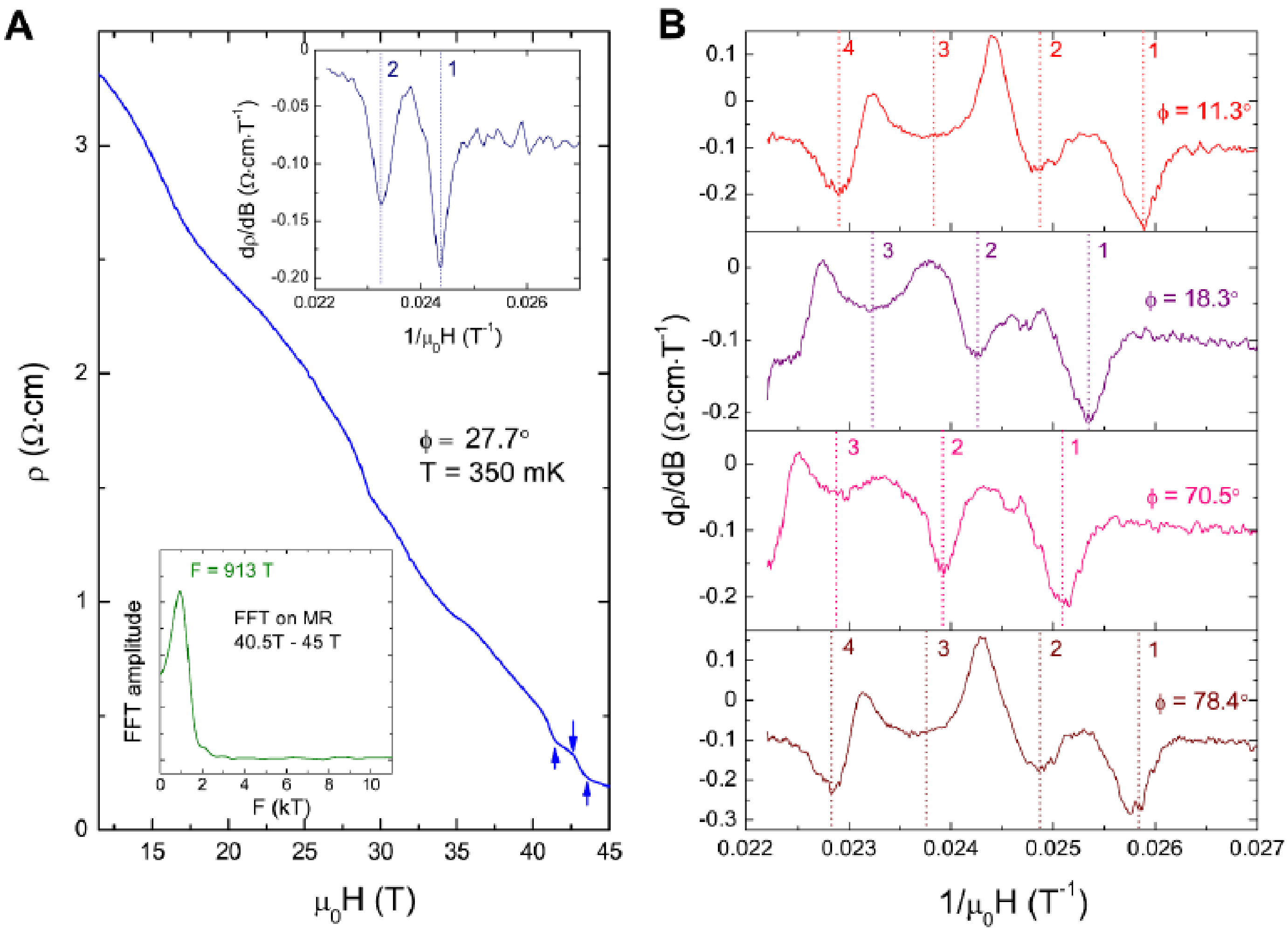
DFT calculation

S. E. Sebastian et al,
Science 349, 287(2015)



Quantum Oscillations in resistivity derivative

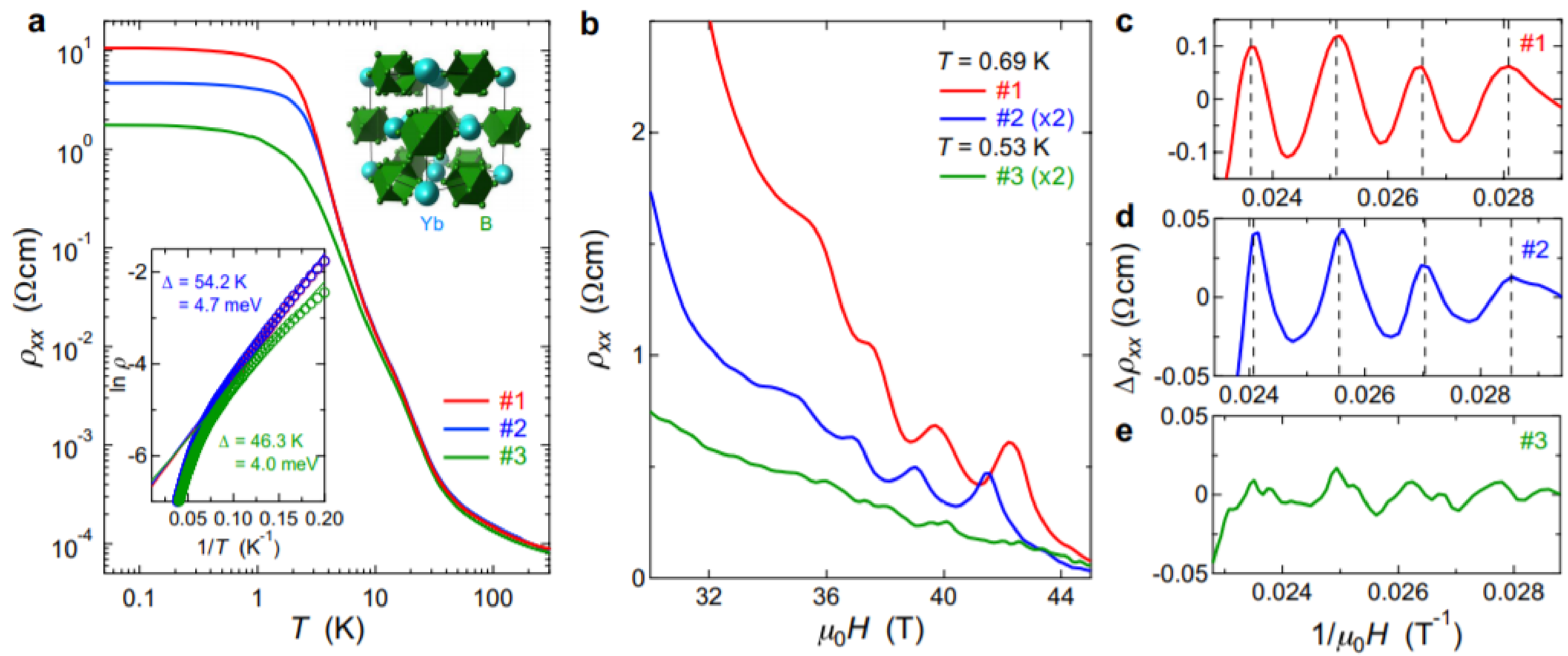
Y. Matsuda, and L. Li etc, Science 362, 65 (2018).



Kondo insulator YbB_{12}

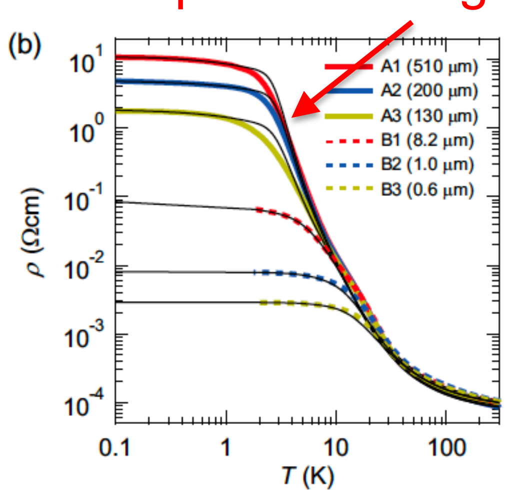
(ytterbium dodecaboride)

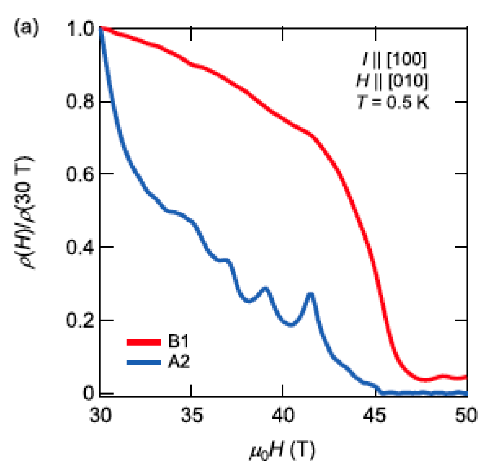
Kondo Insulator YbB_{12}



ρ is larger, oscillation amplitude is larger

Sato, Y. et al. *Nat. Phys.* **15,** 954–959 (2019).

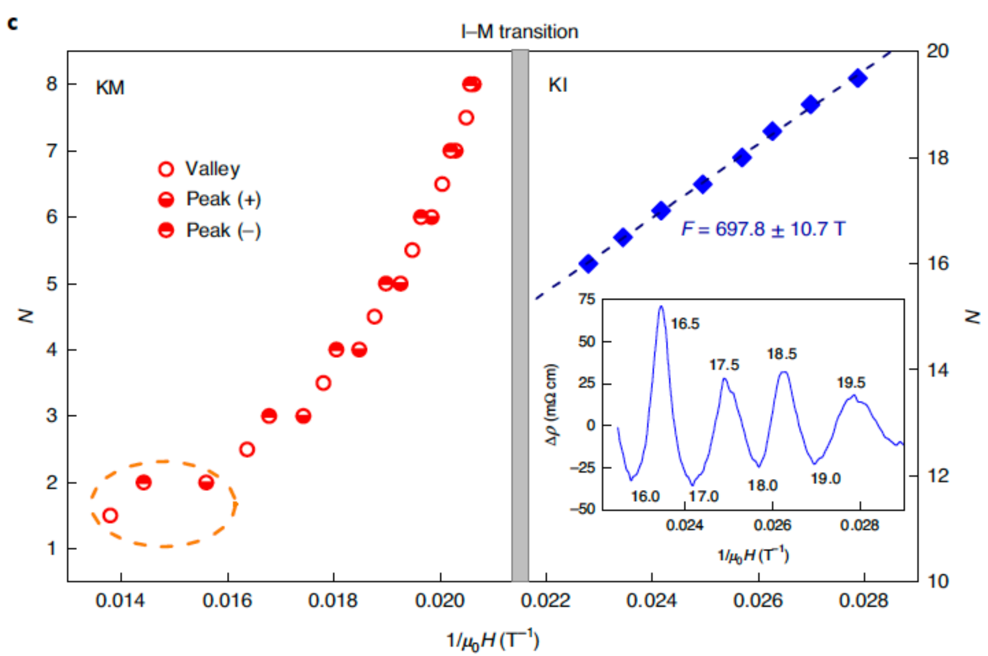


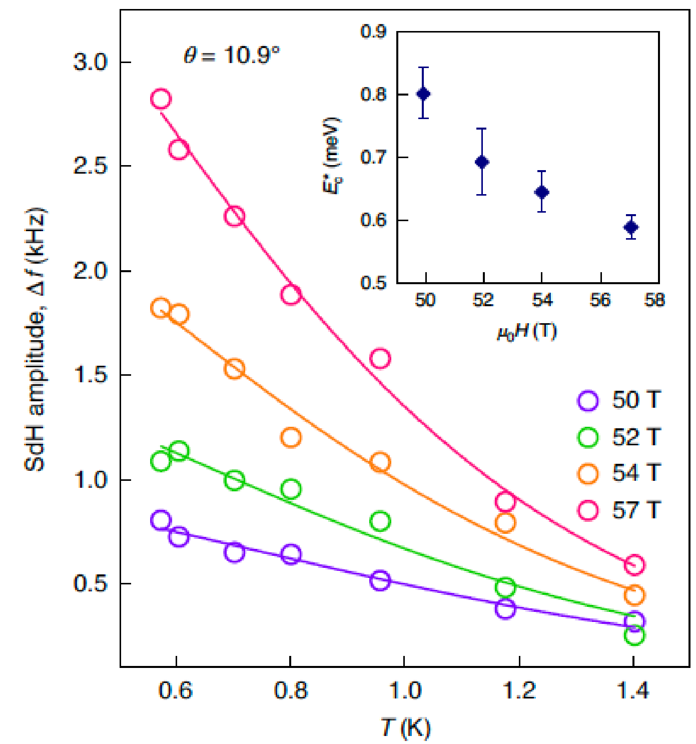


J. Phys. D: Appl. Phys. 54, 404002 (2021)

A2=single crystal

More recent data on Kondo insulator YbB_{12} ：Pulse Magnetic field up to 75T





Under strong fields, it's like a metal in agree with the LK theory

Nature Physics 17, 788 (2021)

Many theories are proposed

*Due to narrow gap

J. Knolle and N. R. Cooper, Phys. Rev. Lett. 115, 146401 (2015); L. Zhang, X. Y. Song, and F. Wang, Phys. Rev. Lett. 116, 046404 (2016).

*Due to surface state

Kondo breakdown, O. Erten, P. Ghaemi, and P. Coleman, Phys. Rev. Lett. 116, 046403 (2016).

*Due to neutral Fermion

Inti Sodemann, Debanjan Chowdhury, T. Senthil, Phys. Rev. B 97, 045152 (2018)

Neutral fermions in mixed-valence insulators

C. M. Varma, Phys. Rev. B 102, 155145, 2020

*Bulk scalar Majorana Fermi Liquid

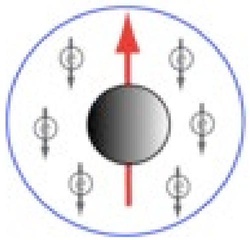
arXiv:1507.03477, G. Baskaran

but none can explain all features observed in expt.

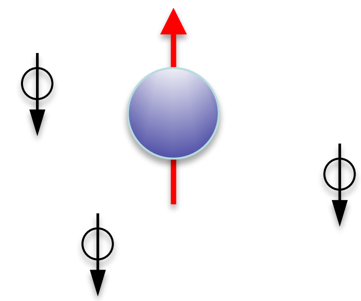
Our theory (Phys. Rev. B 101, 115102, 2020)

Kondo screening itself under goes oscillation

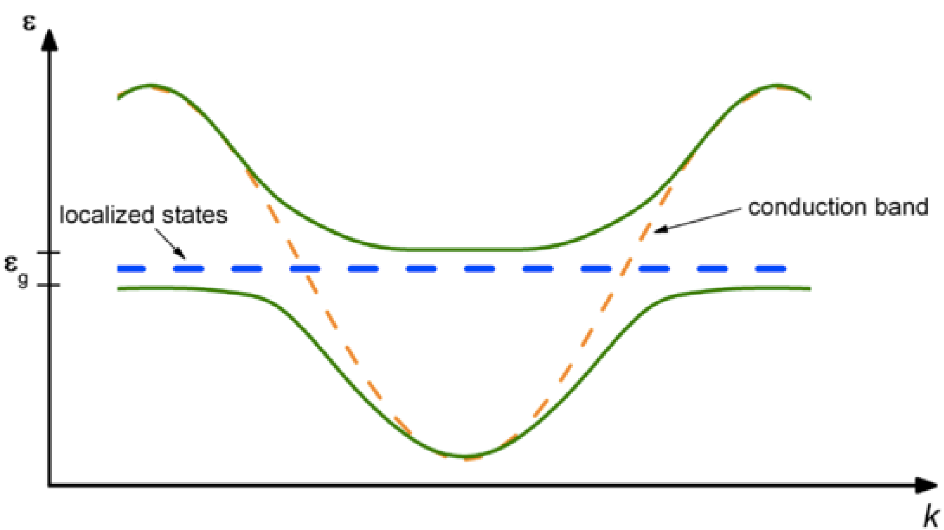
- non-rigidity of band enables the oscillations

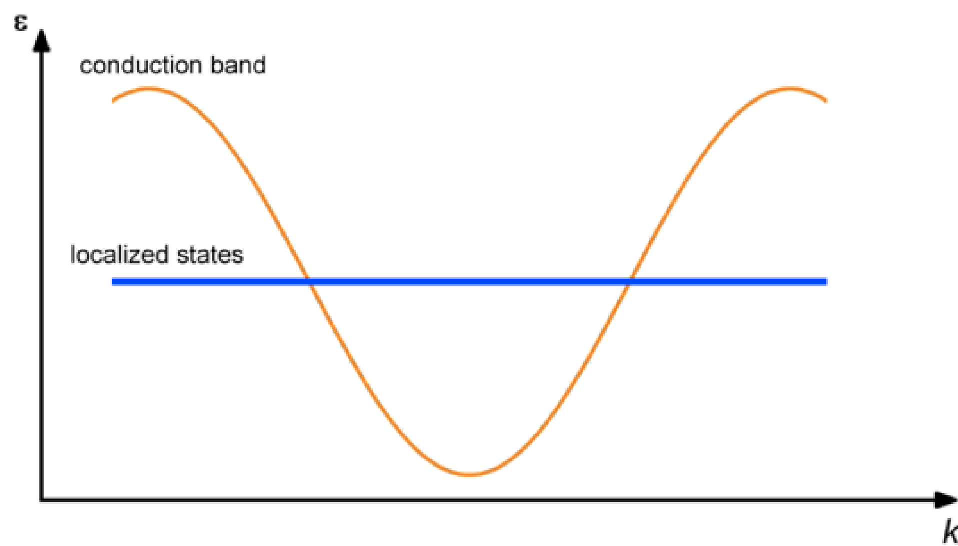


$T < T_K$



$T > T_K$





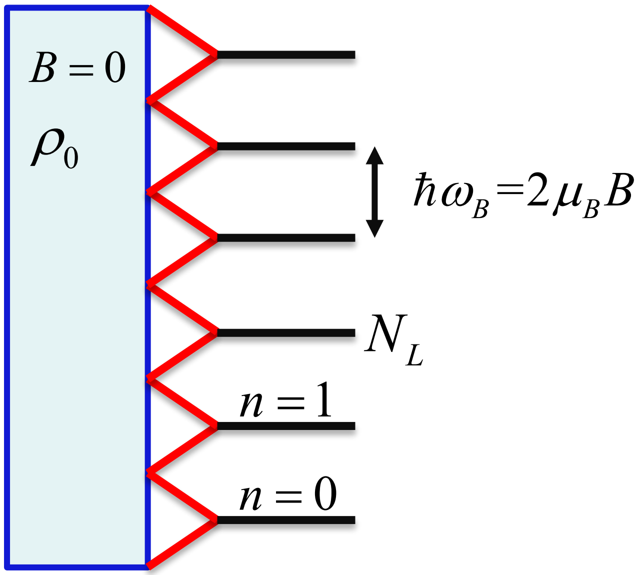
New ingredient: Landau quantization (2D), DOS is discrete

$$\frac{\vec{p}^2}{2m} \to \frac{(\vec{p}+e\vec{A}/c)^2}{2m}.$$

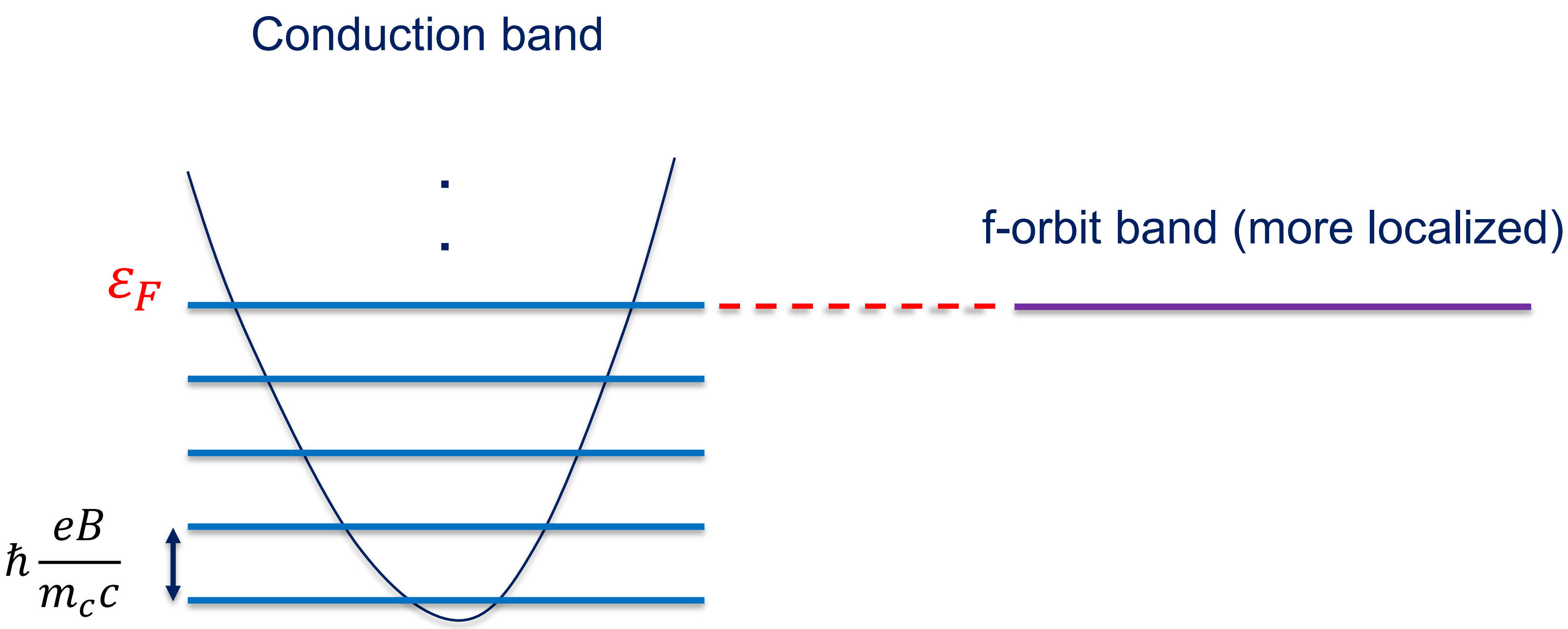
$$\varepsilon_k = \frac{k^2}{2m} \to \varepsilon_n = \hbar\omega_B(n+\frac{1}{2}), \hbar\omega_B = \frac{eB}{mc}.$$

density of states per volume : $\rho_0 = \dfrac{m}{2\pi\hbar^2}$

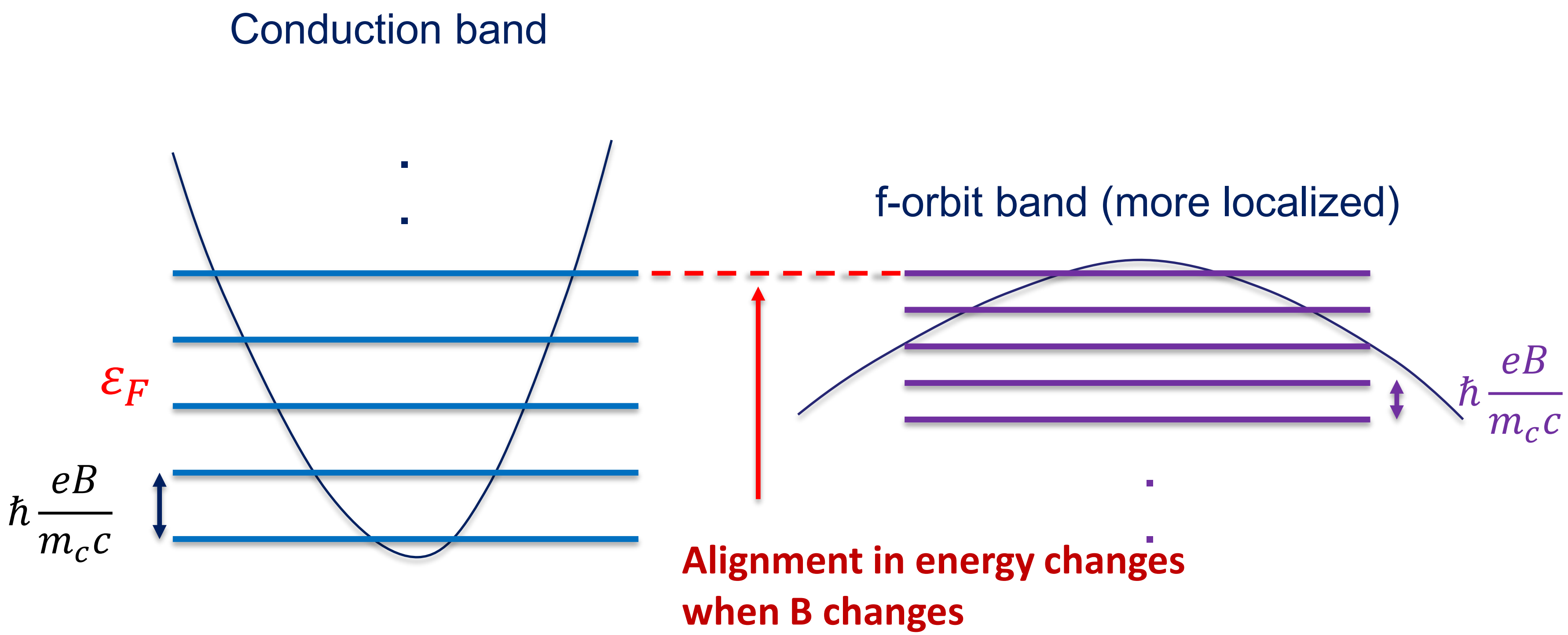
$\to$ Landau degeneracy per volume : $N_L / L^2 = \rho_0 \hbar\omega_B$



Kondo screening itself under goes oscillation
-- due to periodical alignment of Landau levels with f orbit when magnetic field B changes



More realistic model with finite band width f-orbit band



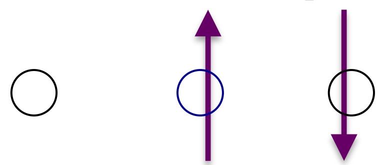
Slave-boson mean field theory

$$H=\sum_{k\sigma}\xi_k c_{k\sigma}^{\dagger}c_{k\sigma}+\xi_k^d d_{k\sigma}^{\dagger}d_{k\sigma}+\sum_{k\sigma}V_k^{\sigma\sigma'}c_{k\sigma}^{\dagger}d_{k\sigma'}+h.c+U\sum_i n_{i\uparrow}^d n_{i\downarrow}^d$$

$$\mathrm{V}_{\mathbf{k}}=v_0 I\ (\text{even parity})\ \text{or}\ 2\lambda_{\mathrm{so}}\sum_{i=x,y,z}\sigma_i\sin k_i$$

$$d_{i\sigma}^{\dagger}=f_{i\sigma}^{\dagger}b_i \qquad 1=\sum_{\sigma}f_{i\sigma}^{\dagger}f_{i\sigma}+b_i^{\dagger}b_i$$

$\langle b_i\rangle = r$ (holon condensate)



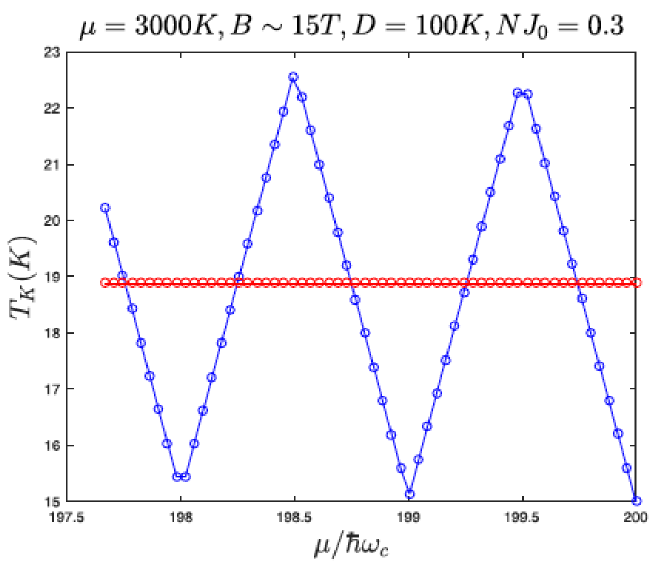
$f_{i\sigma}^{\dagger}$ = spinon

Lagrangian multiplier: $\sum_{i\sigma}\lambda_i(f_{i\sigma}^{\dagger}f_{i\sigma}+b_i^{\dagger}b_i-1),\ \lambda$

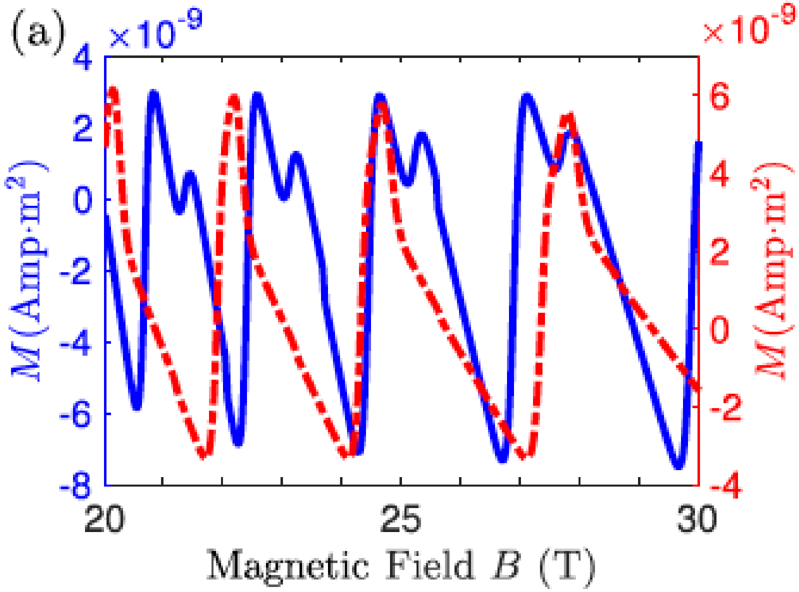
$$\xi_k\to-\mu_c(k_z)+\hbar\omega_c(n+\frac{1}{2}) \qquad \xi_k^d\to-\mu_f(k_z)-\hbar\omega_f(m+\frac{1}{2})$$

Solve λ and r self-consitently

Explain important features observed in Experiments



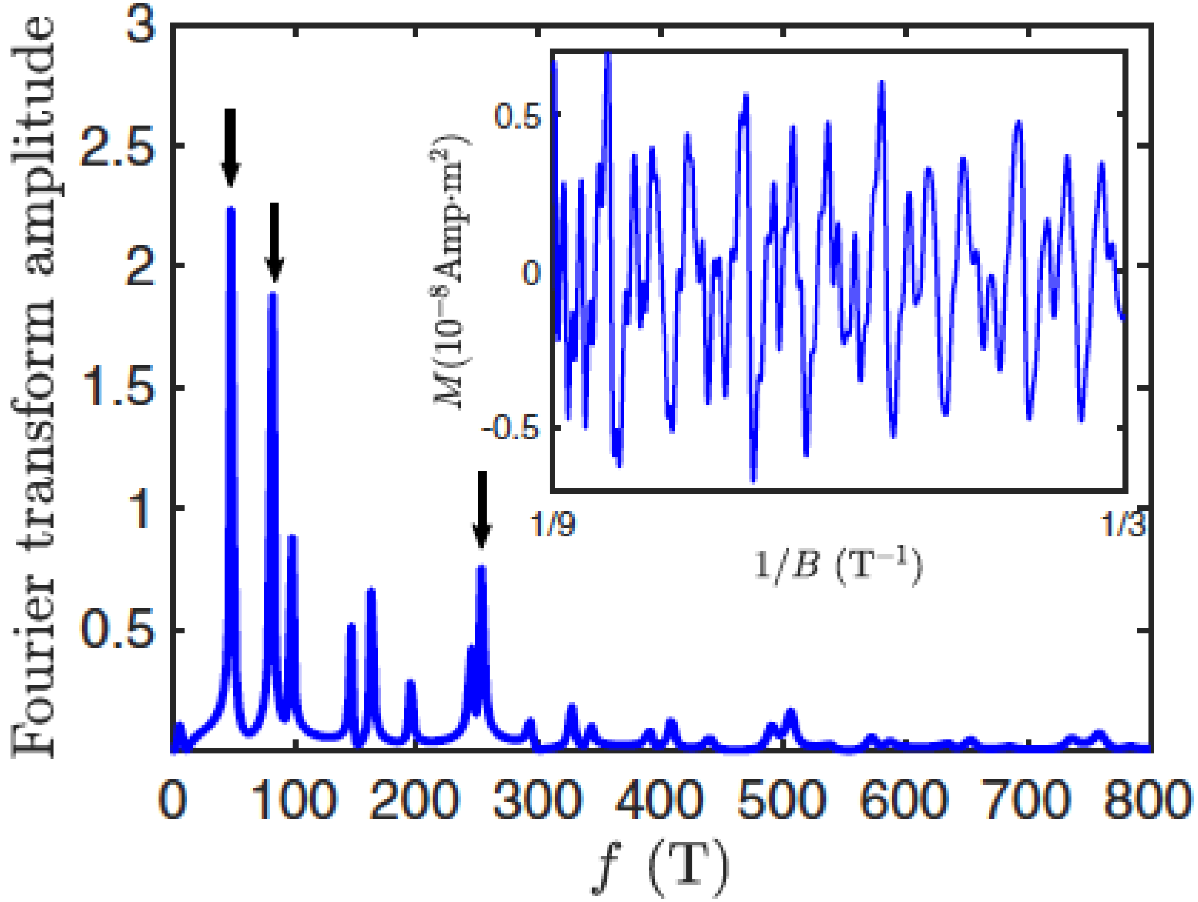
Oscillation of Kondo screening for a single impurity



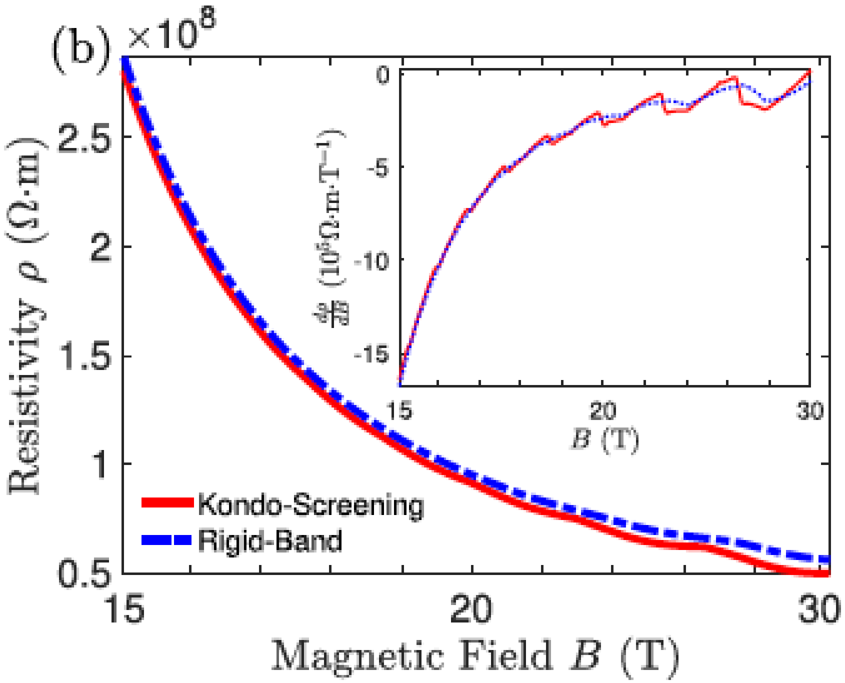
Quantum oscillation in magnetization (moment) for odd (blue)/even (red) parity hybridization.

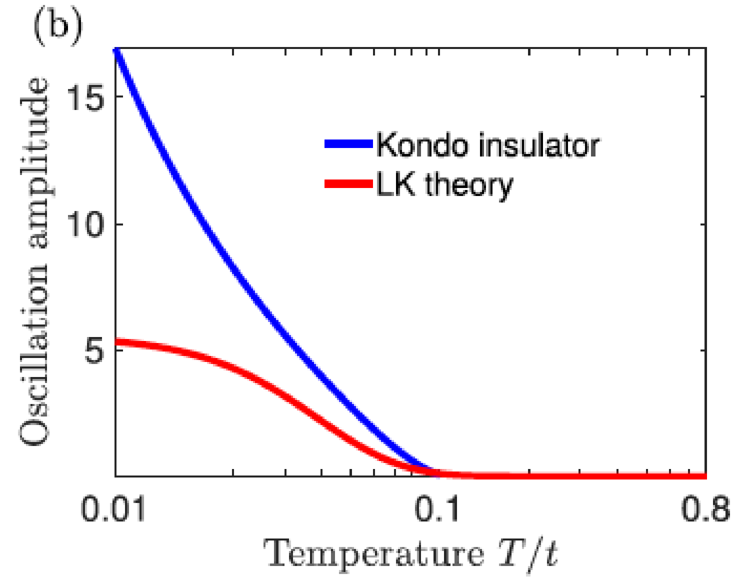
amplitude $\sim 10^{-8}\,Am^2$ consistent with 0.001pF observed in Cantilever magnetometer

Exhibiting Fermi surface



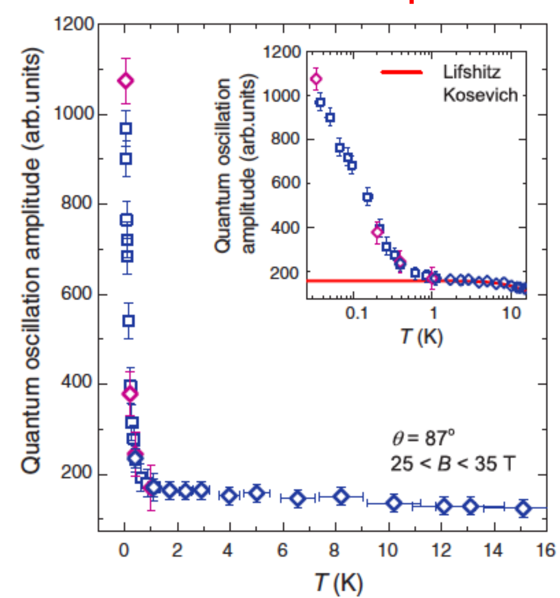
Fourier transformation of quantum oscillation in M when there are 3 conduction-band sections, denoted by $\alpha, \beta,$ and γ. Arrows indicate frequencies that correspond to Fermi surface areas: 55.2T, 92T, and 276T.
Inset: quantum oscillations of M versus 1/B





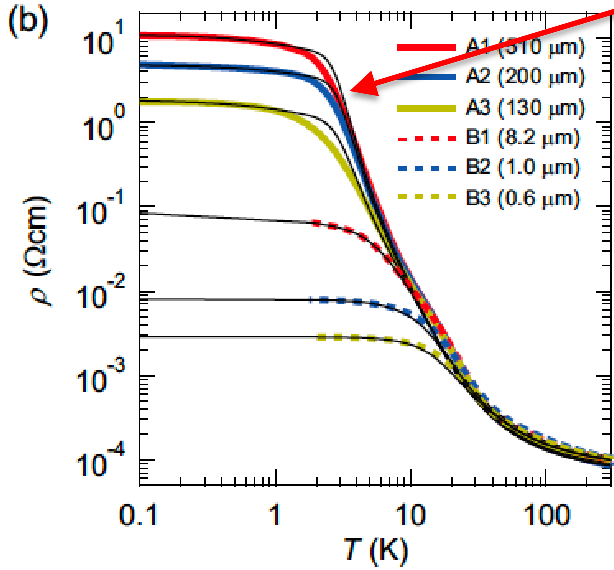
Temperature dependence

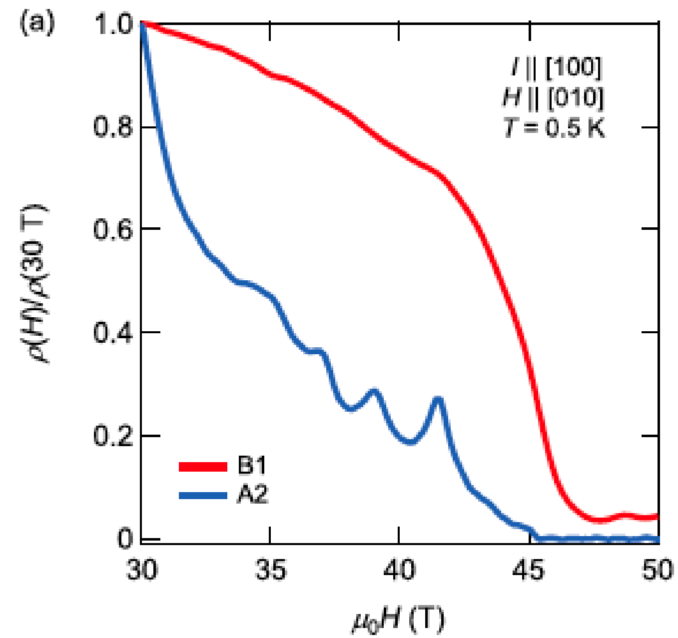
expt

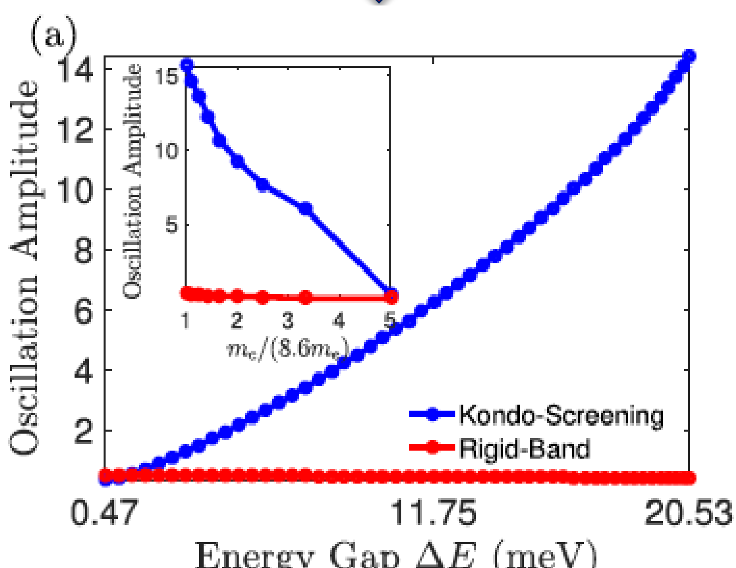


Derivative of resistivity shows oscillation

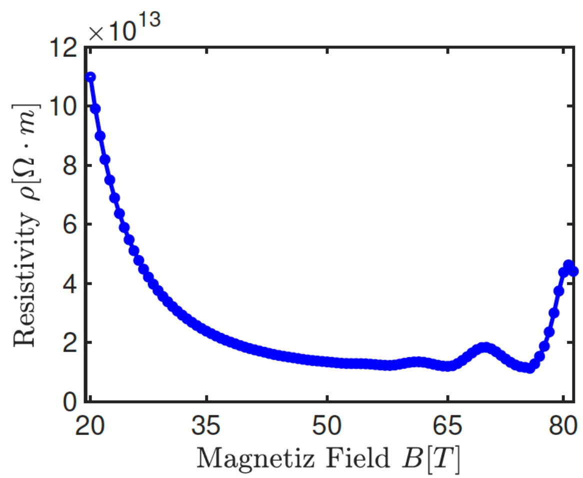
ρ is larger, oscillation amplitude is larger







Our interpretation: it indicates Kondo break down around 45 T ($r \to 0$
seen in our numerical result)



Nor exactly the same
But in the right direction

What are phases that oscillate?

(Phys. Rev. B, 106, 195107, 2022)

What is the ground state for dilute magnetic impurities in Landau quantized system?

(Previous researches for Kondo impurities in magnetic field focus on the Zeeman splitting interaction of impurity, where the conduction band is still treated as continuous band.)

Model Hamiltonian

$$H = H_c + H_V + H_d$$

$$H_c = \sum_\sigma \int C^\dagger_{\vec{r}\sigma} \frac{1}{2m_e}(\vec{p} + \frac{e\vec{A}}{c})^2 C_{\vec{r}\sigma} d\vec{r} + g_c \mu_B B \int s^z_{c,r} d\vec{r}$$

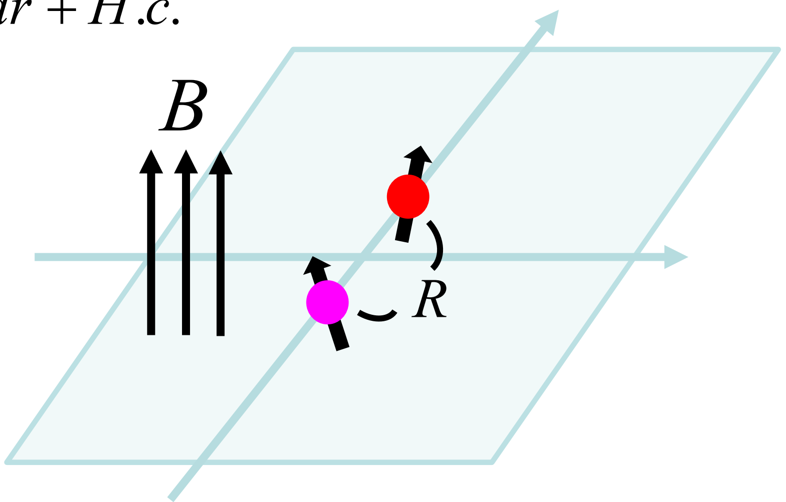
$$H_d = \xi_d \sum_\sigma \left(d^\dagger_{1\sigma} d_{1\sigma} + d^\dagger_{2\sigma} d_{2\sigma} \right) + U \left(n^d_{1\uparrow} n^d_{1\downarrow} + n^d_{2\uparrow} n^d_{2\downarrow} \right) + g_d \mu_B B (s^z_{d_1} + s^z_{d_2})$$

$$H_{hyb} = Va \sum_\sigma \int C^\dagger_{\vec{r}\sigma} \left(\delta(\vec{r} - \vec{r}_1) d_{1\sigma} + \delta(\vec{r} - \vec{r}_2) d_{2\sigma} \right) d\vec{r} + H.c.$$

$$\vec{A} = (0, Bx, 0)$$

$$\vec{r}_1 = (0, R/2)$$

$$\vec{r}_2 = (0, -R/2)$$



Model Hamiltonian in basis of Landau level

Hybridization term

$$H_V = \frac{\tilde{V}}{\sqrt{L}} \sum_{\{n\},k_y\sigma} \phi_n(x_k) e^{ik_yR} d_\sigma^\dagger c_{nk_y\sigma} + \text{H.c.}$$

$$\left(\frac{\Gamma\varepsilon_B}{\pi}\right)^{1/2} \left(\sum_{\{n\},\sigma} d_\sigma^\dagger A_{n\sigma} + \text{H.c.}\right), \quad L \gg l_B$$

$$A_{n\sigma} = \sqrt{\frac{L}{N_L}} \sum_{k_y} e^{ik_yR} \phi_n(x_k) c_{nk_y\sigma}$$

$$H_1 = U d_\uparrow^\dagger d_\uparrow d_\downarrow^\dagger d_\downarrow + \sum_\sigma \xi_\sigma^d d_\sigma^\dagger d_\sigma + \sum_{\{n\},\sigma} \xi_{n\sigma}^c A_{n\sigma}^\dagger A_{n\sigma} + \left(\frac{\Gamma\varepsilon_B}{\pi}\right)^{1/2} \left(\sum_{\{n\},\sigma} d_\sigma^\dagger A_{n\sigma} + \text{H.c.}\right)$$

$$\rho J = \frac{\Gamma}{\pi}\left(\frac{1}{|U+\xi_d|} + \frac{1}{|\xi_d|}\right)$$

Landau Level $\hbar\omega\left(n+\frac{1}{2}\right) - \mu$

$$\Gamma = \rho\pi V^2$$

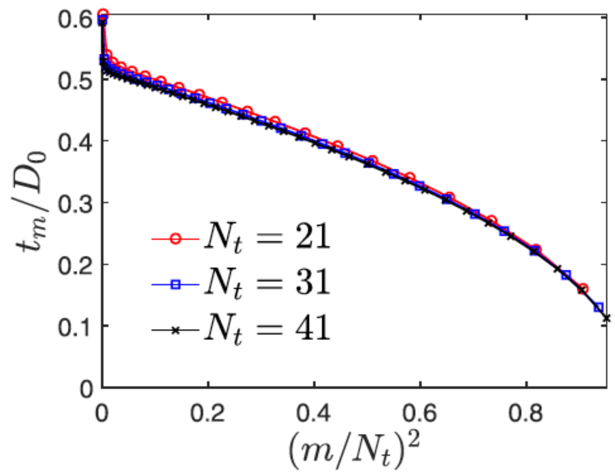
Reduction to a universal 1D chain

$$\sum_{n\sigma} \xi^c_{n\sigma} A^\dagger_{n\sigma} A_{n\sigma} \quad \Rightarrow \quad \sum_{m=1,\sigma}^{N_t} \epsilon_m f^\dagger_{m\sigma} f_{m\sigma} + t_m (f^\dagger_{m\sigma} f_{m+1\sigma} + \mathrm{H.c.})$$

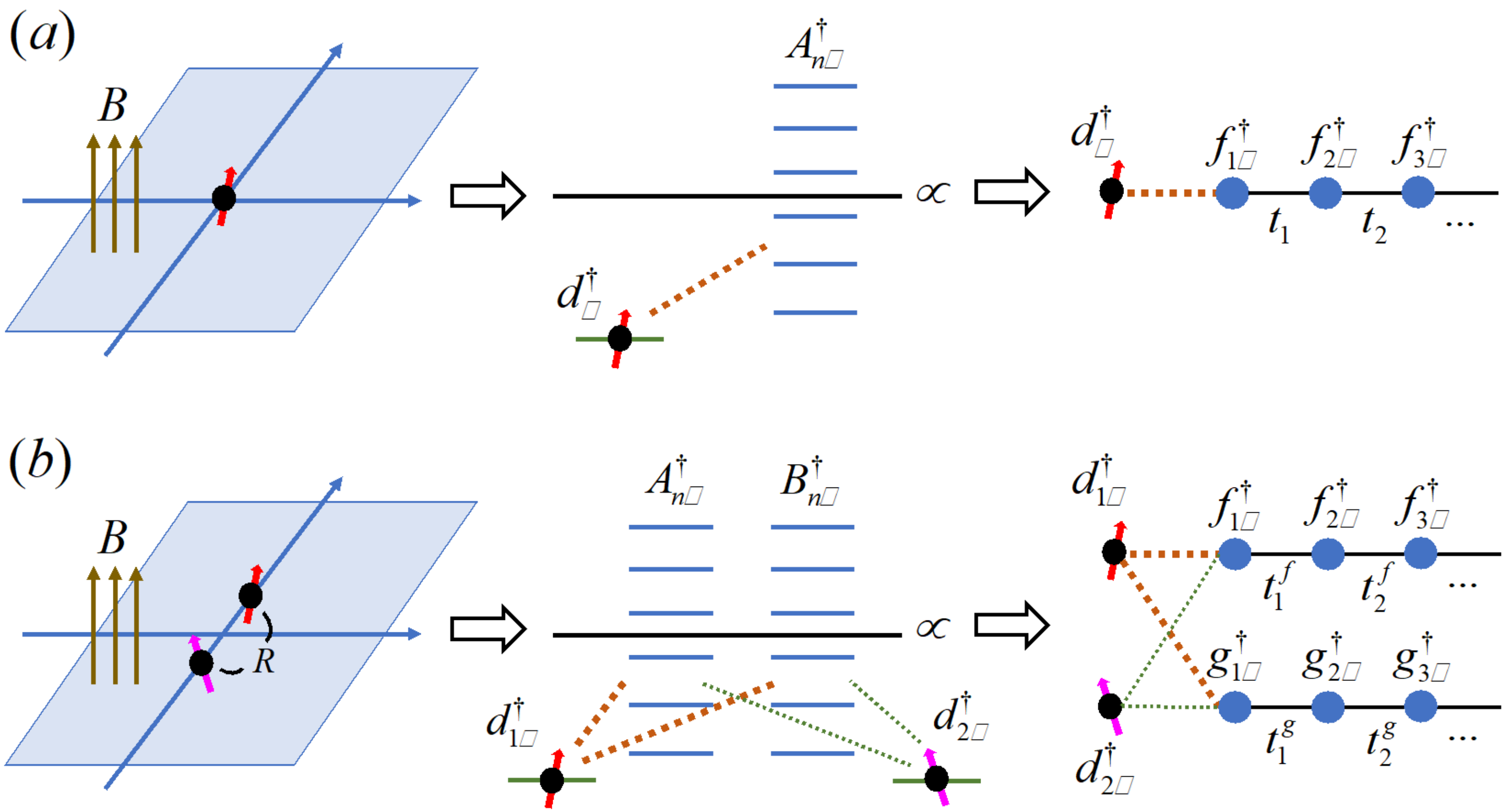
Transformation matrix from $A_{n\sigma}$ to $f_{m\sigma}$: $v_{n,m}$

$$\begin{pmatrix} \epsilon_1 & t_1 & \\ t_1 & \epsilon_2 & t_2 \\ & t_2 & \cdots \end{pmatrix} \begin{pmatrix} v_{1,n} \\ v_{2,n} \\ \cdots \end{pmatrix} = \xi_n \begin{pmatrix} v_{1,n} \\ v_{2,n} \\ \cdots \end{pmatrix}$$

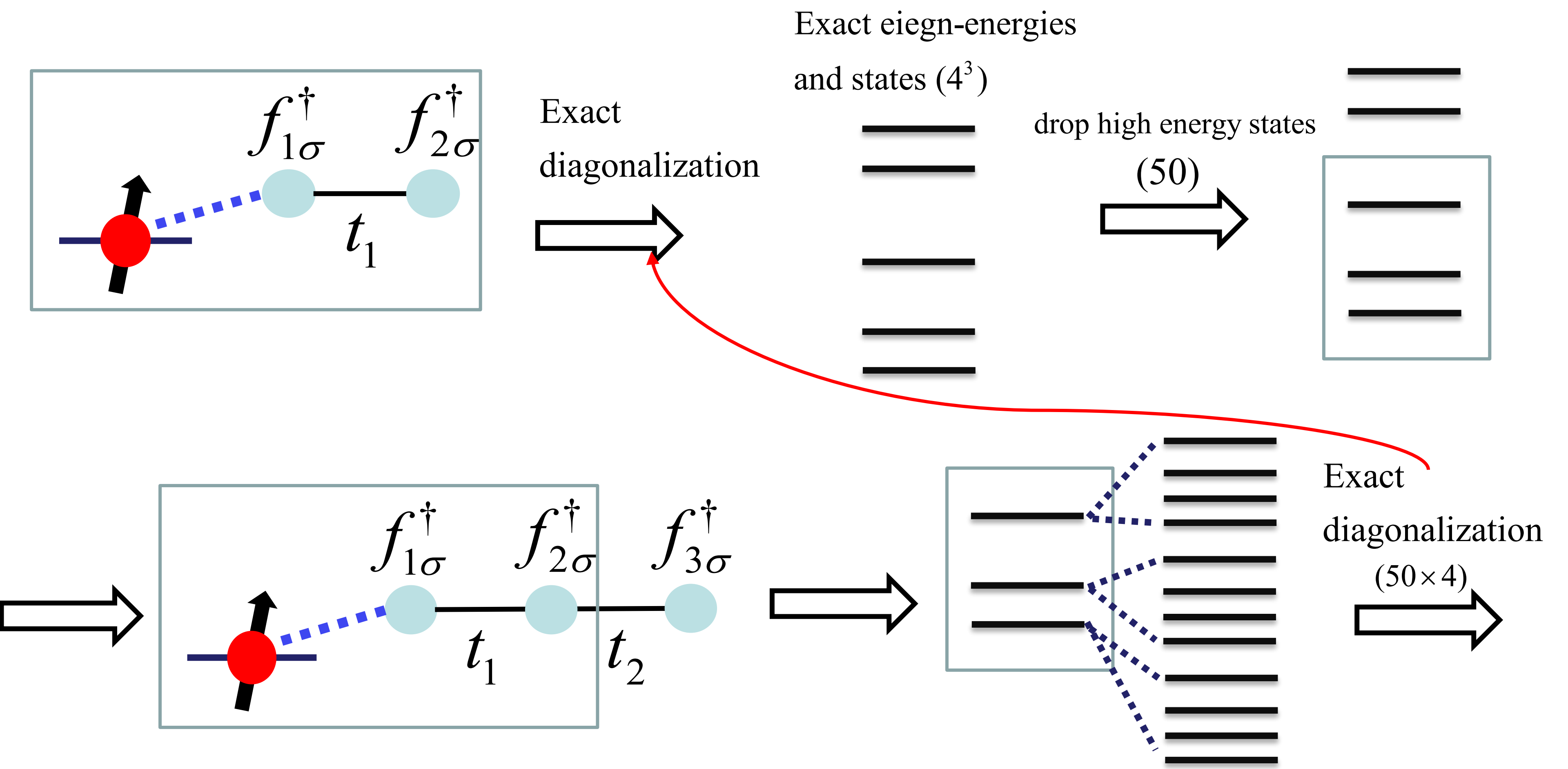
Scaling form of solution



Universal 1D chains



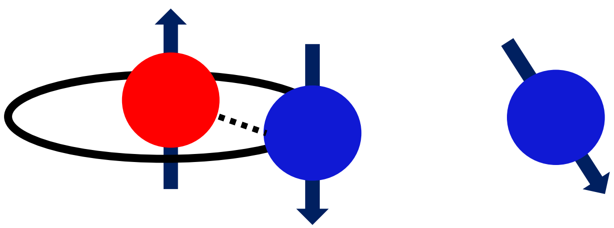
Schematic NRG procedure



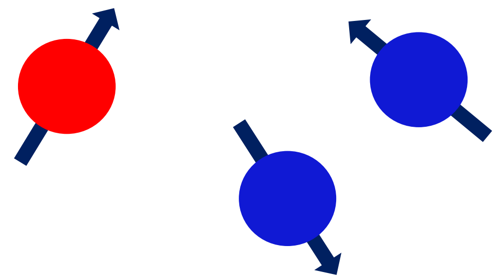
Results: Zero field

Zero field

Singlet
(Screened states):

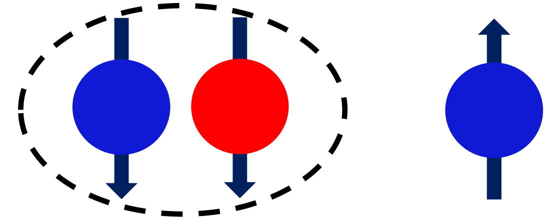


Doublet
(Unscreened state):



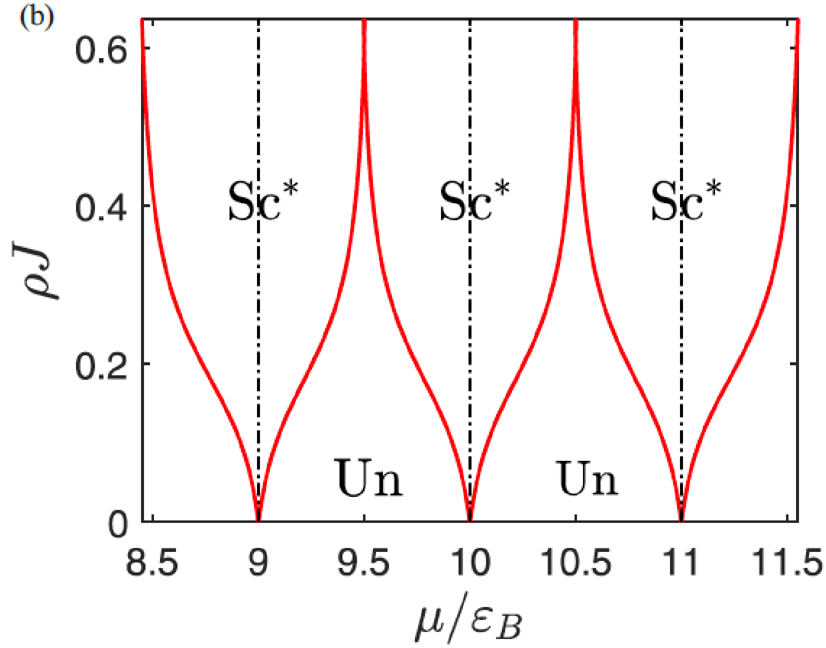
In the presence of Zeeman splitting and non-vanishing B field

Initial state before screening $S_z = -1$
or $S_z = -1/2$
($S_{z,imp} = -1/2$, $S_{z,c} = 0$ or $-1/2$,
depending on whether the Fermi energy is between Zeeman splitting or not)

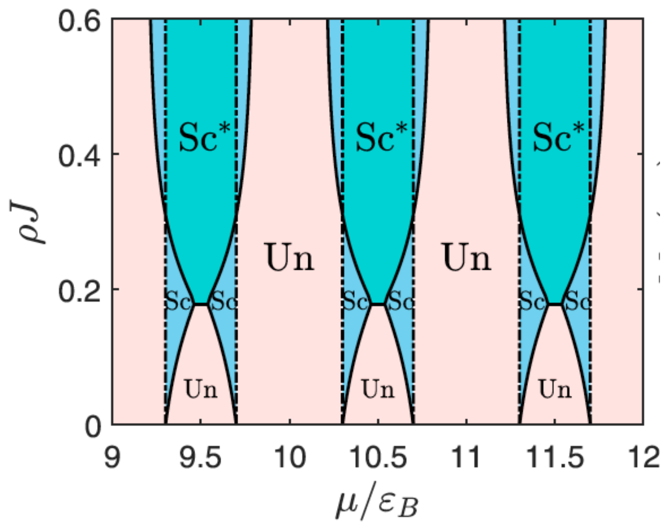


Screening $\Delta S_z = 1/2$ (Sc) or $\Delta S_z = 1$ (Sc*)

Typical Phase diagram



$\widetilde{g_c} = g_c \frac{\mu_B B}{\varepsilon_B} = 2$, $\widetilde{g_d} = g_d \frac{\mu_B B}{\varepsilon_B} = 2$



$\widetilde{g_c} = 0.8$, $\widetilde{g_d} = 2$

$$\Delta s^z \equiv \left\langle s_{tot}^z \right\rangle_\Gamma - \left\langle s_{tot}^z \right\rangle_{\Gamma=0}$$

$\text{Un} : \Delta s^z = 0$

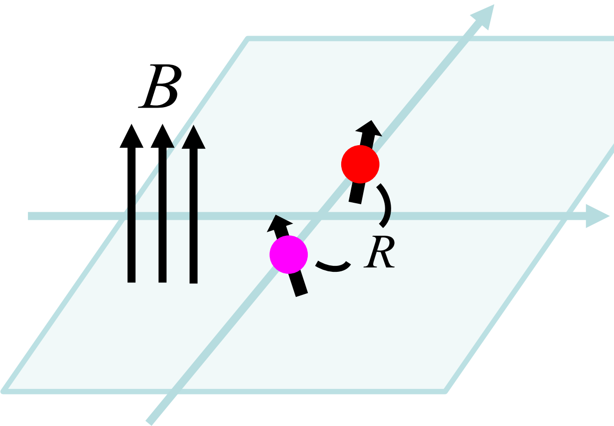
$\text{Sc} : \Delta s^z = 1/2$

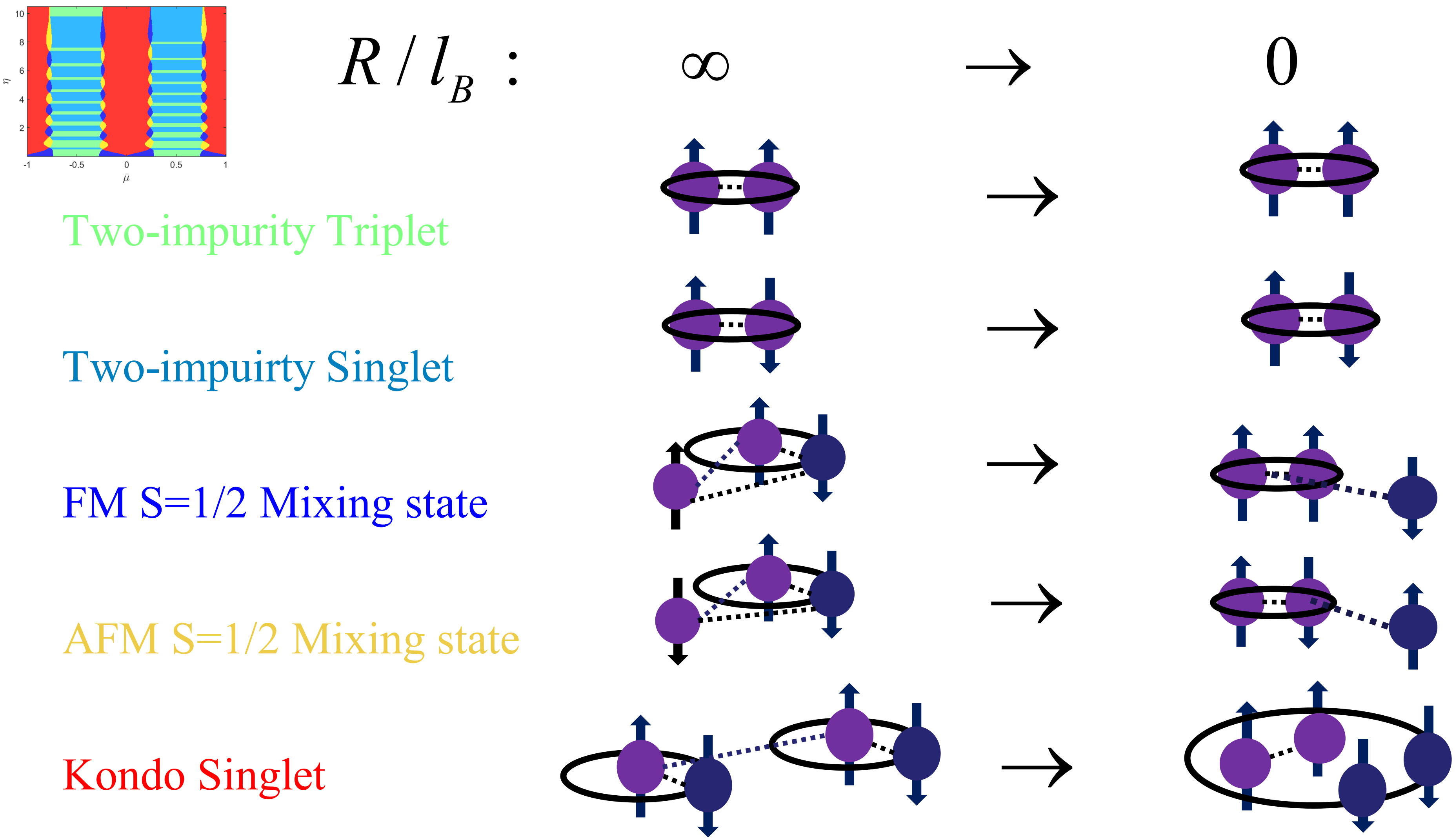
$\text{Sc}^* : \Delta s^z = 1$

Sc(Screened)

Un(Unscreened)

Two impurities





10
8
6
4
2
η
-1
-0.5
0
0.5
1
$\bar{\mu}$
R / l_B :
∞
→
0
Two-impurity Triplet
Two-impuirty Singlet
FM S=1/2 Mixing state
AFM S=1/2 Mixing state
Kondo Singlet

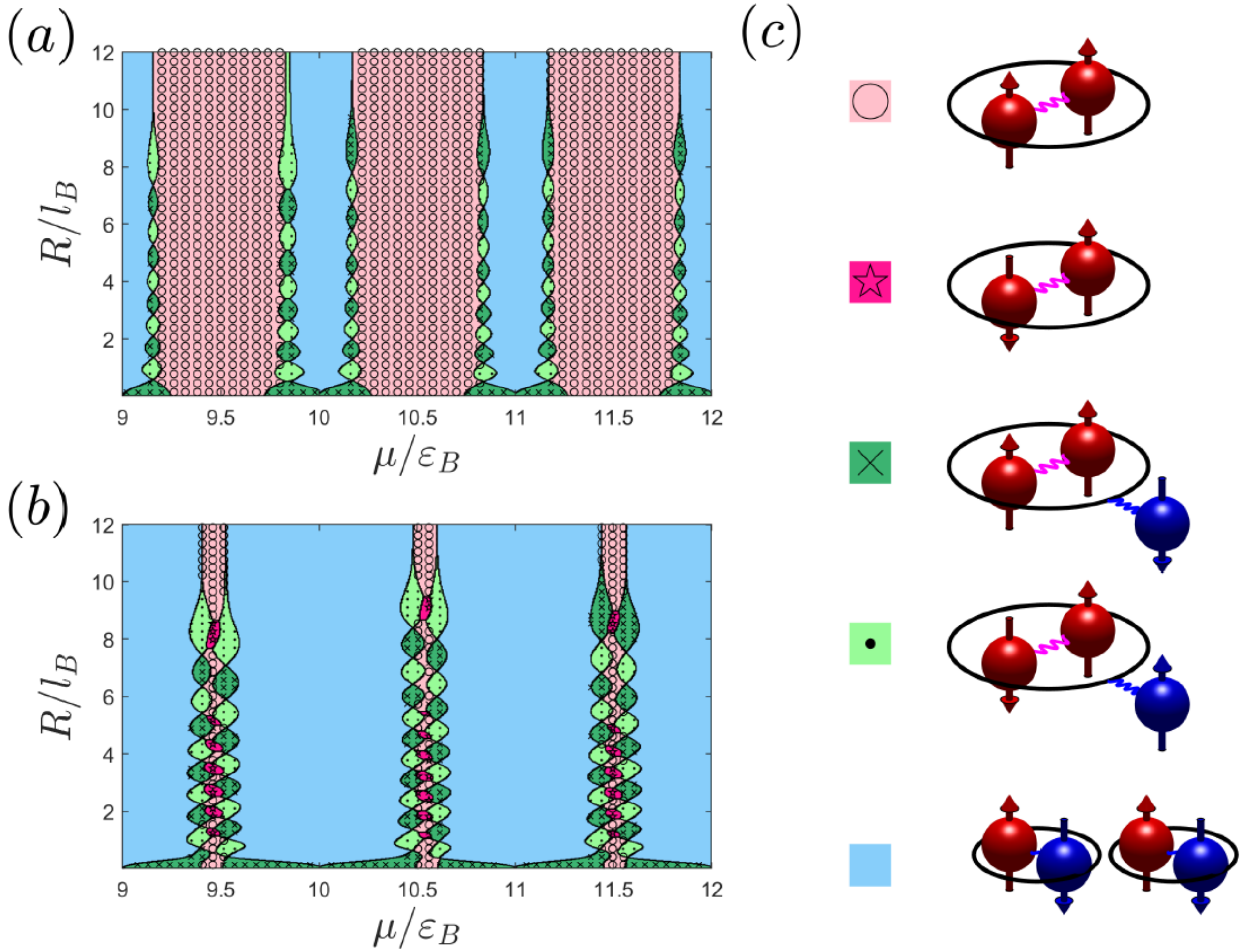
$\tilde{g}_c = \tilde{g}_d = 2$

weak ρJ :

$\rho J = 0.18$

strong ρJ :

$\rho J = 0.45$

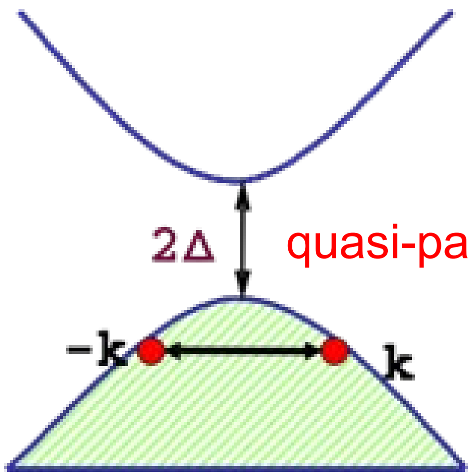


Outline:

- Exotic superconductivity that can arise in topological materials
    - ➢ Topological Kondo superconductivity
      (Communication Physics 7, 253, 2024)
    - ➢ Geometry induced topological superconductivity
      (Phys. Rev. B 103, 014508,2021)
    - ➢ Flat band superconductivity, charge density wave and superconducting pair density wave state
      (Phys. Rev. B 98, 205103, 2018, Phys. Rev. X 11, 041038,2021)
    - ➢ Emergence of O(4) symmetry in cuprate superconductors
      (Submitted to Nature Communication, 2024)

BCS theory – conventional s-wave

$$\Delta_k = -\sum_{k'} V_{k,k'} < c_{-k'\downarrow} c_{k'\uparrow} >$$

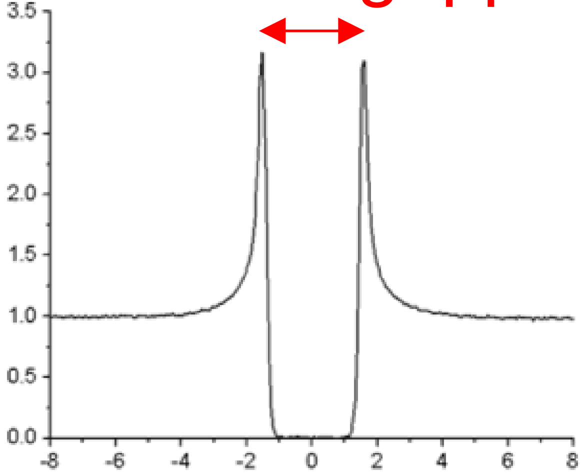


quasi-particle: $E_k = \sqrt{\varepsilon_k^2 + \Delta_k^2}$

pairing symmetry:
s-wave, $\Delta_k = \Delta$

density of state

gapped, 2Δ



$$\Delta_k = -\sum_{k'} V_{k,k'} \frac{\Delta_{k'}}{2E_{k'}} \tanh \beta E_{k'}$$

$$\boxed{\Delta = 0 \;\rightarrow k_B T_c = 1.13\hbar\omega_D e^{-1/Ng} \lesssim k_B \Theta_D}$$

E

N(ε_F) = density of state, $\Theta_D \propto 1/\sqrt{M_{ion}}$

What can other forms of superconductivity exist?

Two electrons: **relative motion**

+ center of mass motion

$$< c_{-k+Q/2\downarrow} c_{k+Q/2\uparrow} >= \phi(k)\psi(Q)$$

Relative motion: pairing symmetry $\phi(k)$ (non s-wave?)

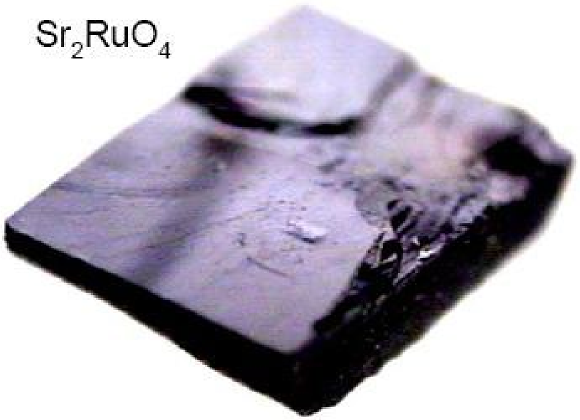
CM momentum: pair density waves $\psi(Q)$

Condensate at finite momentum ($\frac{\hbar^2 Q^2}{2m}$?)

higher Tc? **different mechanism?**

Nature odd-parity superconductors

Superfluid ^3He,
old candidate: Sr_2RuO_4 (?)



Recent proposed candidates: $PrOs_4Sb_{12}$, $Cu_xBi_2Se_3$, Bi_2Te_3 & Sb_2Te_3 (under high pressure), β-$PdBi_2$, $In_xSn_{1-x}Te$, $Cu_x(PbSe)_5Bi_2Se_3$, $Sr_xBi_2Se_3$, Sb_2Te_3

Confirmed candidates are rare!

Outline:

- Exotic superconductivity that can arise in topological materials
  - ➢ Topological Kondo superconductivity

  (Communication Physics 7, 253, 2024)

Topological Kondo Superconductors

Yung-Yeh Chang, Khoe Van Nguyen, Kuang-Lung Chen,
Yen-Wen Lu, Chung-Yu Mou, and Chung-Hou Chung

Offer a qualitative and some quantitative understanding of the spin-triplet superconductivity recently observed in UTe_2

Key idea:
spin-orbit hybridization between d-orbit electrons and f-orbit electrons

- 5d conduction band + 4f more localized band

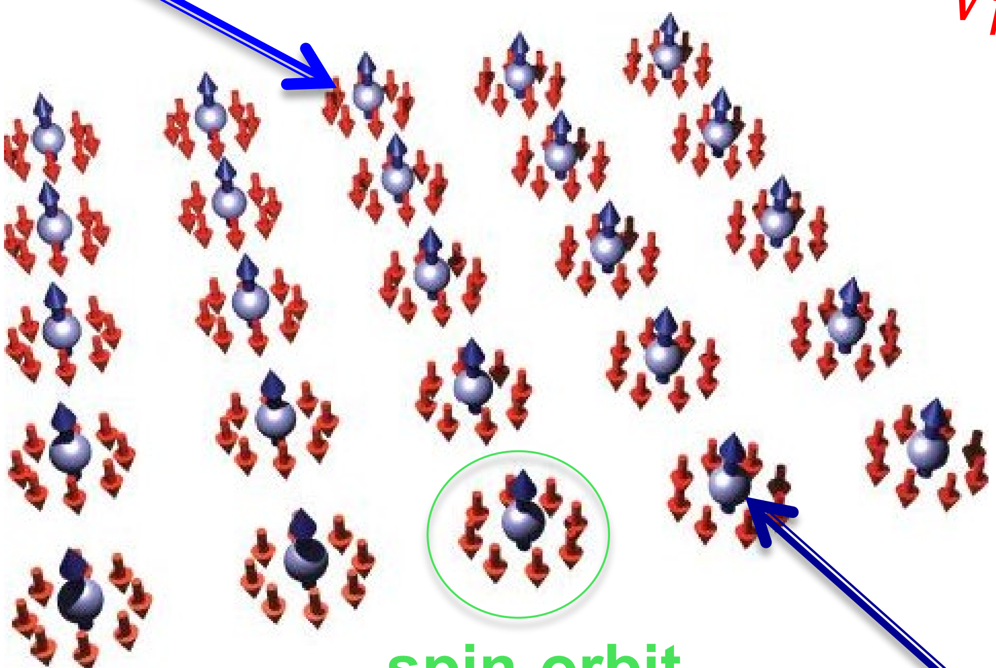
(due to difference in $l = 2$ and $l = 3$)

Kondo lattice with spin-orbit hybridization

$$H = \sum_{k\sigma} \xi_k c_{k\sigma}^{\dagger} c_{k\sigma} + \xi_k^d d_{k\sigma}^{\dagger} d_{k\sigma} + \sum_{k\sigma} V_k^{\sigma\sigma'} c_{k\sigma}^{\dagger} d_{k\sigma'} + h.c + U \sum_i n_{i\uparrow}^d n_{i\downarrow}^d$$

conduction e⁻ $c_{k\sigma}$

$$V_k = 2\lambda_{SO} \sum_o \sigma_i \sin k_i$$



spin-orbit interaction

f-orbit e⁻

$d_{k\sigma} \to f_{k\sigma}$

Kondo-Heisenberg Model with spin-orbit hybridization

U term is replaced by two magnetic interactions:

Kondo spin interaction

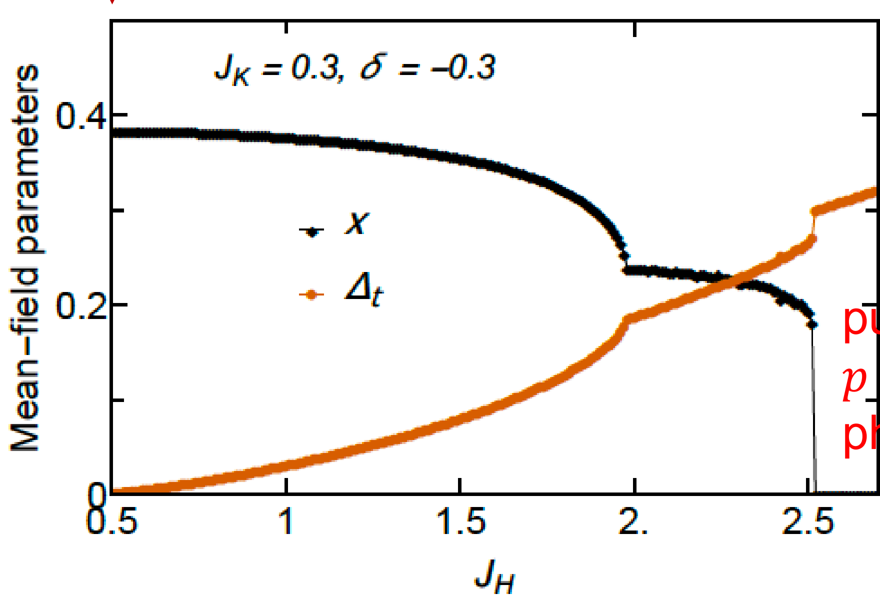
$$H_K = J_K \sum_i \vec{S}_{ic} \cdot \vec{S}_{if}$$

Ferromagnetic RKKY ($J_R > 0$)

$$H_{RKKY} = J_R \sum_{\langle i,j \rangle} \vec{S}_{if} \cdot \vec{S}_{jf}$$

Kondo-Heisenberg Lattice with $p \pm ip$ pairing

Pure Kondo phase



pure $p \pm ip$ SC phase

Fig. 2. The zero-temperature mean-field solutions of t-RVB order parameter Δ_t (brown) and the Kondo correlation x (black) as a function of J_H. We fix $J_K = 0.3$ and doping of the conduction band $\delta = -0.3$ (30 percent hole doping). Without loss of generality, we set $t = 1$. This plot reveals a (co-existing) superconducting ground state with $x \neq 0$, $\Delta_t \neq 0$ for $0 < J_H \lesssim 2.5$ and a pure t-RVB phase where $x = 0$, $\Delta_t \neq 0$ when $J_H \gtrsim 2.52$. A pure Kondo phase ($x \neq 0$, $\Delta_t = 0$) only exists at $J_H = 0$.

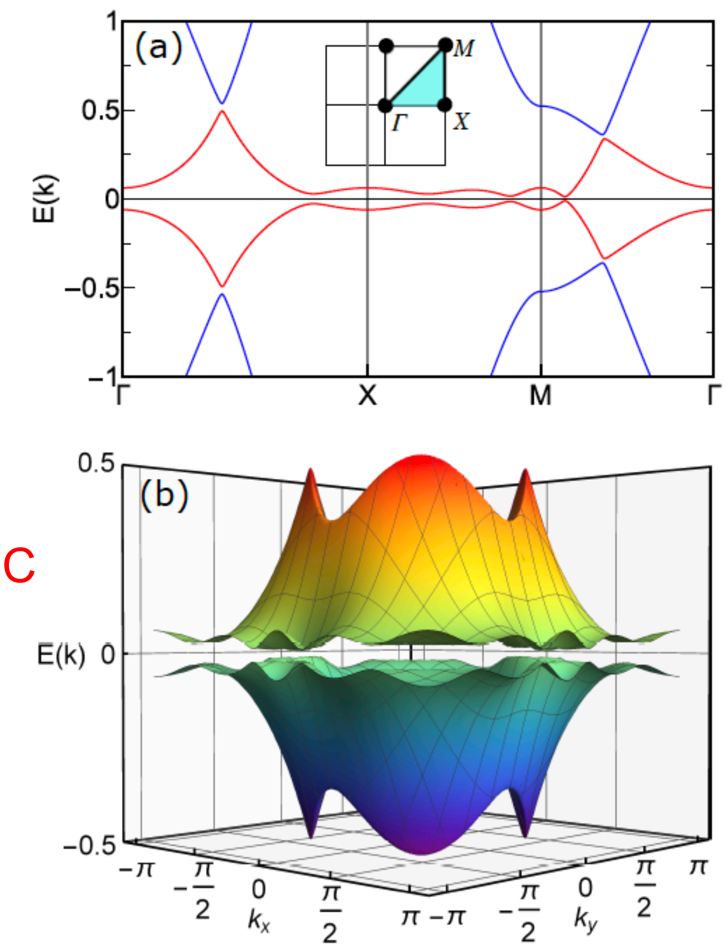


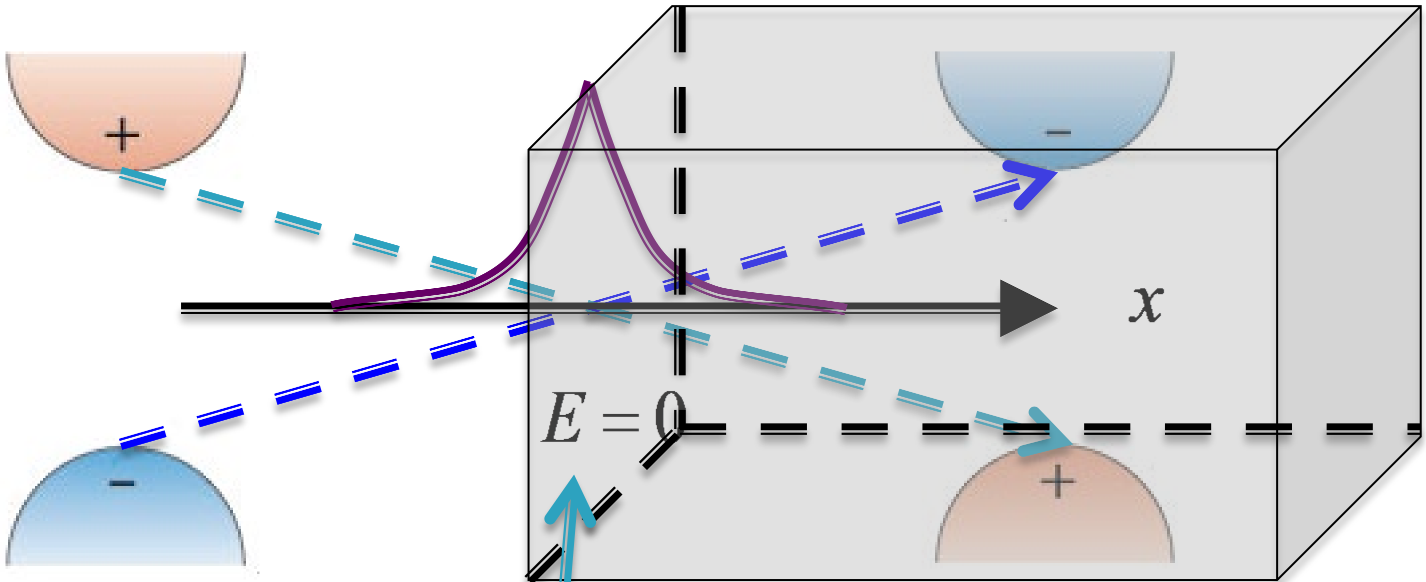
Fig. 3. Figures (a) (red curves) and (b) show the bulk energy spectrum of the co-existing superconducting state near the Fermi level μ. The Fermi level locates at $E(\boldsymbol{k}) = 0$. The coupling constants are $J_K = 0.3$ and $J_H = 1.0$. Inset of (a) displays the First Brillouin zone of a square lattice with indications of high-symmetry points Γ, X, M.

Outline:

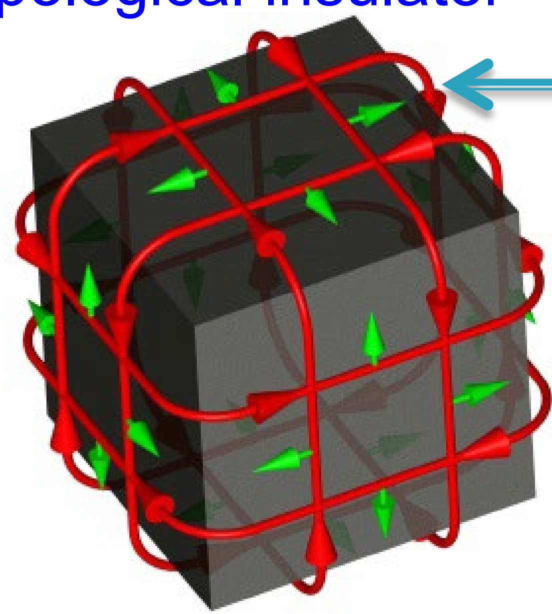
- Exotic superconductivity that can arise in topological materials

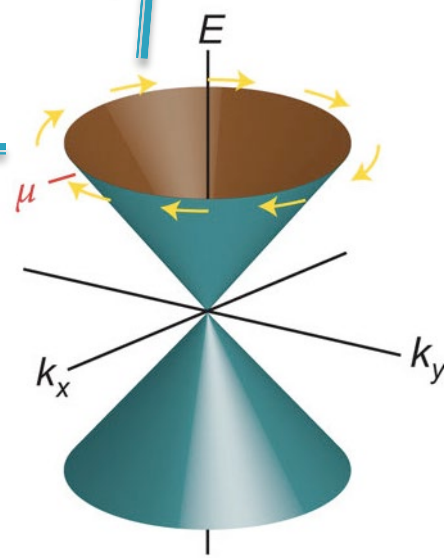
  - ➢ Geometry induced topological superconductivity
(Phys. Rev. B 103, 014508,2021)

New Twist from consideration of topology



3D topological insulator





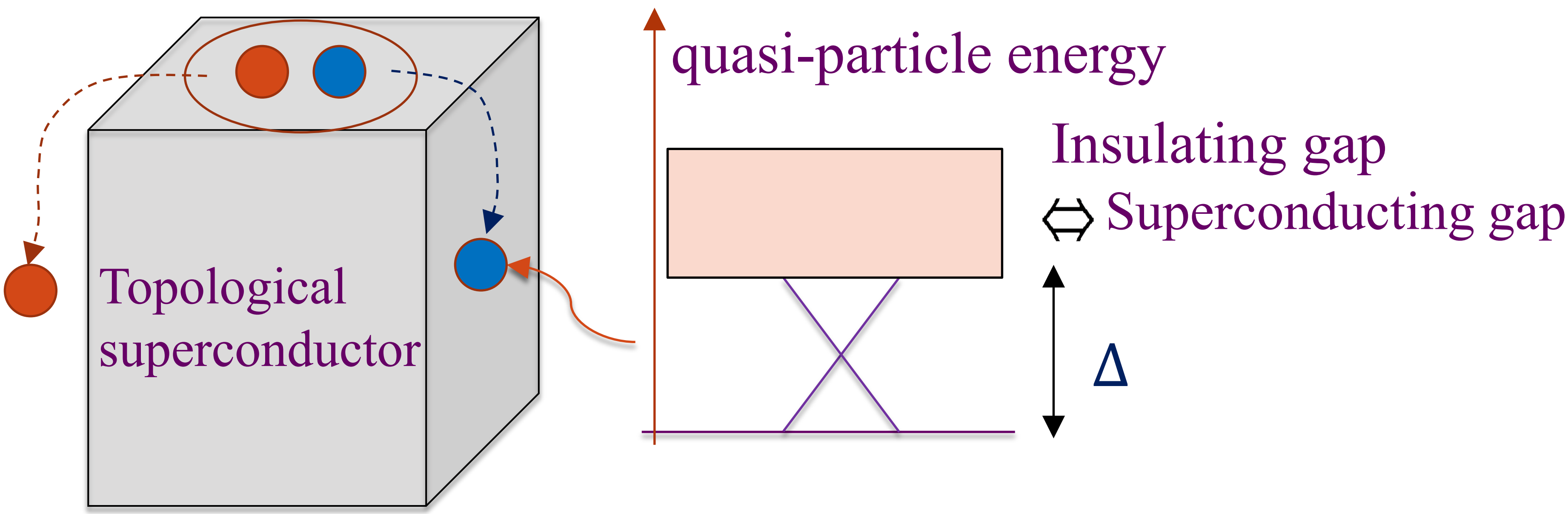
Topological invariant

Z_2 :

Odd number inversion
Even number inversion

Liang Fu, C. L. Kane, and E. J. Mele, 2007

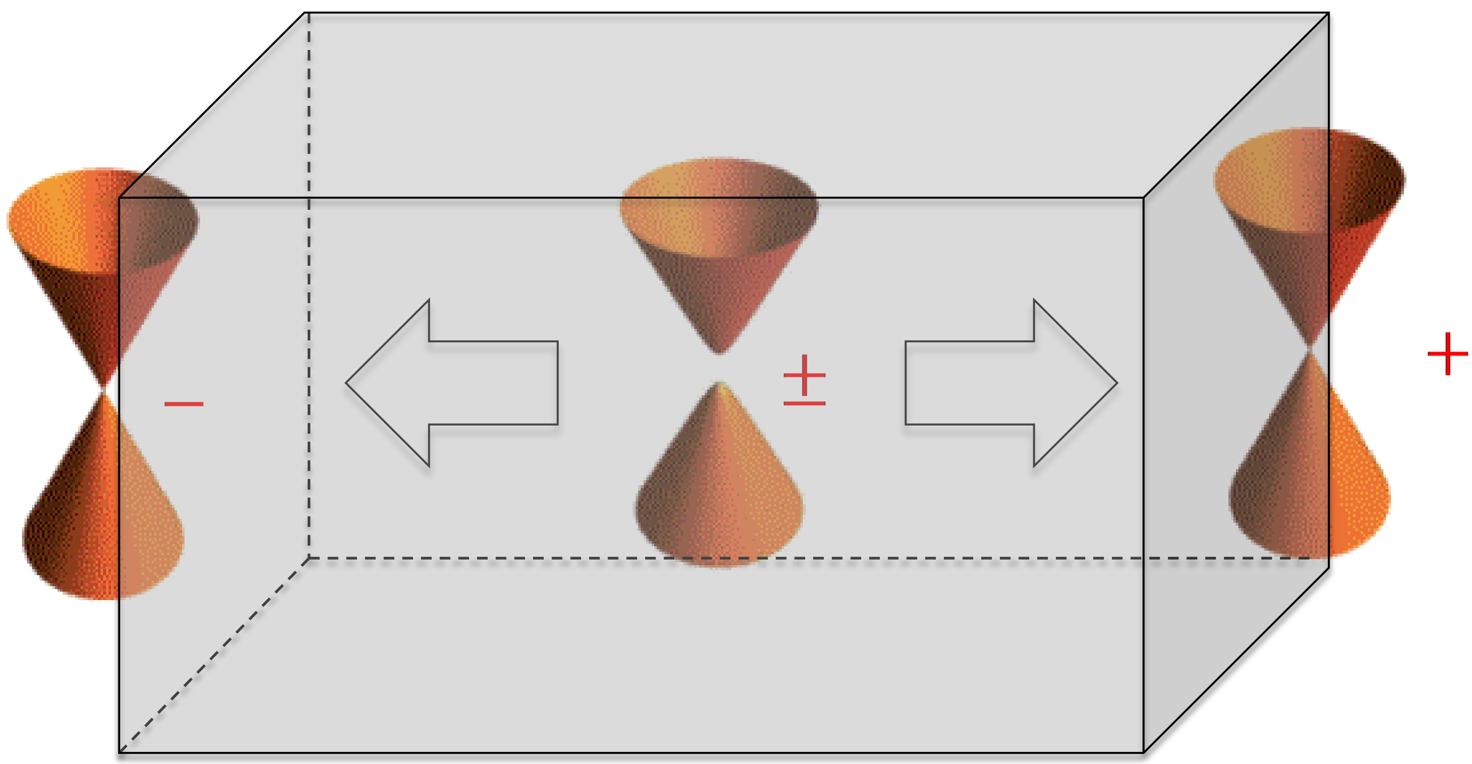
Topological superconductivity



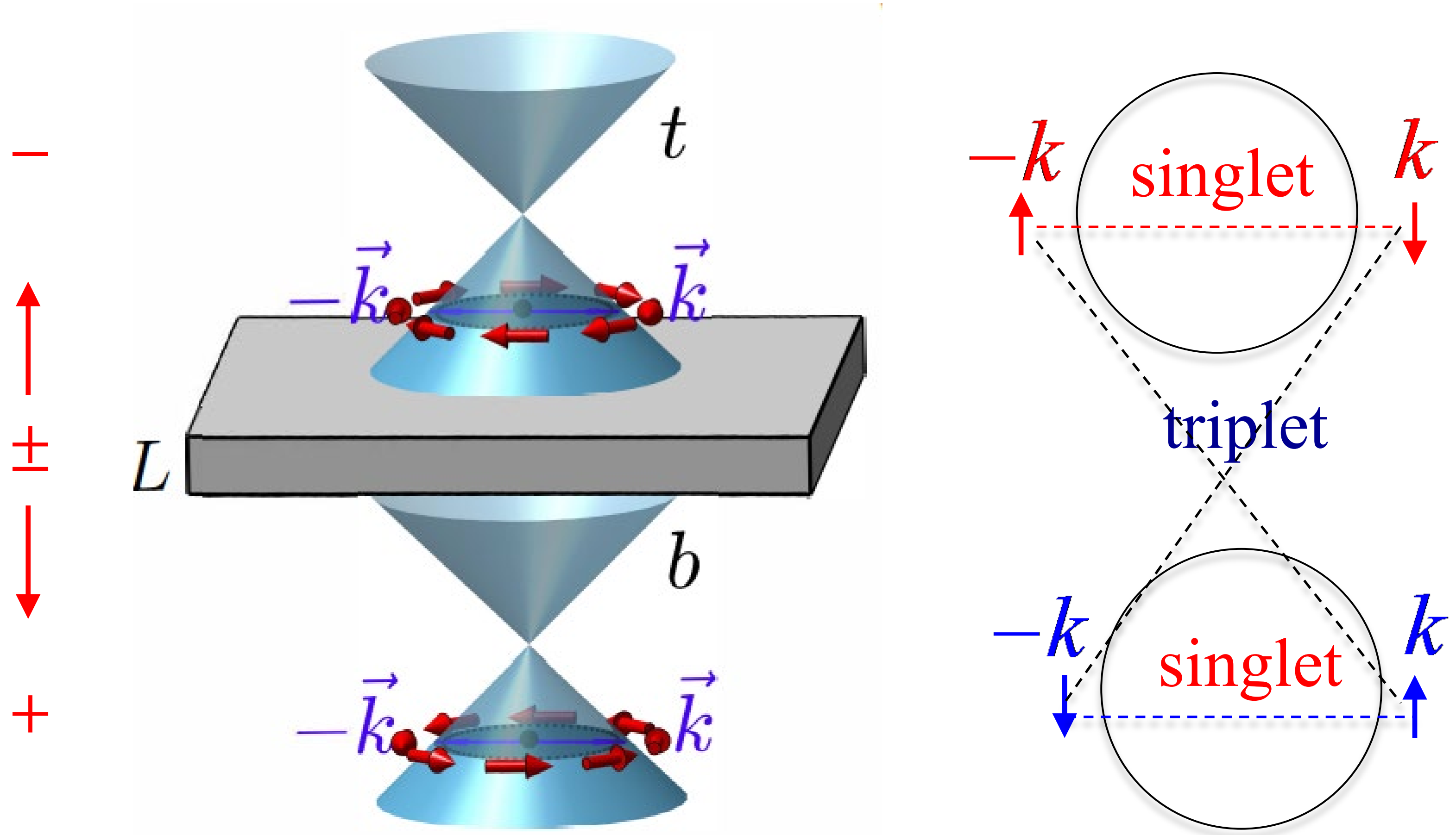
$$H_{SC\uparrow}(k)=\begin{pmatrix} \Lambda_k-\mu & T_k & 0 & \Delta_k \\ T_k^* & -\Lambda_k-\mu & -\Delta_{-k} & 0 \\ 0 & -\Delta_{-k}^* & -\Lambda_k+\mu & T_k \\ \Delta_k^* & 0 & T_k^* & \Lambda_k+\mu \end{pmatrix} \quad \psi_{FM}=\begin{pmatrix} C_{Ak\uparrow} \\ C_{Bk\uparrow} \\ C_{Ak\downarrow} \\ C_{Bk\downarrow} \end{pmatrix} \text{ or } \psi_{FM}=\begin{pmatrix} C_{Ak\uparrow} \\ C_{Bk\uparrow} \\ C_{Ak\downarrow} \\ C_{Bk\downarrow} \end{pmatrix}$$

Qi & Zhang, Rev. Mod. Phys. 83, 1057 (2011); Hasan & Kane 82, 3045 (2010).

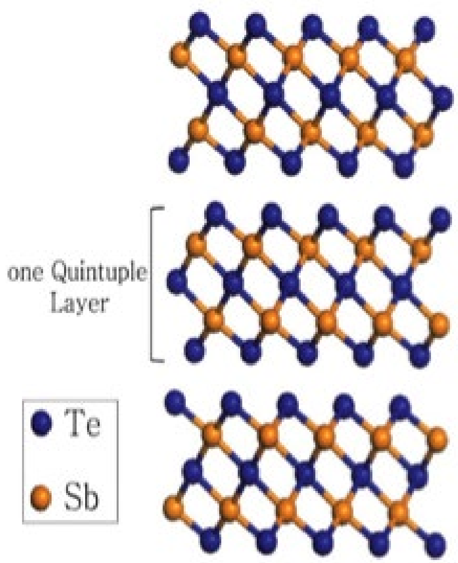
Unique feature of topological Insulators: chirality separation in real space without invoking symmetry breaking

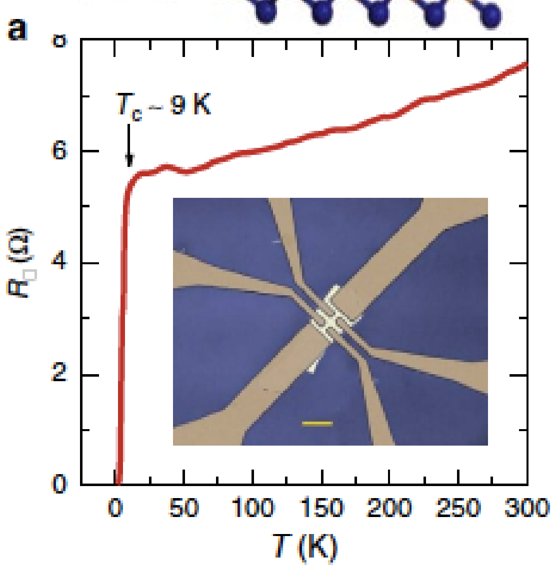


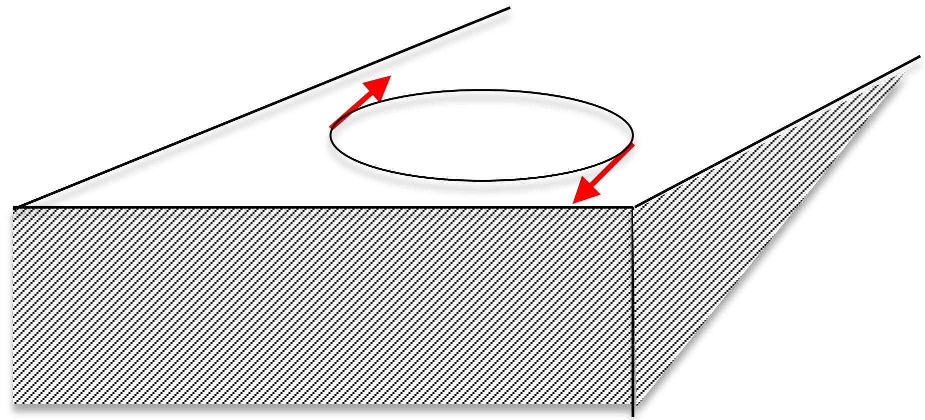
Thin film geometry:
competition of intra-surface (singlet) and inter-surface (triplet) through thickness dependence of interaction



Feasibility: surface superconductivity on flat surface of Sb_2Te_3 (hole-doped single Weyl cone)







$$= \frac{1}{2}\left[e^{-i\phi}\,|\uparrow\uparrow\rangle - e^{i\phi}\,|\downarrow\downarrow\rangle\right] - \frac{1}{2}\left[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right]$$

Equal strength of singlet and triplet pairing!

Marginal topological superconductivity!

L. Zhao et al, Nat. Commun. 6, 8279 (2015).

Additional effect on curved space:
spin connection effect

$$\partial_\mu \to \partial_\mu + igA_\mu \qquad A_\mu = \frac{1}{4}\omega_\mu^{ab}\sigma_{ab} \qquad \nabla \times \vec{A} = \vec{B}_{eff}$$

$\sigma_{ab} = -\frac{i}{2}[\gamma_a, \gamma_b]$ $\quad \omega_\mu^{ab}$ = spin connection

$\int gA_\mu dx^\mu$ = **Berry phase due to different orientation of Dirac cone**

Sphere:
A. A. Abrikosov, Int. J. Mod. Phys. A17, 885, (2002)
D.-H. Lee, Phys. Rev. Lett. 103, 196804 (2009).

Local spin up $-1/2$ **Local spin down** $+1/2$

Only $\uparrow\uparrow$ or $\downarrow\downarrow$ **sees** $\vec{B}_{eff}$!

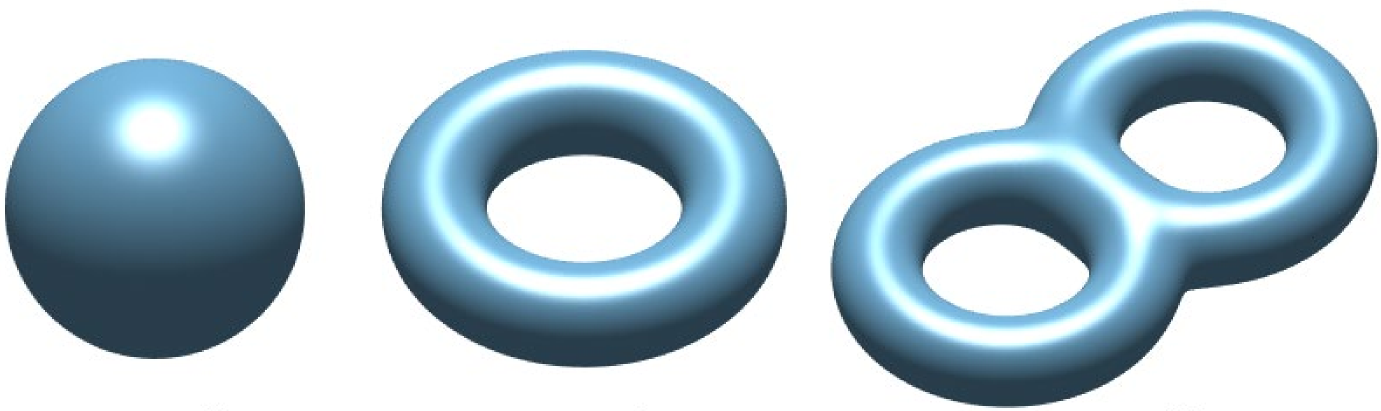
Our extension: $\vec{B}_{eff} = \pm\frac{1}{2}K\hat{n}$

K = Gauss curvature

$\hat{n}$ = unit normal vector to the surface

Gauss-Bonnet theorem: $\oint_S \vec{B}_{eff} \cdot d\vec{a} = \pm 2\pi(1-g)$

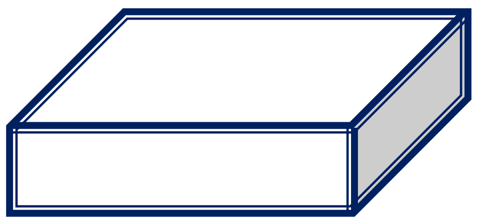
$S =$



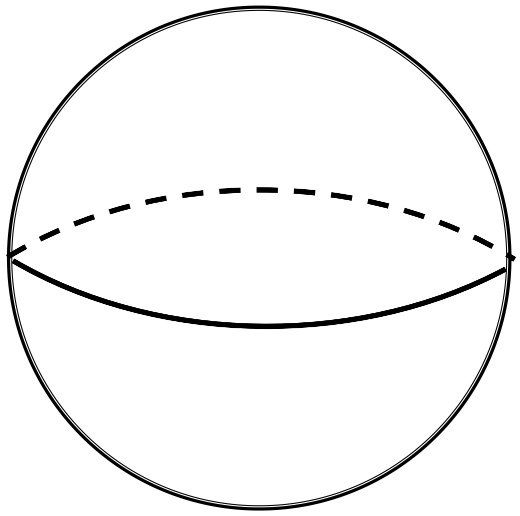
$g=0$ $g=1$ $g=2$ …

Illustration on two $g = 0$ surfaces

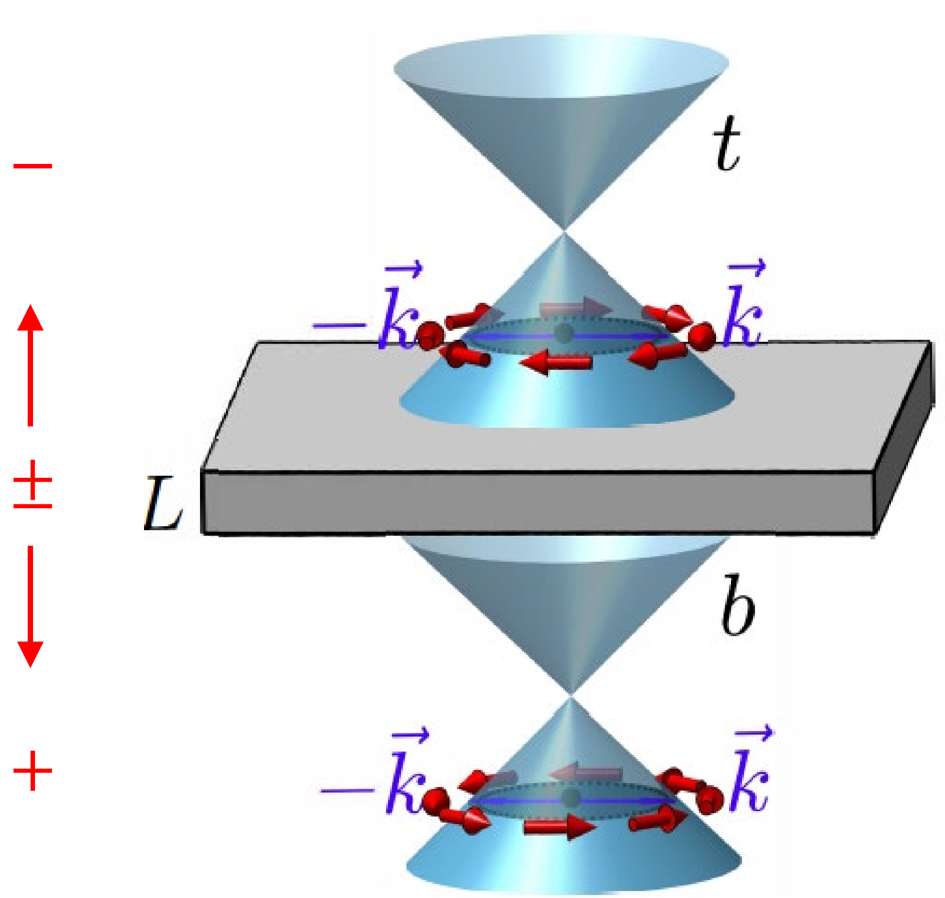
(i) thin film geometry
(two surfaces,
thickness can be tuned)

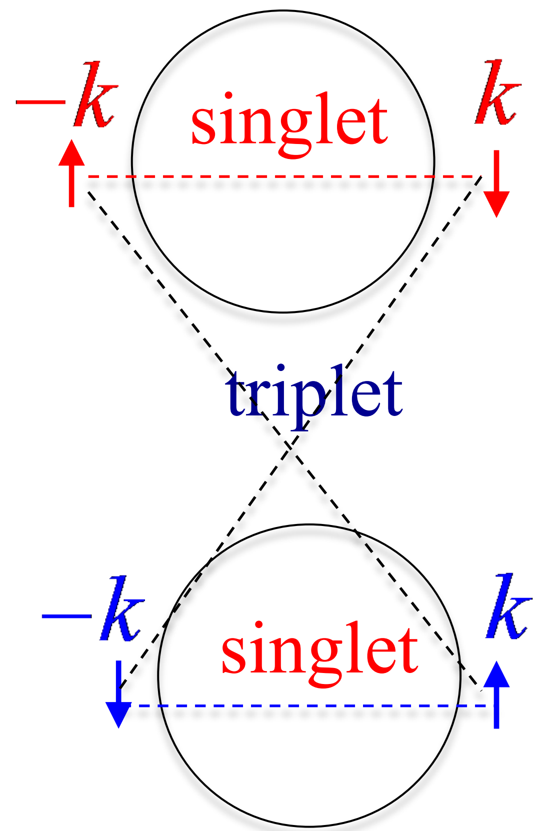


(ii) spherical geometry
(curvature can be tuned)

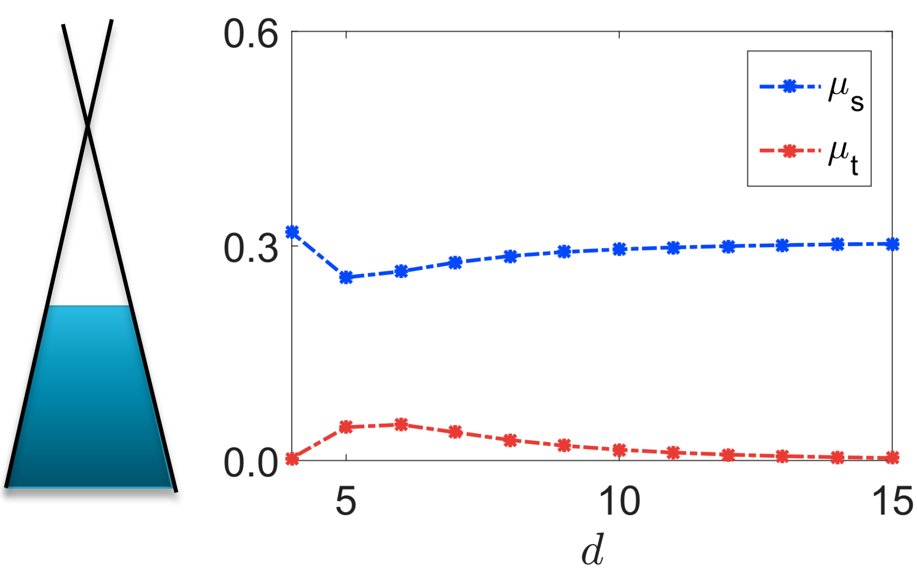


Thin film geometry:
competition of intra-surface (singlet) and inter-surface (triplet) through thickness dependence of interaction



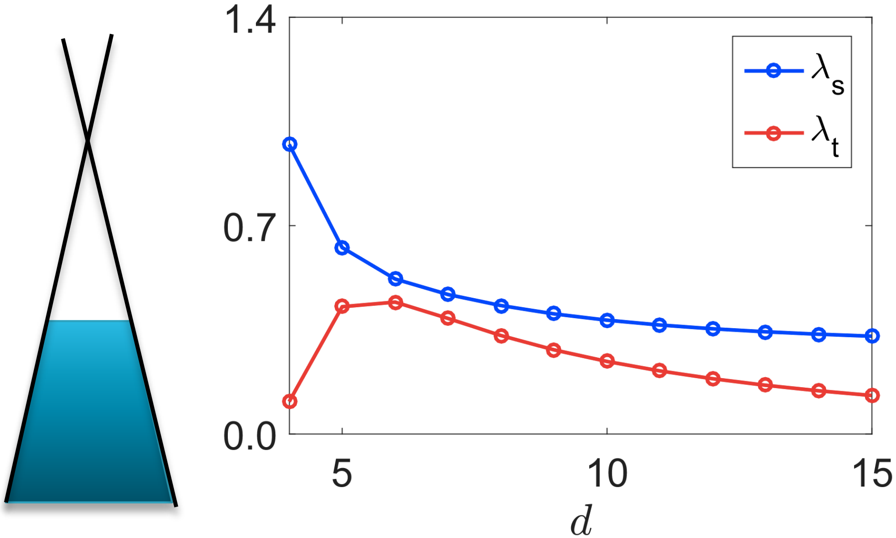


Coulomb interaction (average over Fermi surface)



$$\mu_\alpha = \oint g_\alpha^C(k_F, k_F)$$

Electron-phonon coupling



$$\lambda_\alpha = \oint g_\alpha^P(k_F, k_F)$$

Exclusive singlet and triplet pairing

$$H_\Delta = \sum_k \Delta_s(k) e^{-i\phi_k} (c^\dagger_{kt} c^\dagger_{-kt} - c^\dagger_{kb} c^\dagger_{-kb}) + \Delta_t(k) e^{-i\phi_k} (c^\dagger_{kt} c^\dagger_{-kb} + c^\dagger_{kb} c^\dagger_{-kt}) + h.c$$

Both singlet and triplet paring are determined by the same quasi-particle energy

$$E(k) = \sqrt{\xi_k^2 + \Delta_s^2(k) + \Delta_t^2(k)}$$

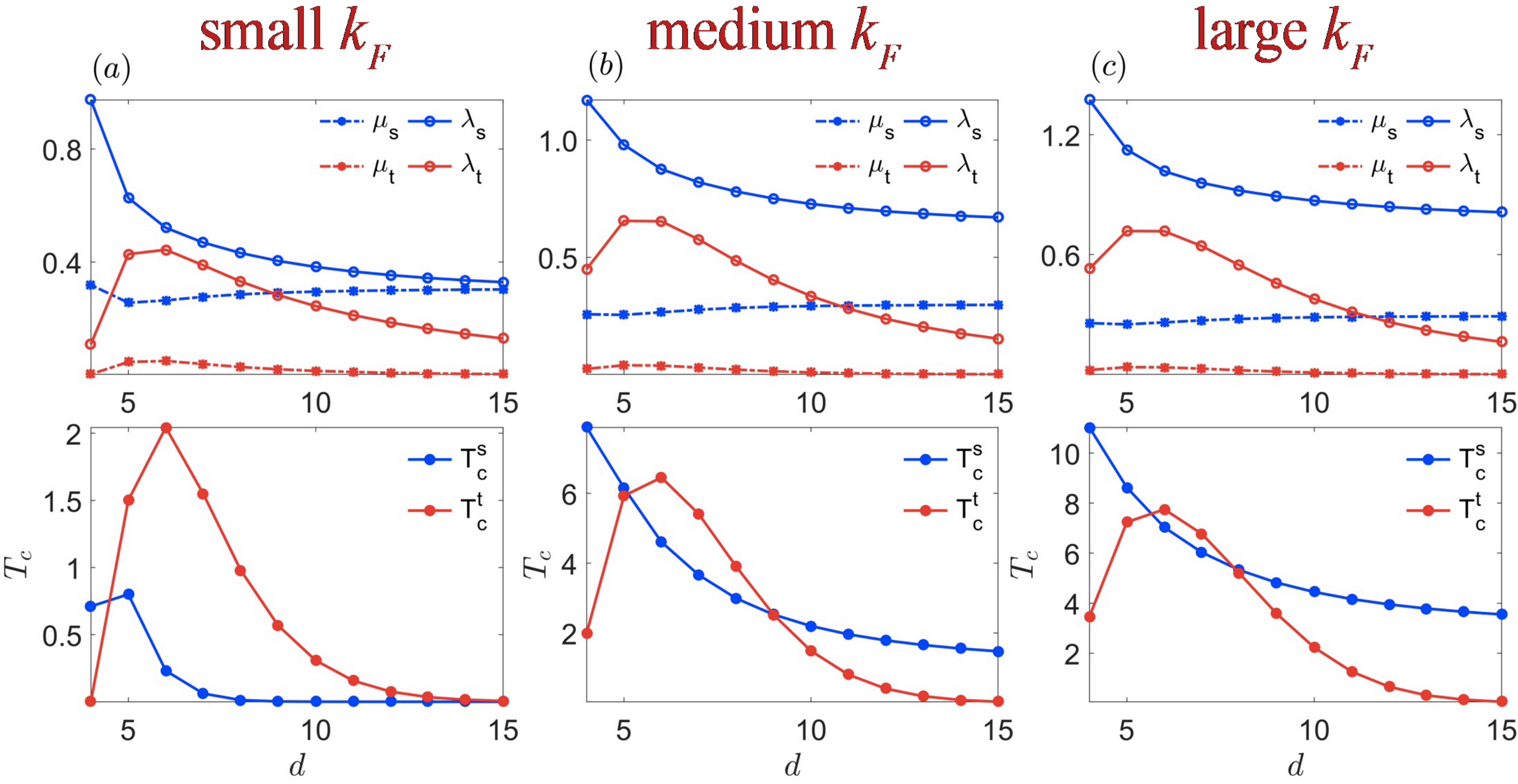
$$\Delta_s(k) = \sum_{k'} g_s(k,k') \frac{\Delta_s(k')}{2E_{k'}} \tanh(\beta E_{k'})$$

$$\Delta_t(k) = \sum_{k'} g_t(k,k') \frac{\Delta_t(k')}{2E_{k'}} \tanh(\beta E_{k'})$$

$\Rightarrow$ can not be satisfied simultaneously!

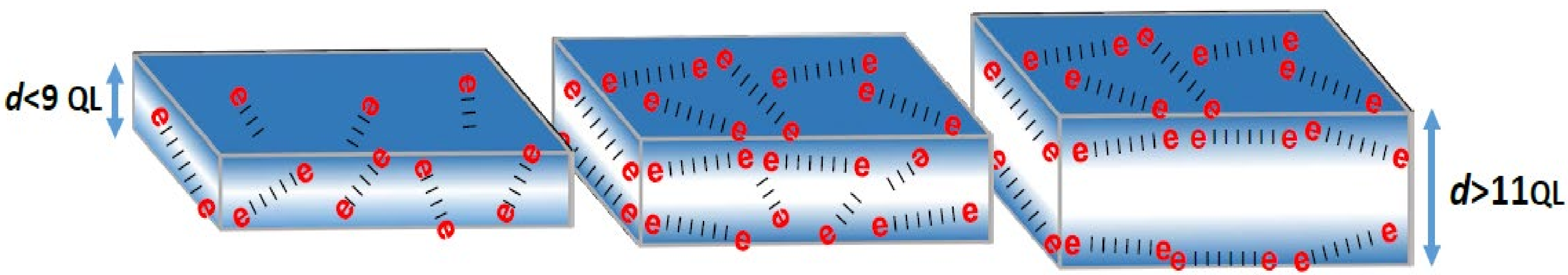
Theoretical results for Sb_2Te_3 films

McMillan formula: $T_c = \frac{\theta_D}{1.45}\exp\left[-\frac{1.04(1+\lambda)}{\lambda-\mu^*(1+1.62\lambda)}\right], \mu^* = \mu[1+\ln(\Lambda/\omega_c)]$

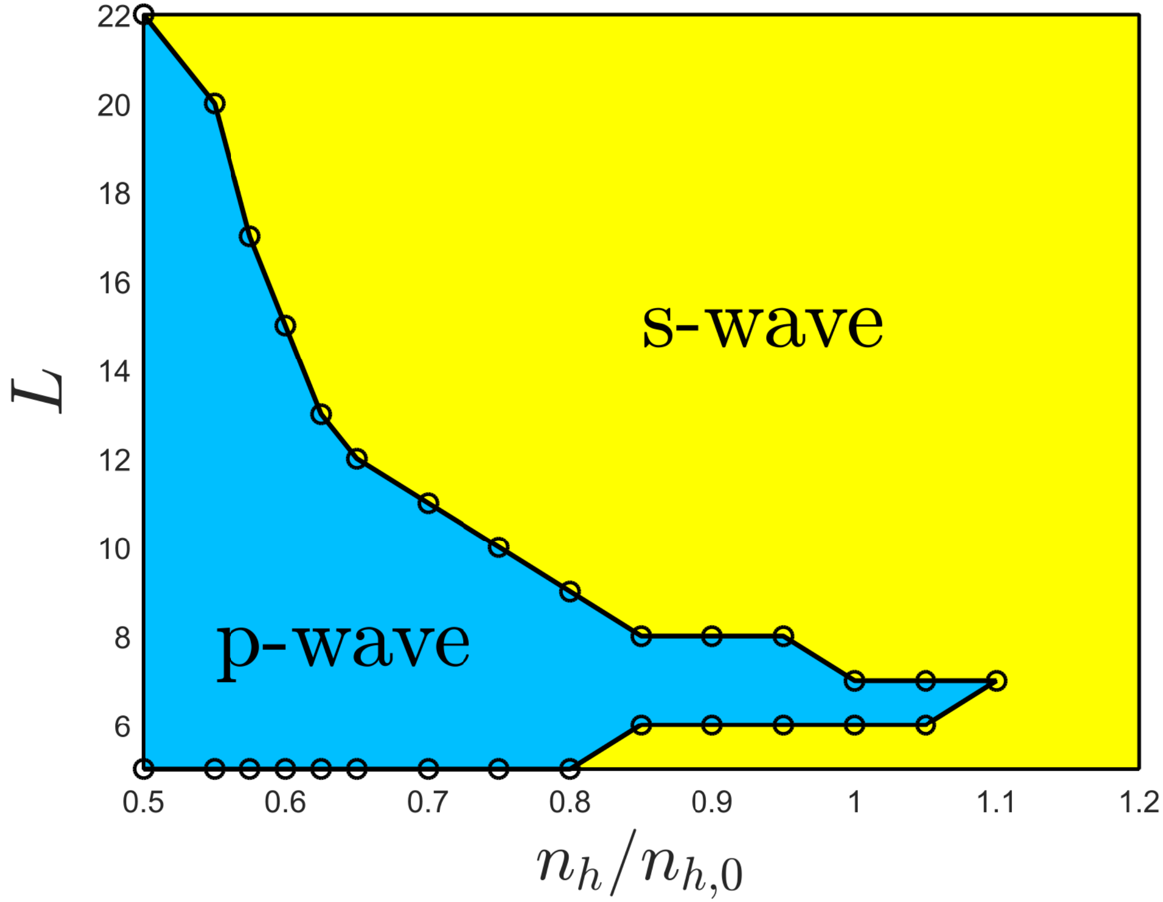


Experimental observations on superconductivity in Sb_2Te_3 nanoflakes

-- Yang-Yuan Chen's group Academia Sinica

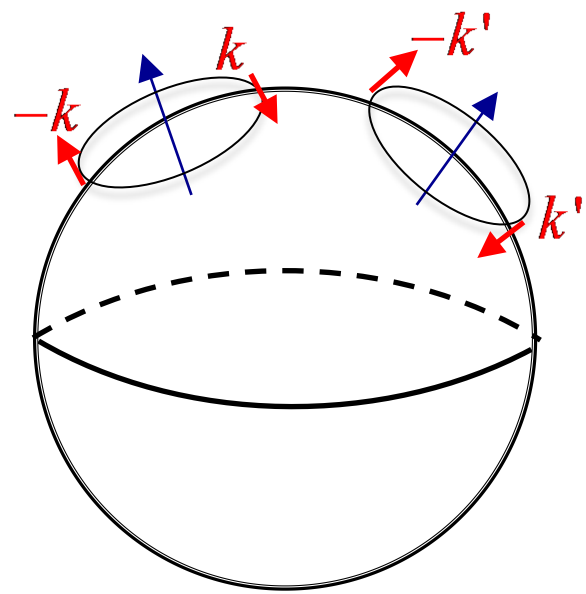


Phase diagram



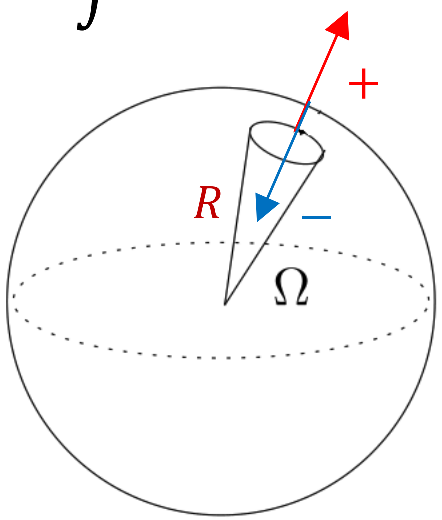
Spherical geometry:

Competition of singlet pairing at same site and triplet pairing at different sites through change of curvature



General Hamiltonian for superconductivity on sphere

$$H = \int d\Omega\, \Psi_\Omega^\dagger (h - \mu)\, \Psi_\Omega + \frac{1}{2} \iint d\Omega d\Omega'\, V(\Omega, \Omega') (\Psi_\Omega^\dagger \Psi_\Omega)(\Psi_{\Omega'}^\dagger \Psi_{\Omega'})$$



Local spinor $\Psi_\Omega^\dagger = (c_{\Omega,+}^\dagger, c_{\Omega,-}^\dagger)$

$$h = \frac{\lambda_{so}}{R} \begin{pmatrix} 0 & D_- \\ D_+ & 0 \end{pmatrix}$$

$$D_\pm = e^{\pm i\phi} (\pm \partial_\theta + \frac{i}{\sin\theta} \partial_\phi \mp \frac{1}{2} \tan\frac{\theta}{2})$$

$$V(\Omega, \Omega') = V_c(\Omega, \Omega') + V_{ph}(\Omega, \Omega') \qquad V_{ph}(\Omega, \Omega') = -V_{ph} \exp(-\alpha_{ph} \Delta\Omega^2)$$

$$V_c(\Omega, \Omega') = \frac{V_C}{2R|\sin\frac{\Delta\Omega}{2}|} \exp(-\alpha_c |\sin\frac{\Delta\Omega}{2}|) \qquad \Delta\Omega = \Omega - \Omega'$$

Mean field theory

$$H = \int d\Omega\, \Psi_\Omega^\dagger (h-\mu)\, \Psi_\Omega + \frac{1}{2}\iint d\Omega d\Omega'\, \Delta_{\Omega,\Omega'}^{s,s'} C_{\Omega,s}^\dagger C_{\Omega',s'}^\dagger + h.c.$$

$$\Delta_{\Omega,\Omega'}^{s,s'} = V(\Omega,\Omega')\, \langle C_{\Omega,s} C_{\Omega',s'} \rangle$$

Cooper pair: Center of Mass $\bar{\Omega} = \dfrac{\Omega + \Omega'}{q}$

$$\Delta_{\Omega,\Omega'}^{s,s'} = \Delta_s(\bar{\Omega}) S(\Omega,\Omega') + \Delta_p(\bar{\Omega}) P(\Omega,\Omega') + \;\ldots$$

$\boldsymbol{s, s' = \pm}$

Local spinor

$|+\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$ $|-\rangle = \begin{pmatrix} -\alpha^* \\ \beta^* \end{pmatrix}$

$S(\Omega,\Omega')$ = constant (s-wave)

$(P+iP)(\Omega,\Omega') = \alpha\beta' - \beta\alpha'$ (p+ip wave)

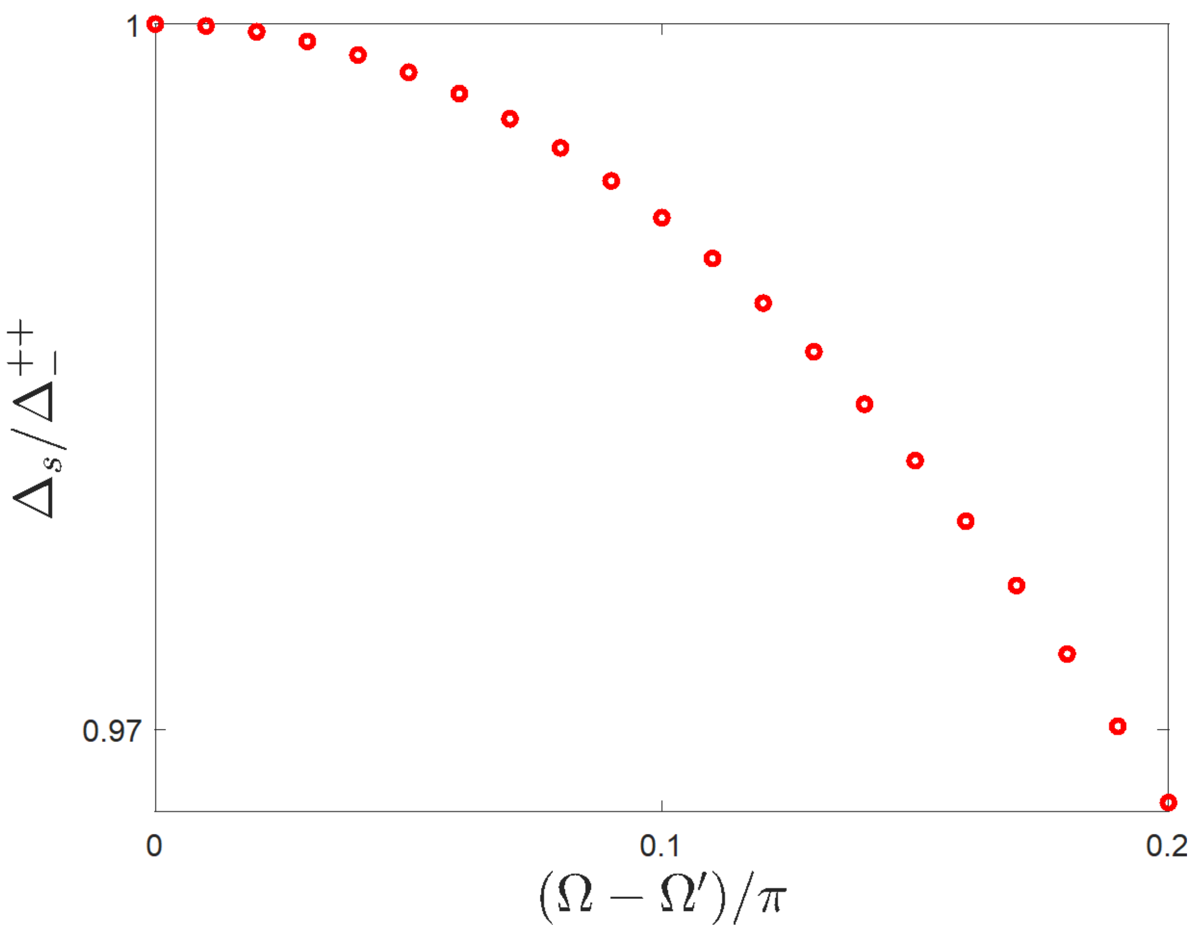
$(P-iP)(\Omega,\Omega') = \alpha\beta'^* - \beta\alpha'^*$ (p-ip wave)

Meissner Phase : triplet dominates

Singlet: Δ_s

Triplet: $\Delta^{++} = \Delta_{-}^{++}(p_x - ip_y) + \Delta_{+}^{++}(p_x + ip_y) = \Delta^{--}$

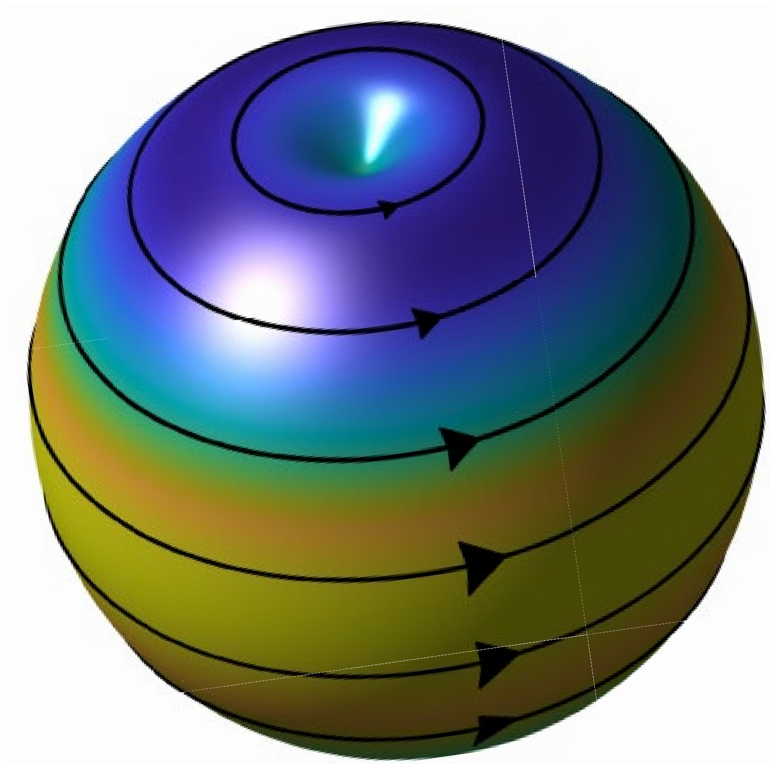
$\Delta^{--} = \Delta_{-}^{--}(p_x - ip_y) + \Delta_{+}^{--}(p_x + ip_y)$



Curvature induced vortex states

Vortex phase

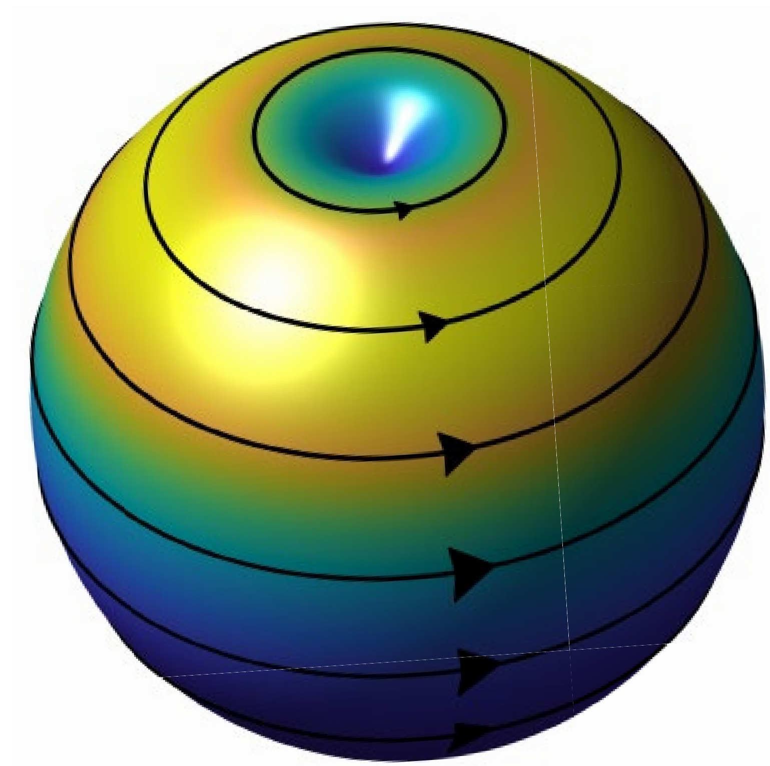
$Q = 1$



$Q = 1$

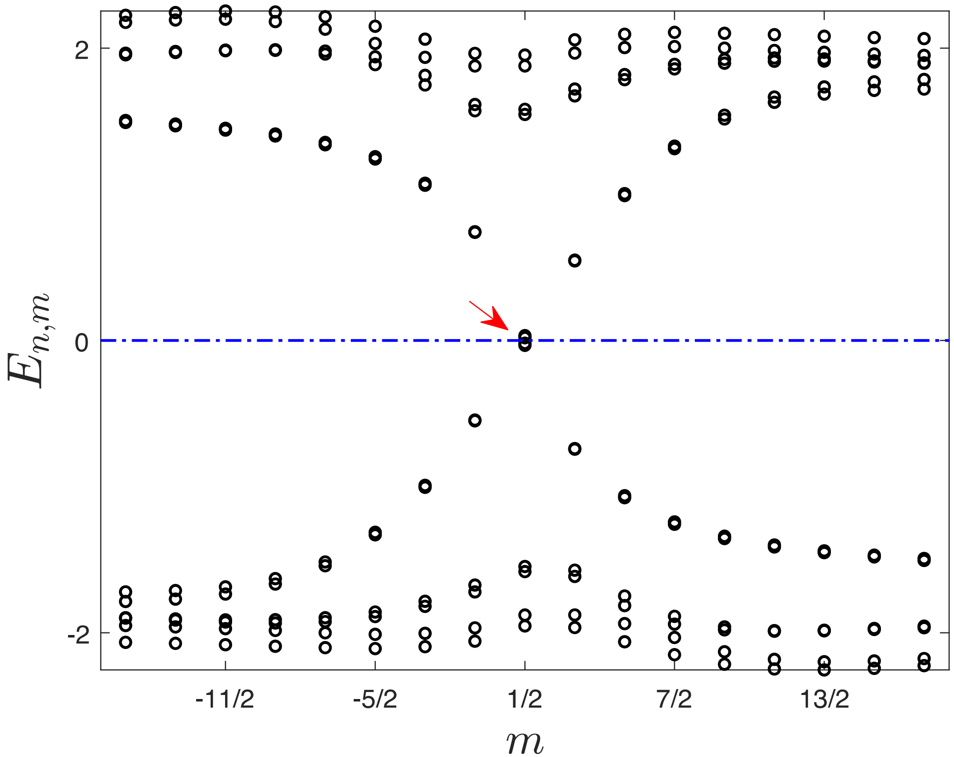
Vortex* phase

$Q = 2$

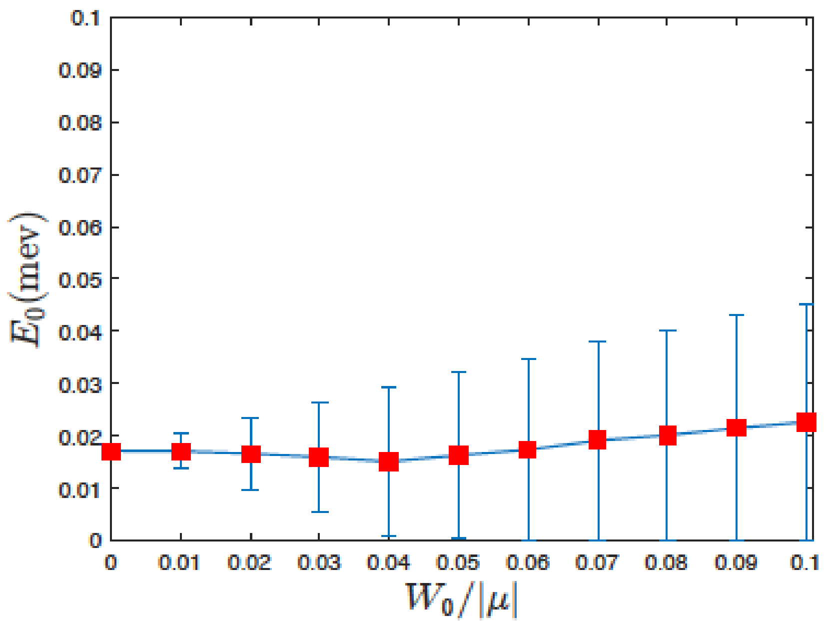


$Q = 0$

Majorana zero mode (only for $Q = \pm 1$)



Disorder effect



disorder strength

Majorana mode in the vortex on a sphere:
spinless p+ip, S. Moroz et al. Phys. Rev. B 93, 024521, (2016).
proximity effect, L. H. Hu et al. Phys. Rev. B 94, 224501, (2016)

Poincare-Hopf theorem and vortex formation

Poincare-Hopf theorem
(Hairy ball theorem) :
$\vec{v}$ vector field on a manifold M
$\vec{r}_i$ isolated points that $\vec{v} = 0$

A hair whorl

$\sum_{\vec{r}_i} index(\vec{v}) = \chi(M)$ (Euler characteristic of M)

superconducting state: $\vec{v}$ = supercurrent density
vortex: $index(\vec{v})$ = winding number
general surface: $\chi(M) = 2(1 - g)$

Given a surface with genus g
$\Longrightarrow$ Minimum number of vortex:$2(1 - g)$

Vortex formation: curvature + energetics

Example: Sphere $g = 0$

$\Longrightarrow$ Minimum number of vortex: 2

$Q = 1$, number of vortices = 2

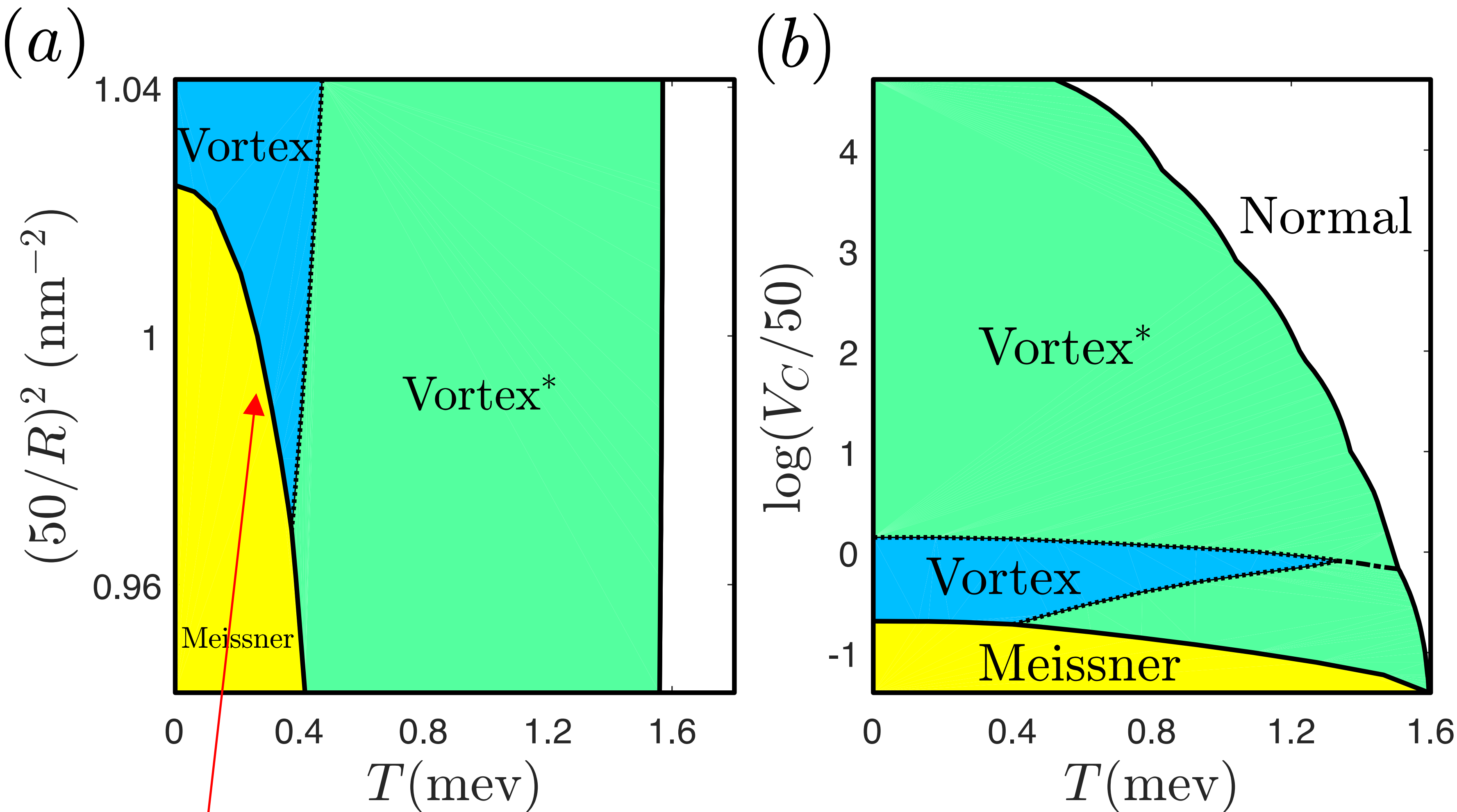
or $Q = 2$, number of vortices = 1

In general, one can add vortex-pairs, $Q = \pm 1$, to satisfy the Poincare-Hopf theorem. However, it costs energy determined by curvature as $\vec{B}_{eff} = \pm \frac{1}{2} K \hat{n}$

threshold curvature: $\epsilon \ell - B_{eff} \int b \, d^3 r = 0$

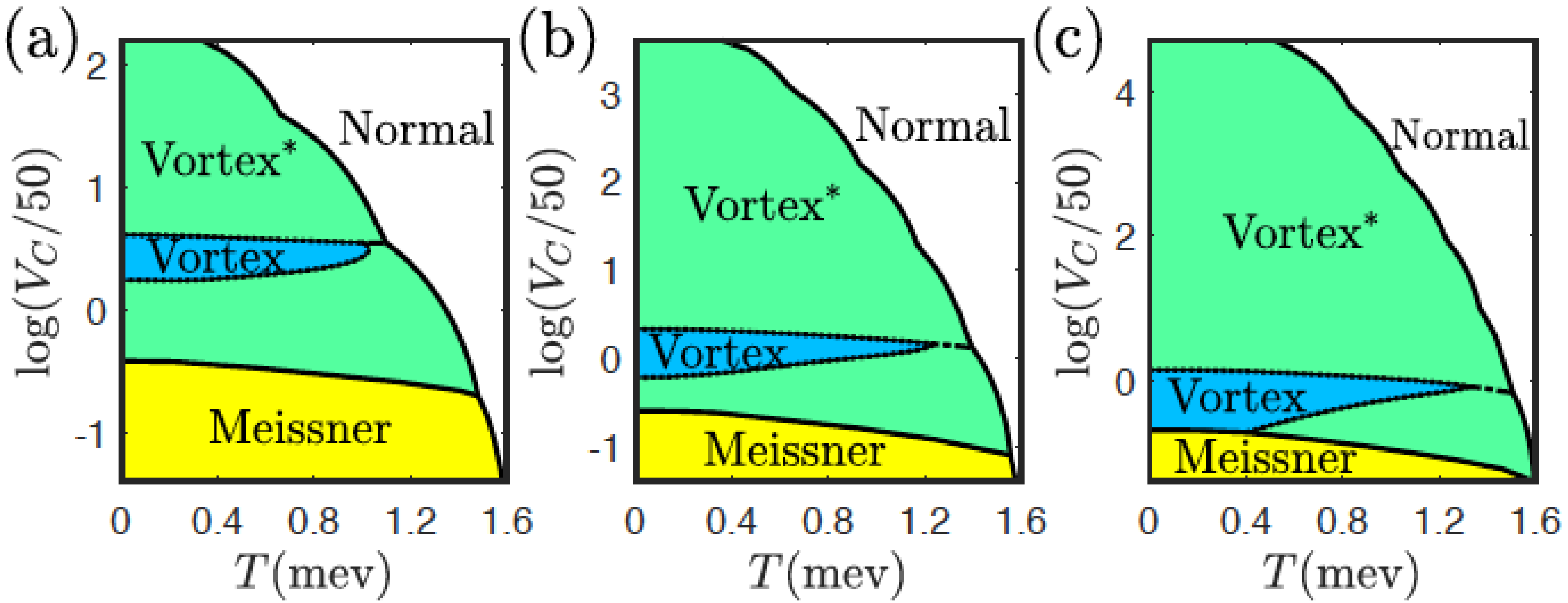
$$K_c = \frac{8\pi\epsilon}{\phi_0}$$

Phase diagram



~ critical (threshold) curvature for forming a vortex

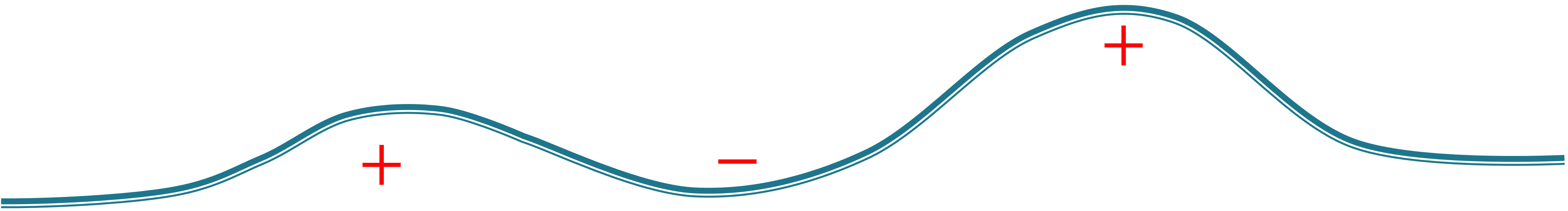
Phase diagram with different phonon strength

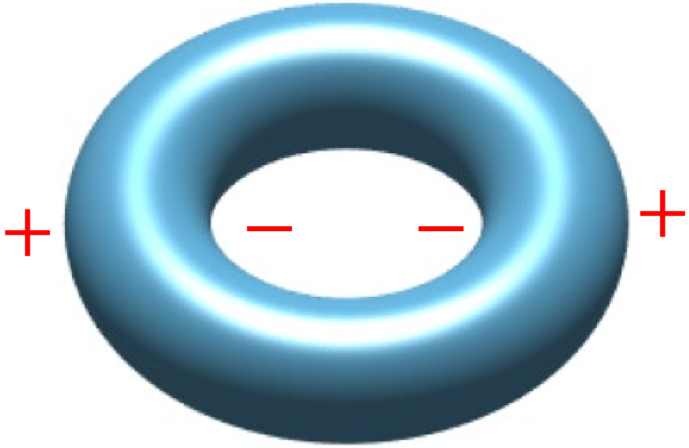


(a) $\xi_{ph} = 30\text{nm}, V_{ph} = 9.425\text{meV}$ (b) $\xi_{ph} = 50\text{nm}, V_{ph} = 7.76\text{meV}$ (c) $\xi_{ph} = 70\text{nm}, V_{ph} = 7.2845\text{meV}$

$\lambda_{so} = 35\text{mev} \cdot \text{nm},\ \xi_C = 4\text{nm},\ R = 50\text{nm},\ V_C = 50\ \text{meV}\cdot\text{nm},\ \mu = -9.5\text{meV}$

Extension to surface roughness/bump, …





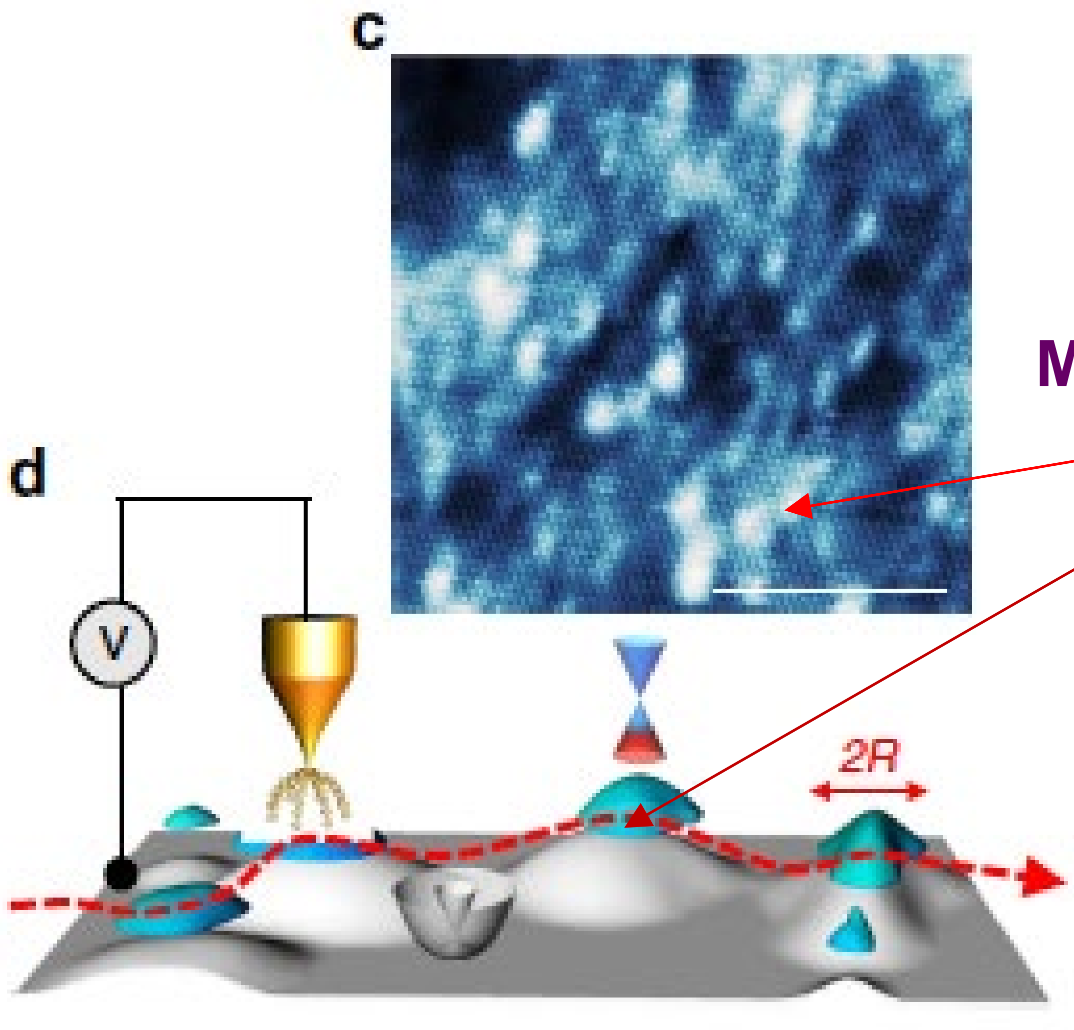
Threshold: $K_c \sim 1/(50\mathrm{nm})^2$

Minimum Free energy:

One vortex occurs at bump with largest curvature

Experimental detection:

surface superconductivity in Sb_2Te_3 with surface roughness (R = 50 nm or less, below 9K)



Majorana zero mode ?

L. Zhao et al,
Nat .Commun. 6, 8279 (2015).

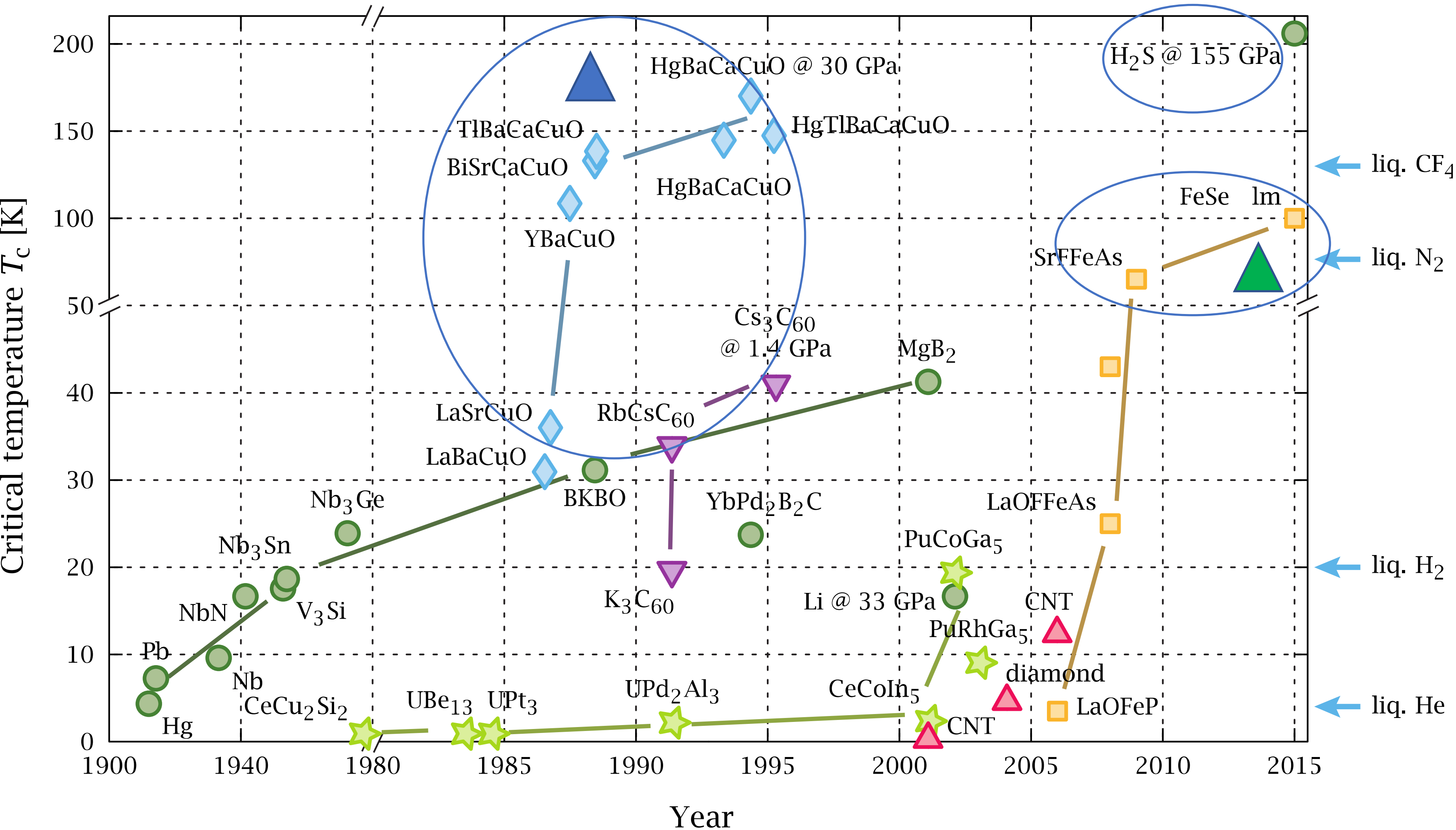
Outline:

- Exotic superconductivity that can arise in topological materials

  - Flat band superconductivity, charge density wave and superconducting pair density wave state
  (Phys. Rev. B 98, 205103, 2018)

Routes to high Tc

Debye 2-3x10^2 meV
For metallic hydrogen



By PJRay - Own work, CC BY-SA 4.0,
https://commons.wikimedia.org/w/index.php?curid=46193149

Tc due to intermediate boson

$$k_B T_c = \hbar\omega_D e^{-1/Ng}$$

or $k_B T_c = \Lambda\, e^{-1/Ng}$

Λ ~ the bandwidth of intermediated boson

T_c is limited by Λ, not by the strength of attractive interaction g!

Flat-band superconductivity

BCS Mean Field Theory:

$$\Delta_k = -\sum_{k'} V_{k,k'} \frac{\Delta_{k'}}{2E_{k'}} \tanh \beta E_{k'} \qquad E_k = \sqrt{\xi_k^2 + \Delta_k^2} \quad \xi_k = \varepsilon_k - \mu$$

Flat band at Fermi energy: $\xi_k = \varepsilon_k - \mu = 0$

s-wave: $\Delta_k = \Delta, V_{k,k'} = -g/N$

$$\Delta_k = -\sum_{k'} V_{k,k'} \frac{\Delta_{k'}}{2E_{k'}} \tanh \beta E_{k'} \Rightarrow 1 = g(\frac{1}{N}\sum_{k'}) \lim_{\Delta \to 0} \frac{\tanh \beta_c \Delta}{2\Delta}$$

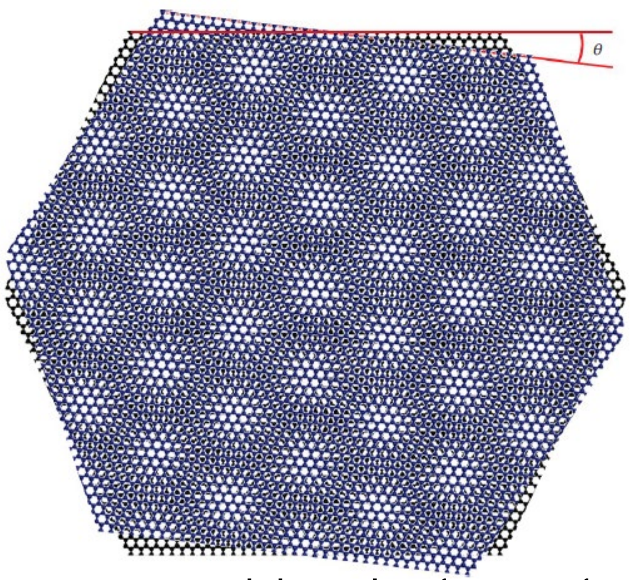
$$k_B T_c = \frac{g}{2} \quad \Leftrightarrow \quad k_B T_c = \hbar \omega_D e^{-1/Ng}$$

T_c **is limited by** g **!** (g $\lesssim$ 0.1eV for phonon)

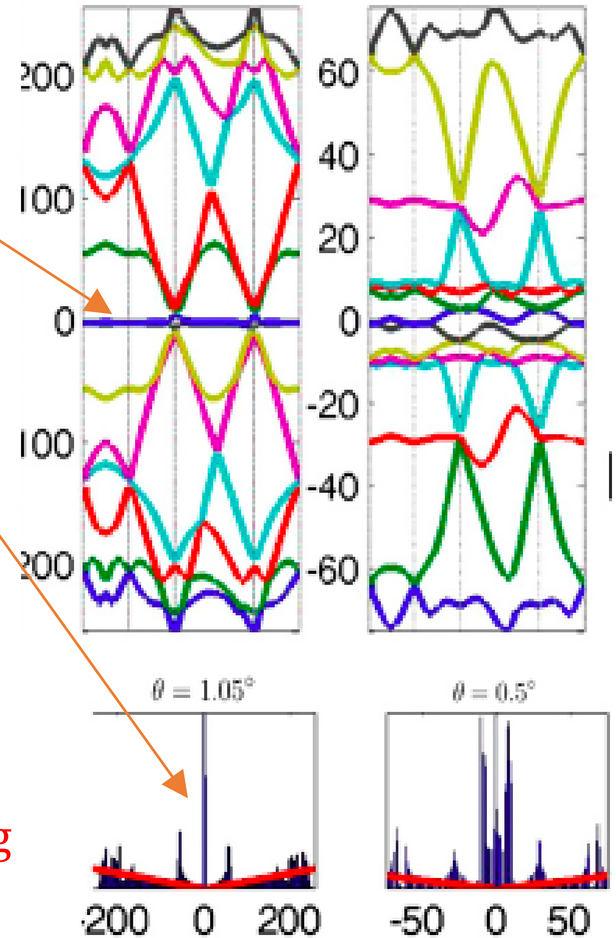
(S Peotta,Nat. com. 6, 8944, 2015; V. J. Kauppila, PRB 93, 214505, 2016)

Surprised superconductivity in bi-layer graphene

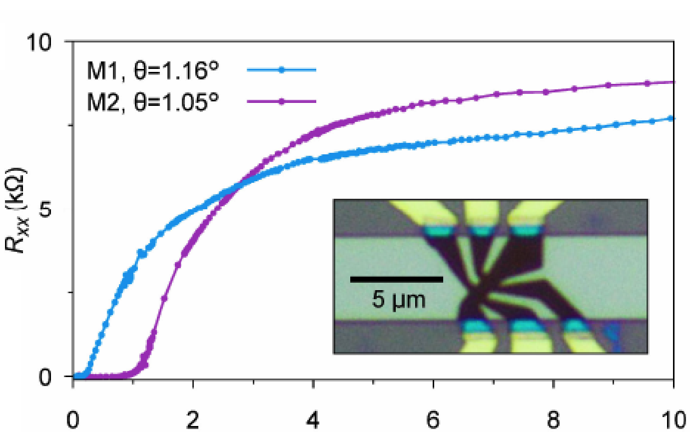
Flat band of bi-layer graphene
twisted by $\theta = 1.1°$



(Kinetic energy vanishes due to quantum interference
R Bristritzer,and A. H. MacDonald, PNAS 108, 12233, 2011)



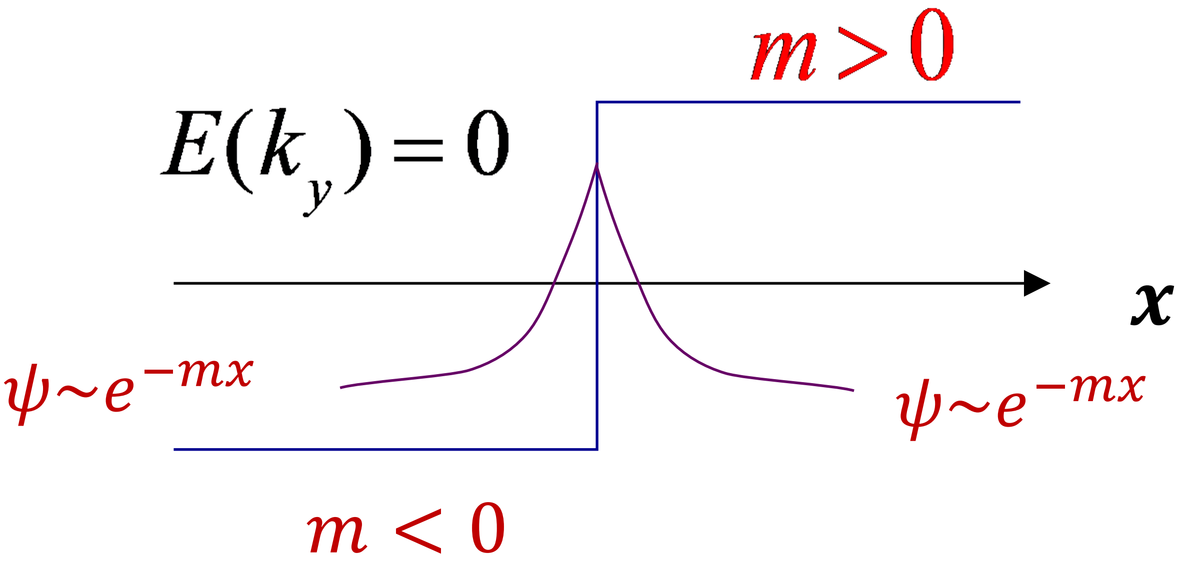
$\boldsymbol{E(meV)}$



Graphene
non-superconducting
$\rightarrow \boldsymbol{T_c = 1.7K}$

(Pablo Jarrillo-Herrero's group),
http://dx.doi.org/10.1038/nature26160, 2018)

Topological flat band (domain wall Fermi



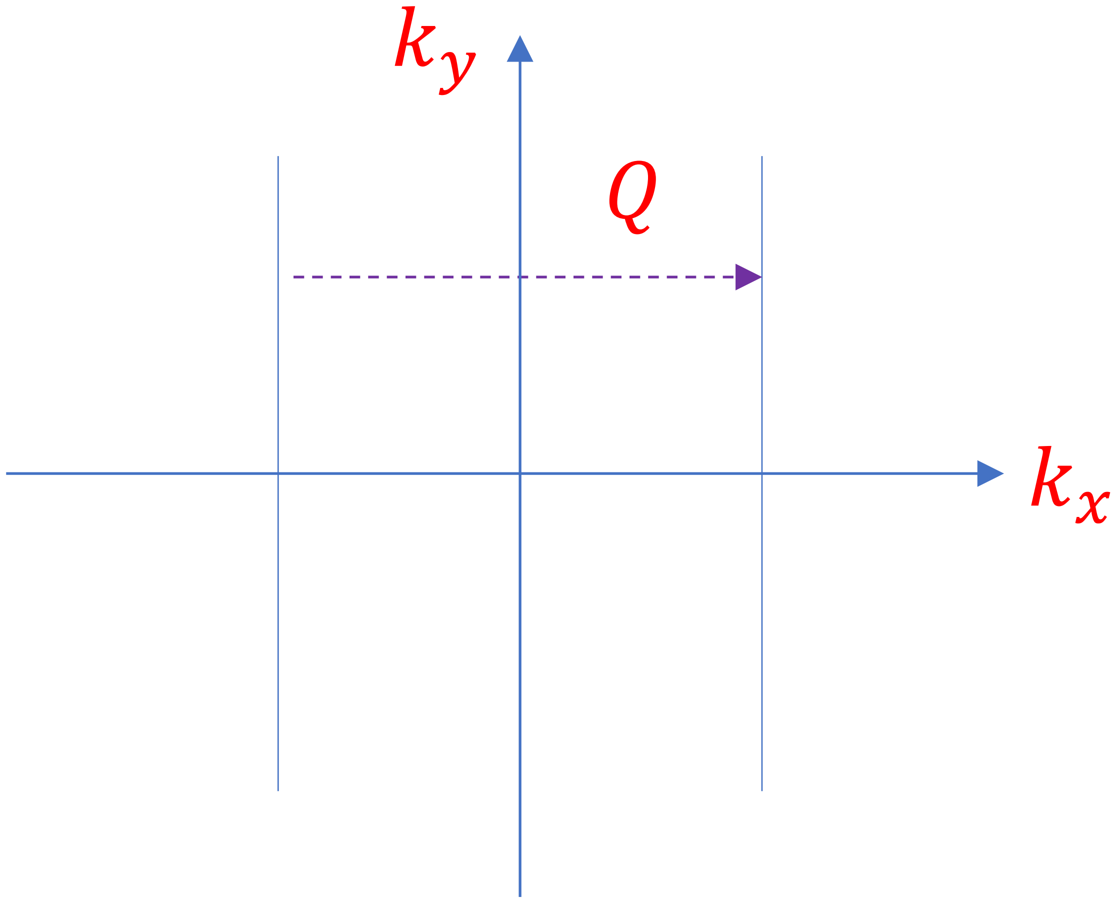
$$\left(\frac{\partial}{\partial x} + m\right)\psi = 0$$

Dirac Hamiltonian

Flat band

$$E(k_y) = 0$$

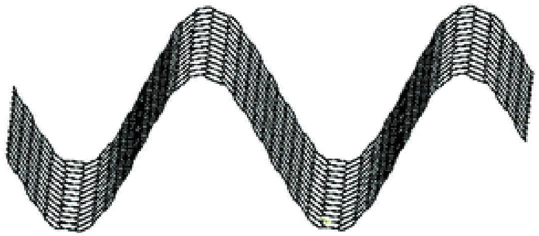
Problems: competing orders ?

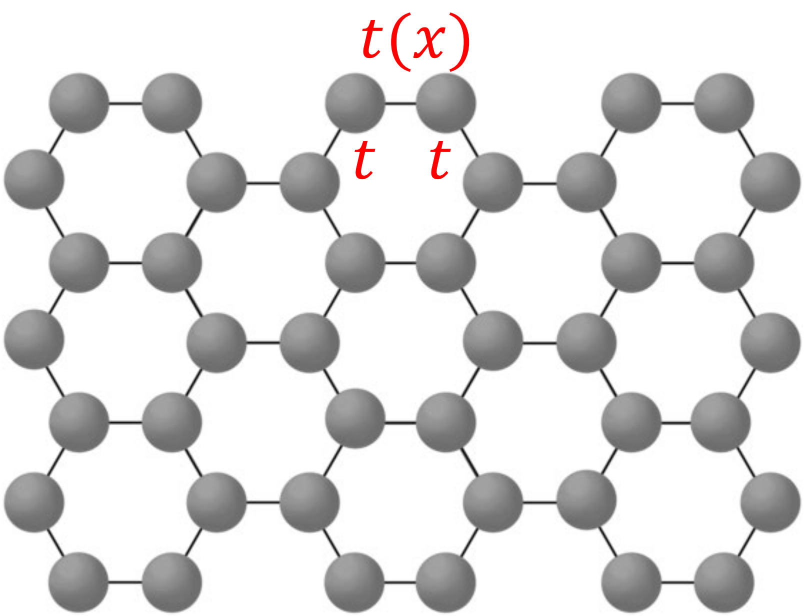


charge density wave, spin density wave, ….

Creating Flat-bands in Strained Graphene

(Phys. Rev. B 98, 205103, 2018)

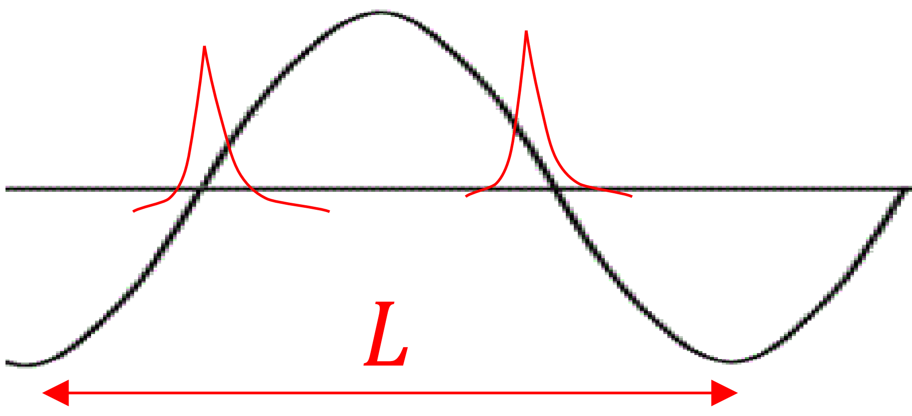




Strain due to ripples

$$t(x) = t(1 + \alpha \cos Qx)$$

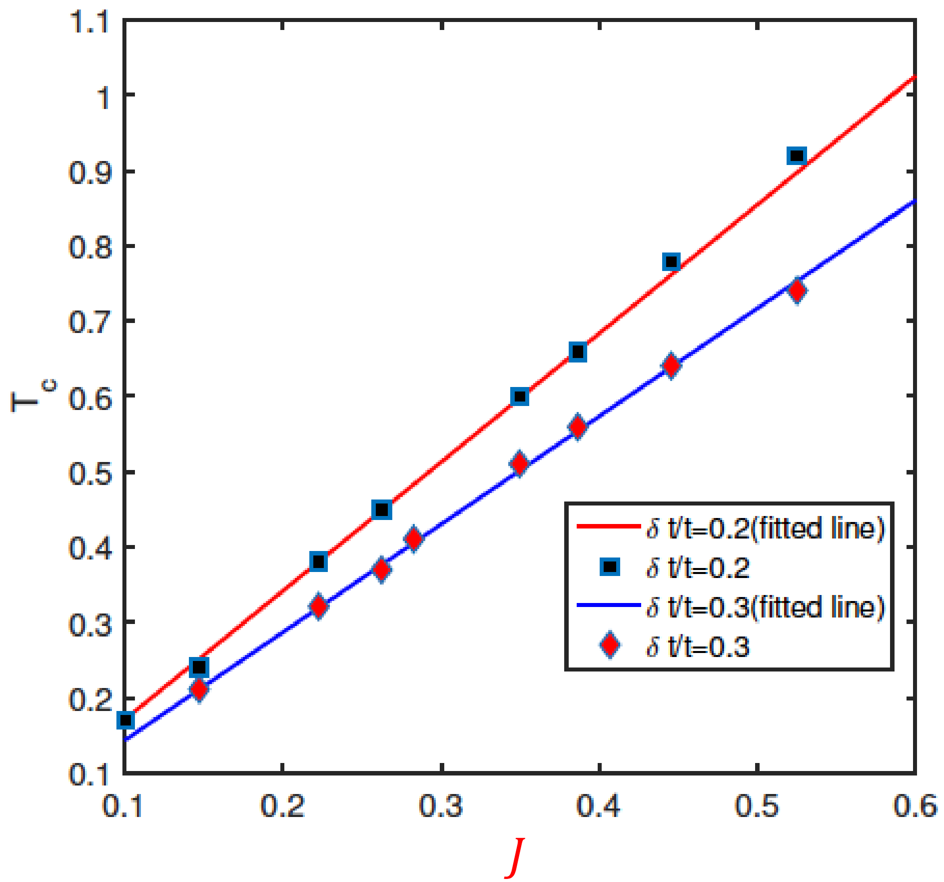
$$Q = 2\pi/L$$



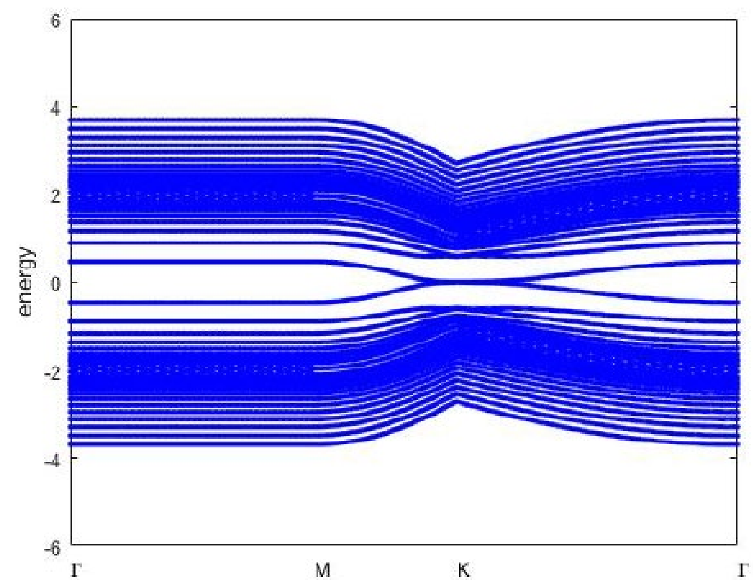
$$H = \sum_{<i,j>} -t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + h.c. + J(\vec{s}_i \cdot \vec{s}_j - \frac{1}{4} n_i n_j)$$

$$\sum_{\sigma} c_{i\sigma}^{\dagger} c_{i\sigma} \leq 1$$

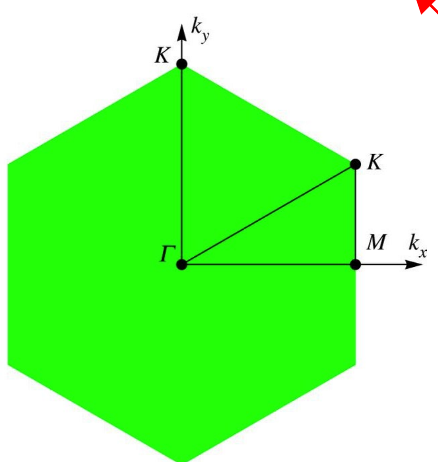
Enhanced T_c due to flat bands in large strain



$\alpha = 0.4, \mathrm{period} = 25$



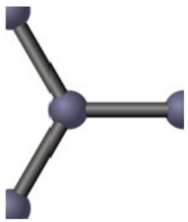
Dirac point



Anomalous density wave state

Mean fields: $\chi_{ij} = \sum_\sigma \left\langle c^\dagger_{j\sigma} c_{i\sigma} \right\rangle, \Delta_{ij} = \left\langle c_{j\downarrow} c_{i\uparrow} - c_{j\uparrow} c_{i\downarrow} \right\rangle$

$\Delta_1(x)$



$\Delta_3(x)$

$\Delta_2(x) = \Delta_1^*(x)$

$$\Delta_s(x) \equiv \frac{1}{\sqrt{3}}(\Delta_1(x) + \Delta_2(x) + \Delta_3(x))$$

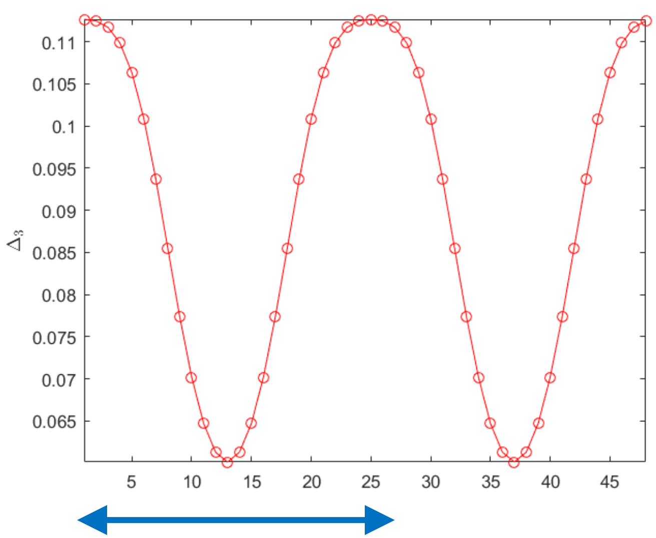
$$\Delta_{d_{x^2-y^2}}(x) \equiv \frac{-1}{\sqrt{6}}(\Delta_1(x) + \Delta_2(x) - 2\Delta_3(x))$$

$$\Delta_{d_{xy}}(x) \equiv \frac{-\mathrm{Im}}{\sqrt{2}}(\Delta_1(x) - \Delta_2(x))$$

Expected: $Q = 2\pi/L$, 2Q, 3Q,….

$\Delta_3(x)$

$A:$

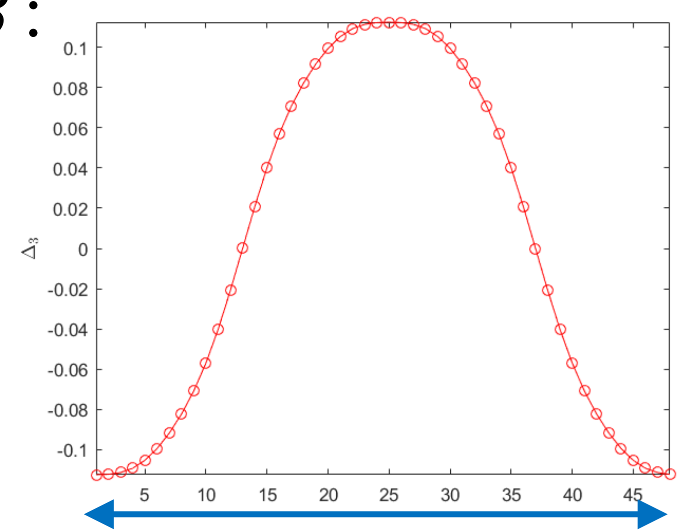


L

Anomalous: Q/2

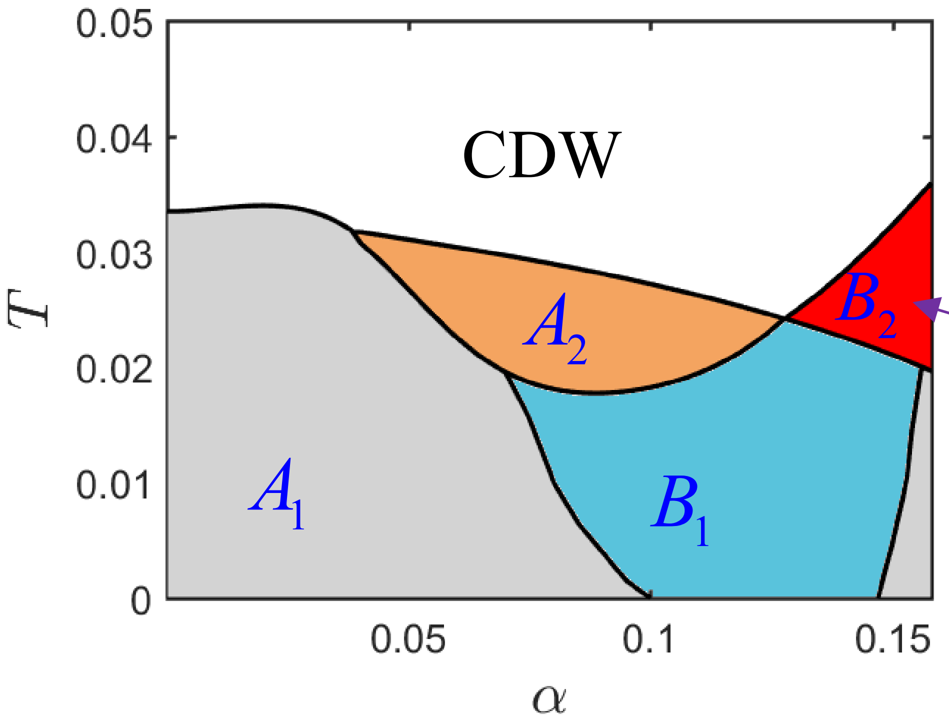
$\Delta_3(x)$

$B:$



$2L$

Typical Phase Diagram (hole doping $\delta = 0.15, L = 16$) --- with complicated density waves



A_1, A_2, and B_1 :
Non-vanishing uniform SC

B_2 :
only PDW (Q/2)
+CDW(Q) !

A_1 $S(0,Q), d_{x^2-y^2} + id_{xy}(0,Q)$
CDW $(0,Q)$

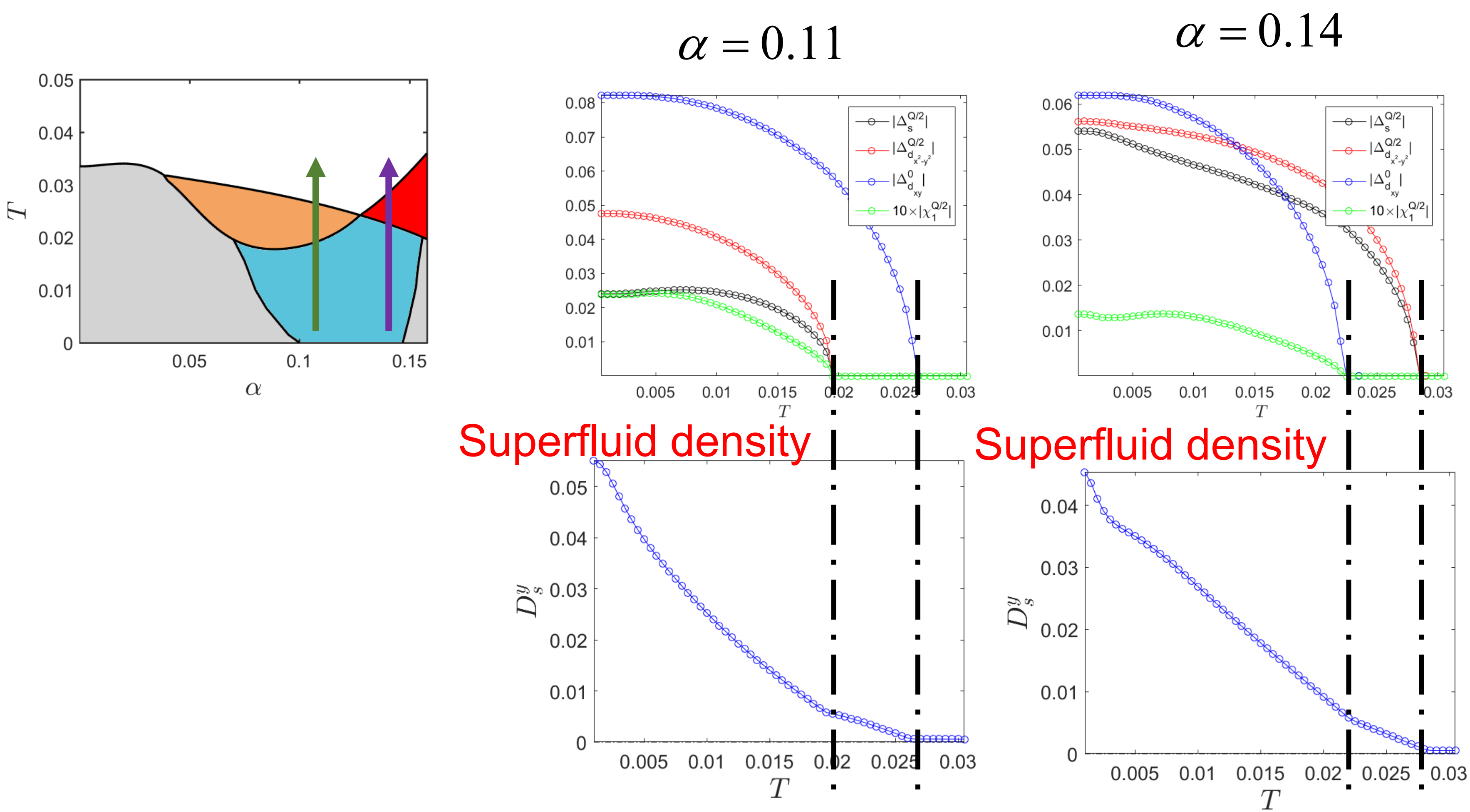
B_1 $S\left(\frac{Q}{2}\right), d_{x^2-y^2}\left(\frac{Q}{2}\right), id_{xy}(0,Q)$
CDW $(0,Q,Q/2)$

A_2 $d_{xy}(0,Q)$
CDW $(0,Q)$

B_2 $S\left(\frac{Q}{2}\right), d_{x^2-y^2}\left(\frac{Q}{2}\right)$
CDW(Q)

Stablized Cooper pair at finite Q: superconducting pair density wave state

Gain energy through : $-\rho(Q)\Delta(-\frac{Q}{2})\Delta(-\frac{Q}{2})$



Conclusion and Summary

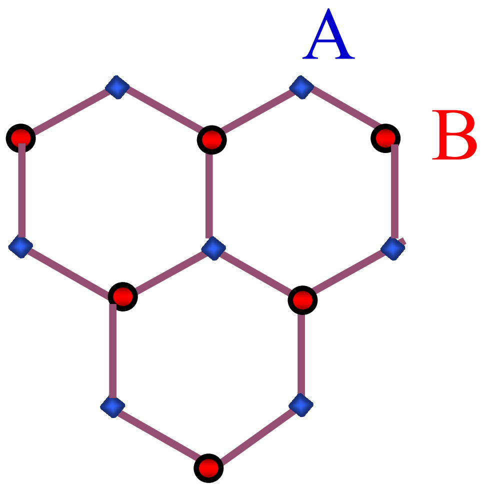
1. Quantum Oscillations in Kondo insulators:

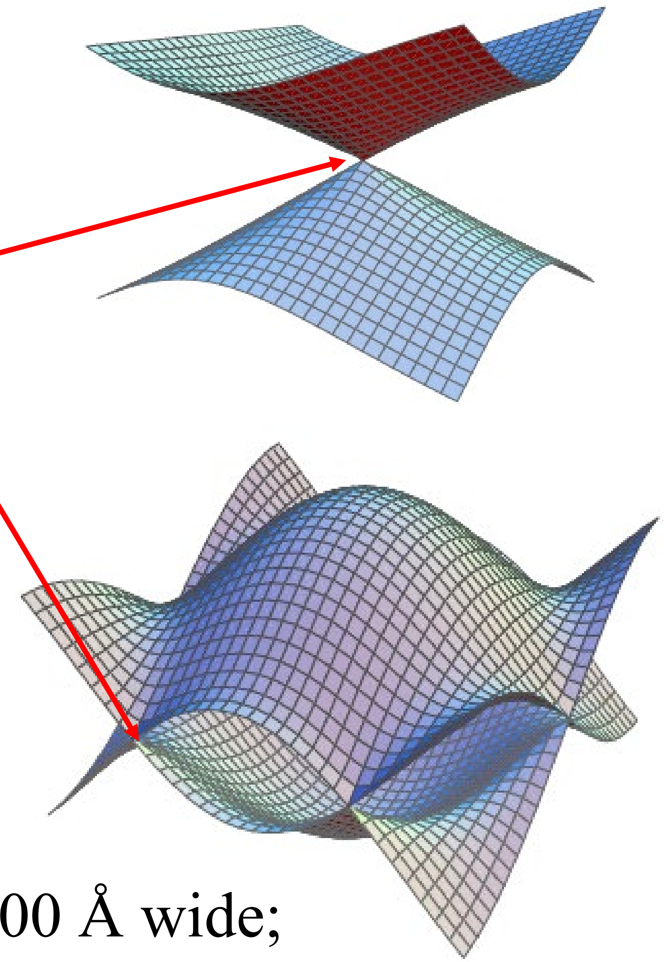
Kondo screening itself under goes oscillation in the presence of magnetic fields. It explains important features observed in experiments.

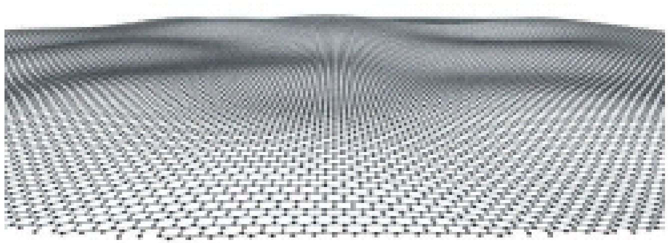
2. Unconventional Superconductivity

1. Spin-orbit hybridization in Kondo lattice provides a route to p-wave superconductivity characterized by Z_2 topological index.
2. A new route to topological superconductivity is possible through inter-surface pairing.
3. Singlet and triplet pairings are differentiated through thickness dependence. The spinfull triplet p+ip pairing dominates for thin films of topological insulators with thickness below 9-10QLs.
4. Experimental evidences of spinfull p-wave for Sb_2Te_3 nanoflakes are observed.
5. Curvature helps in converting surface superconductivity into topological superconductivity
6. Vortices can be spontaneously generated on a sphere and host Majorana zero mode.

2D Dirac Fermions in Graphene

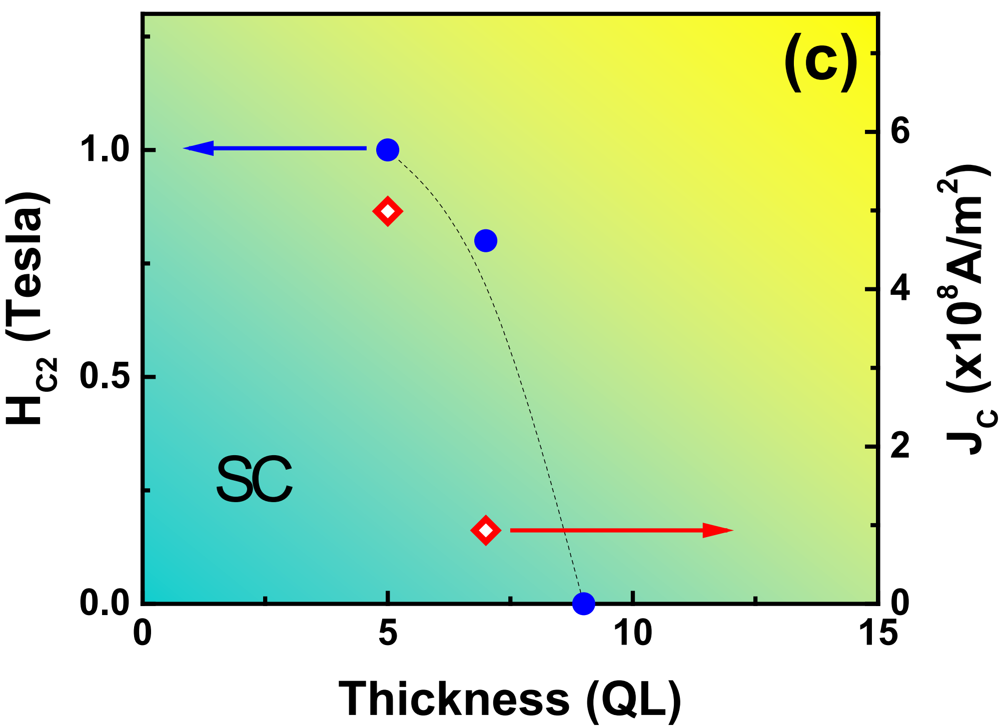






Ripples are of order 2–20 Å high and 20–200 Å wide;
Meyer et al., Nature 446, 60, (2007);
Fasolinao et al., Nature Materials 6, 858 (2007)

Strong thickness dependent properties: critical current and fields



$$H_{c_2}^{\perp}(0) = \frac{\phi_0}{2\pi\xi^2}$$

$$\xi = 0.885\sqrt{\xi_0 \ell},\ \ell = d$$

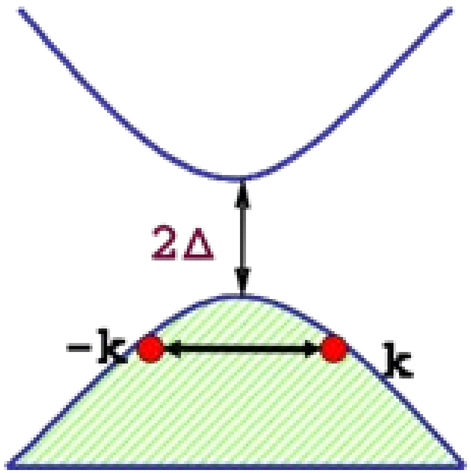
$$\xi_0 = \hbar\upsilon_F / \Delta \propto 1/T_c$$

$$H_{c_2}^{\perp}(0) \propto T_c / d$$

$J_c \propto$ current distribution factor

ratio of $J_c \approx$ ratio of conductivity in normal state

Conventional superconductors



$$\Delta_k = -\sum_{k'} V_{k,k'} < c_{-k\downarrow} c_{k\uparrow} >$$

s-wave: $\Delta_k = \Delta$

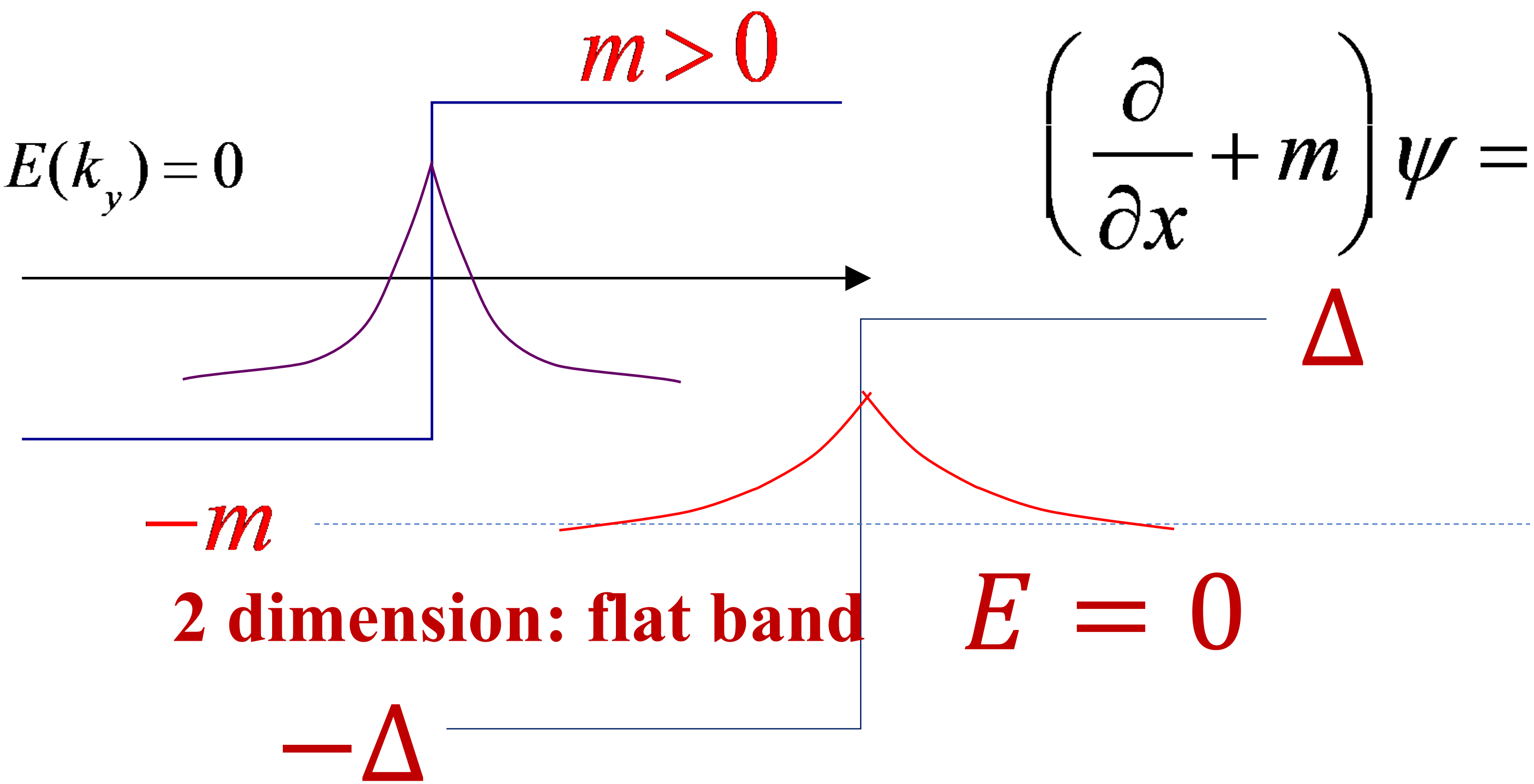
$$= -\sum_{k'} V_{k,k'} \frac{\Delta_{k'}}{2E_{k'}} \tanh \beta E_{k'}$$

Mean field:

$$H = \sum_{k,\sigma} (\epsilon_k - \mu) c_{k\sigma}^{\dagger} c_{k\sigma} - \Delta_k c_{k\uparrow}^{\dagger} c_{-k\downarrow}^{\dagger} - \Delta_k^{*} c_{-k\downarrow} c_{k\uparrow}$$

$k_B T_c = \hbar \omega_D e^{-1/Ng}$ N(ε_F) = density of state

Domain wall fermions and flat-band

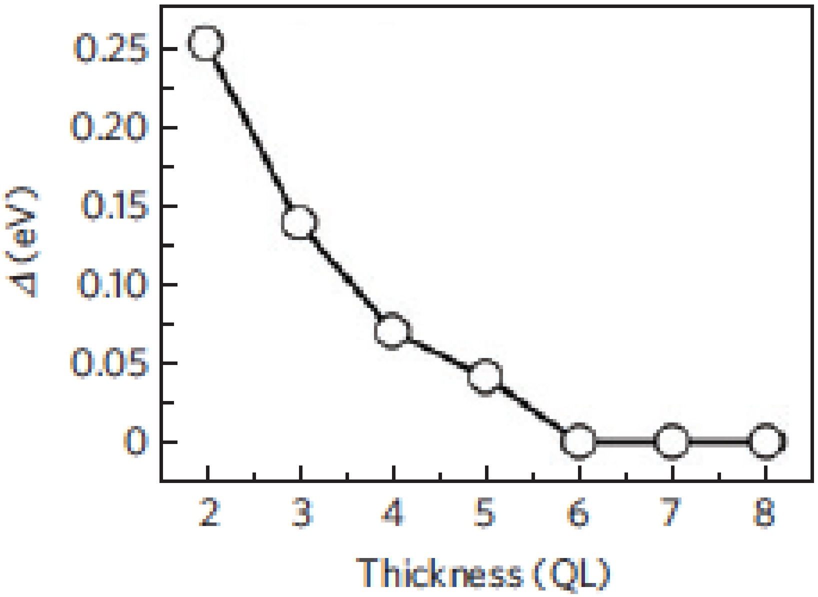


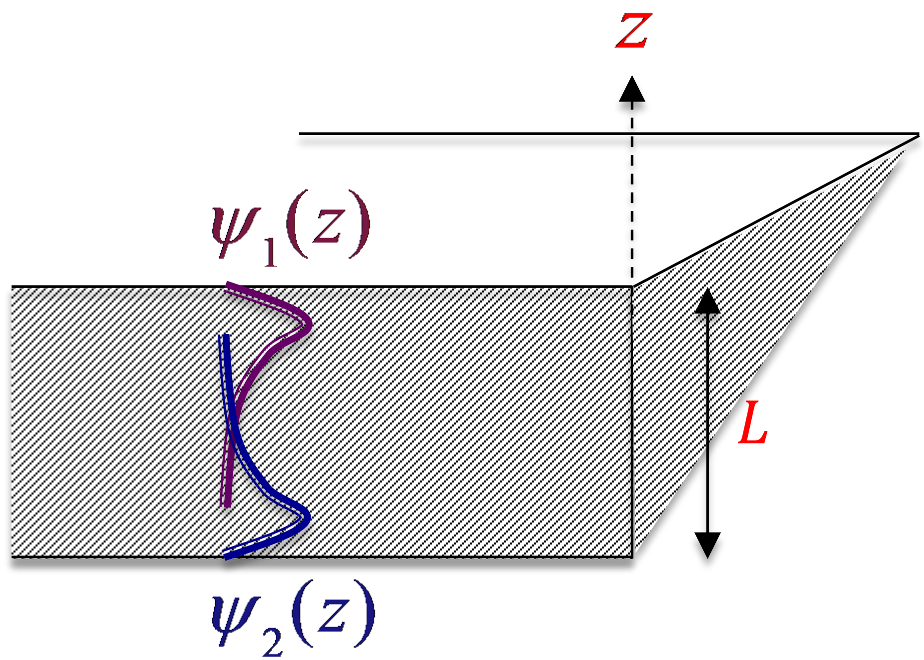
$$\left(\frac{\partial}{\partial x} + m \right) \psi = 0$$

Origin of thickness dependence

Overlap of edge states: hybridization gap arises

$\Longrightarrow$ Change of density of state





Zhang, Y. et al. Nat. Phys. 6, 584, 2010

Origin of thickness dependence

Coulomb interaction:

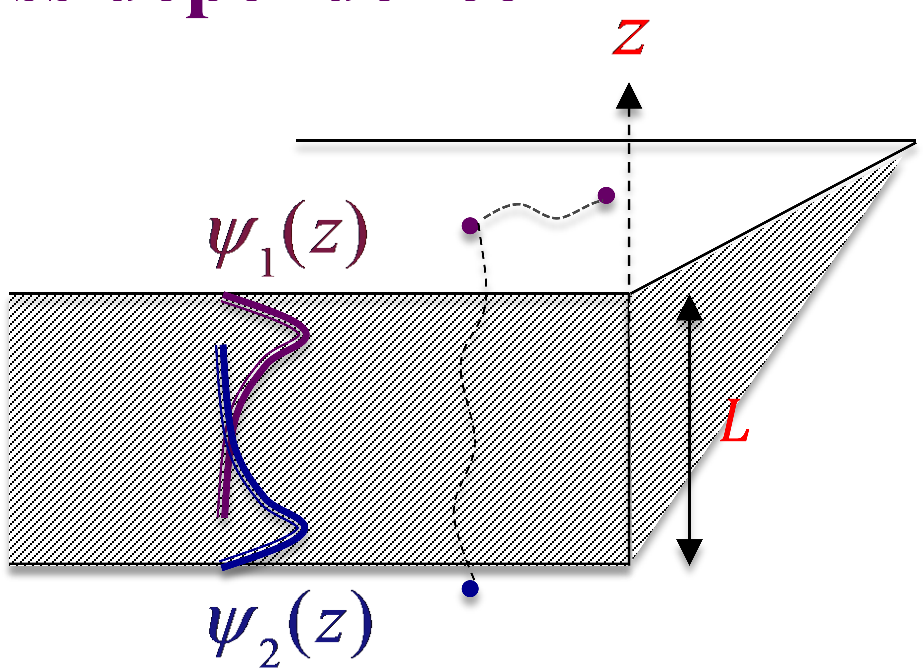
intra surface

(min separation = 0)

versus

inter surface

(min separation = L)



Fermi-energy dependent screened Coulomb interaction $V_q^C(z,z')$

$$G_q(z-z') = \frac{4\pi e^2}{\kappa}\frac{e^{-q|z-z'|}}{2q}$$

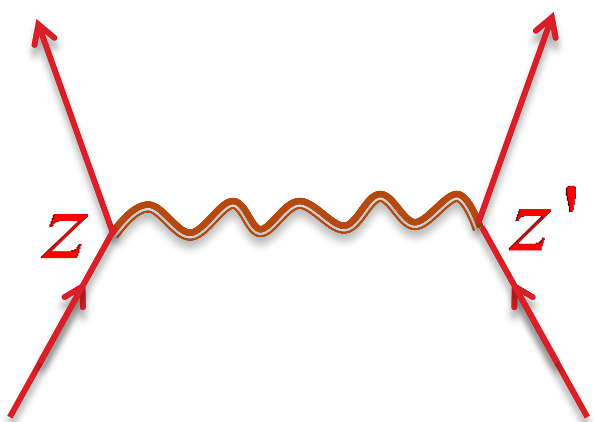
$$\left(\frac{d^2}{dz^2} - q^2\right)V_q^C(z,z') = -\frac{4\pi}{\kappa}\delta(z-z')$$

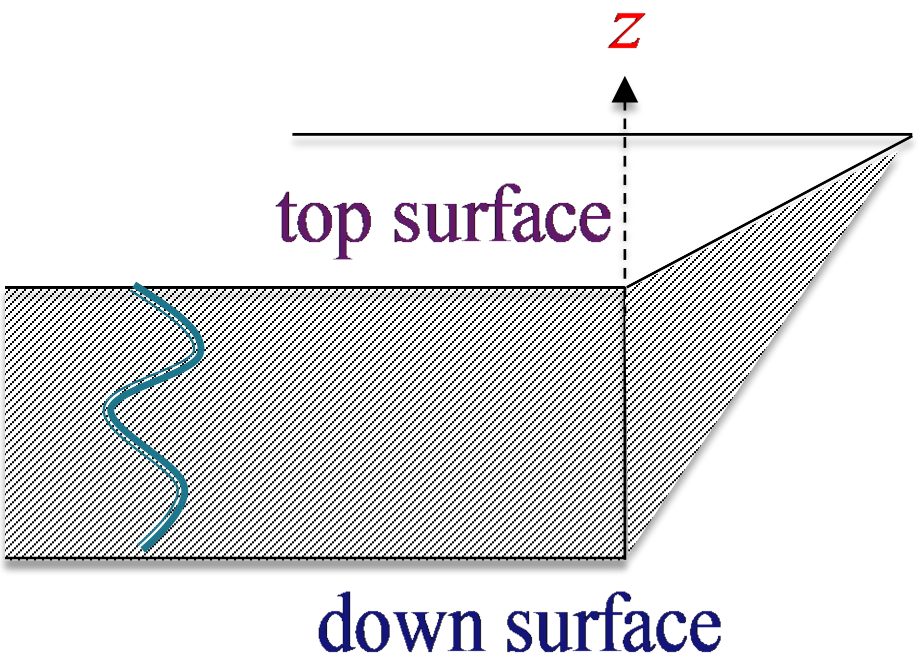
$$+2q_{TF}\,|\psi_1(z)|^2\,V_1(z') + 2q_{TF}\,|\psi_2(z)|^2\,V_1(z')$$

$$V_n(z) = \int dz' V_q^C(z',z)\,|\psi_n(z')|^2$$

Origin of thickness dependence

Electron-Phonon interaction





Phonon propagation: intra-surface versus inter-surface

$$V_q^P(z,z') = -\frac{[Z\hbar q\overline{G_q}]^2}{Ma^2}\sum_E \frac{\phi_E(z)\phi_E(z')}{E^2+(\upsilon q)^2}$$

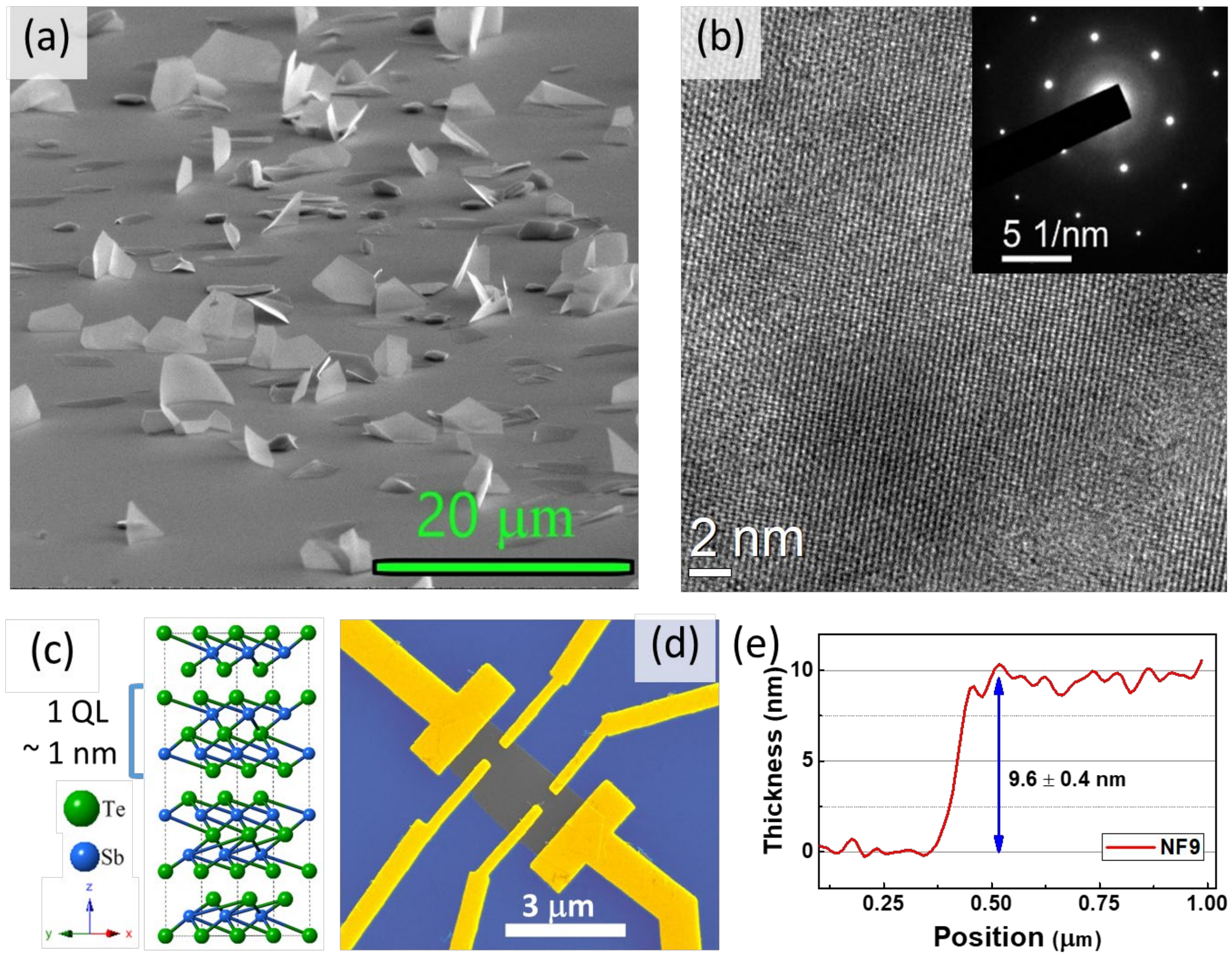
$\phi_E(z)$ = phonon wavefunction

$$\overline{G_q} = \iint dz dz' G_q(z,z')$$

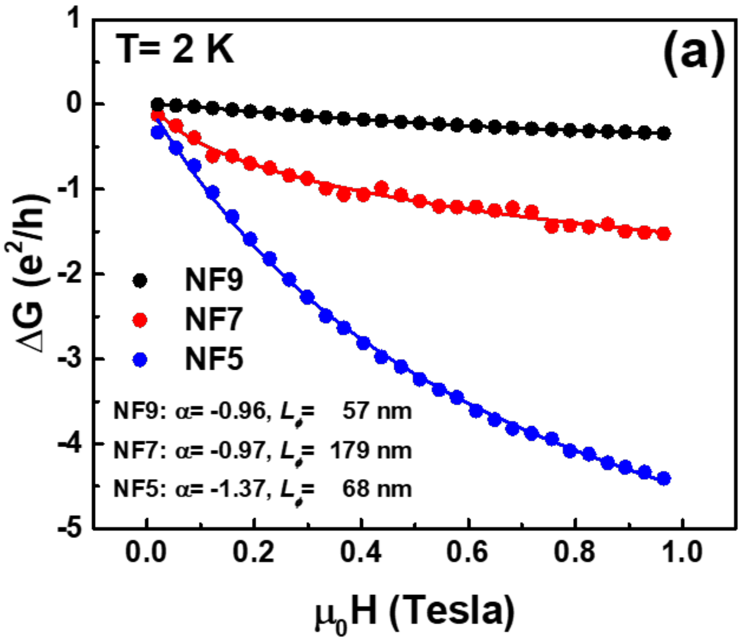
z direction: standing wave

Experimental Evidences in Sb_2Te_3 nanoflakes

Physical vapor deposition (PVD)
Using polycrystalline Sb_2Te_3 on SiO_2/Si substrate

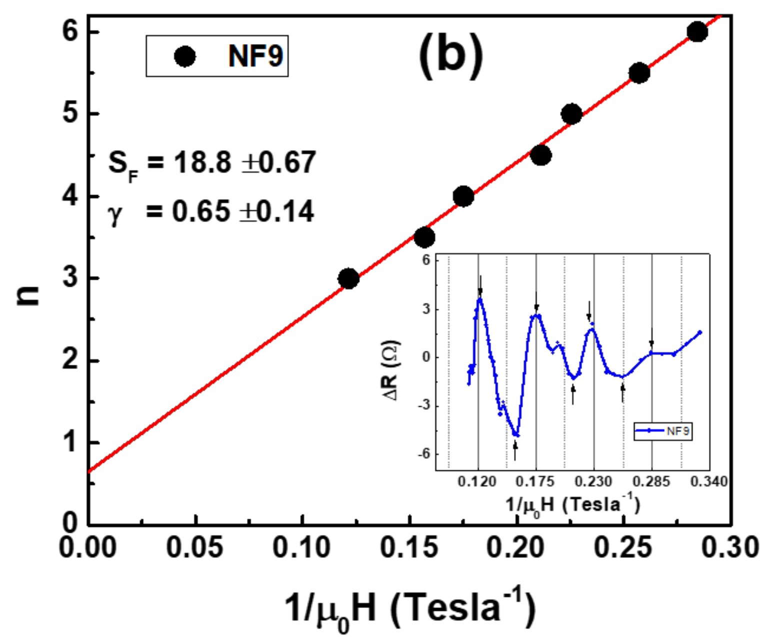


Evidences of surface states



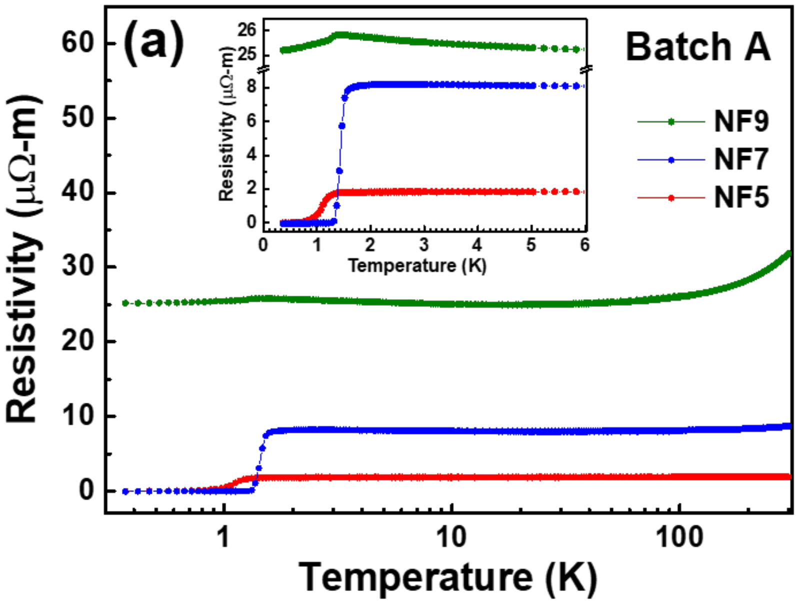
Weak anti-localization

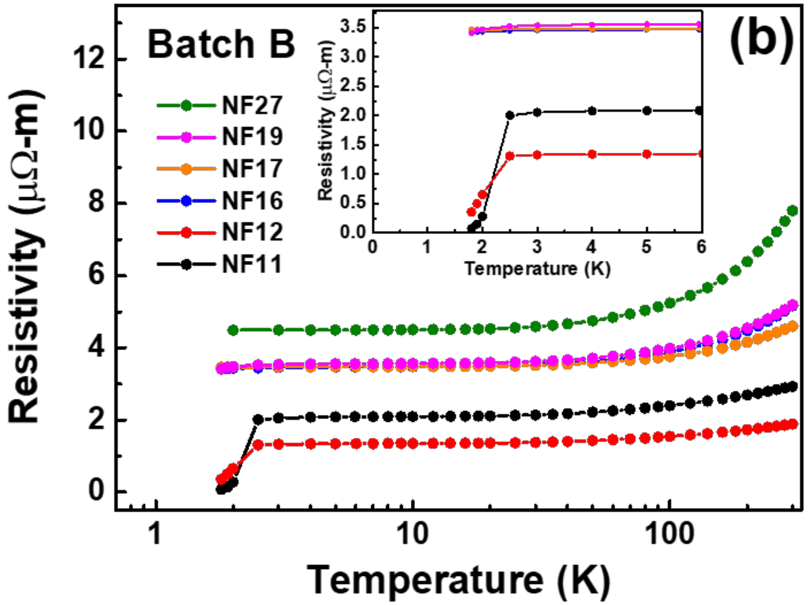
$$\Delta G = -\frac{\alpha e^2}{2\pi^2\hbar}\left[\ln\left(\frac{\hbar}{4eL_\phi^2 B}\right) - \psi\left(\frac{1}{2} + \frac{\hbar}{4eL_\phi^2 B}\right)\right]$$



Shubnikov-de Haas oscillations due to Landau levels

Transport Measurements





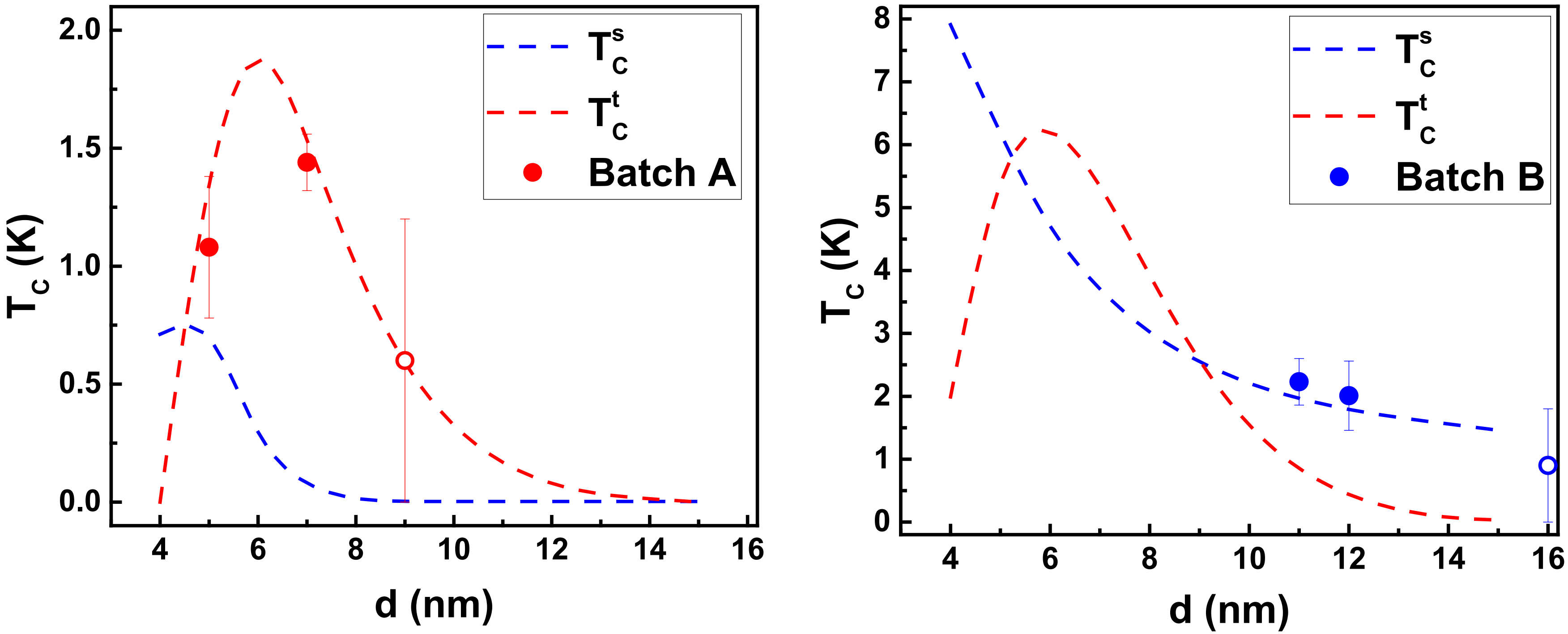
Superconducting transition ≤ 2.5K

Two batches of samples grown under different condition (Te vapor pressure)

Batch A, smaller k_F

Batch B, larger k_F

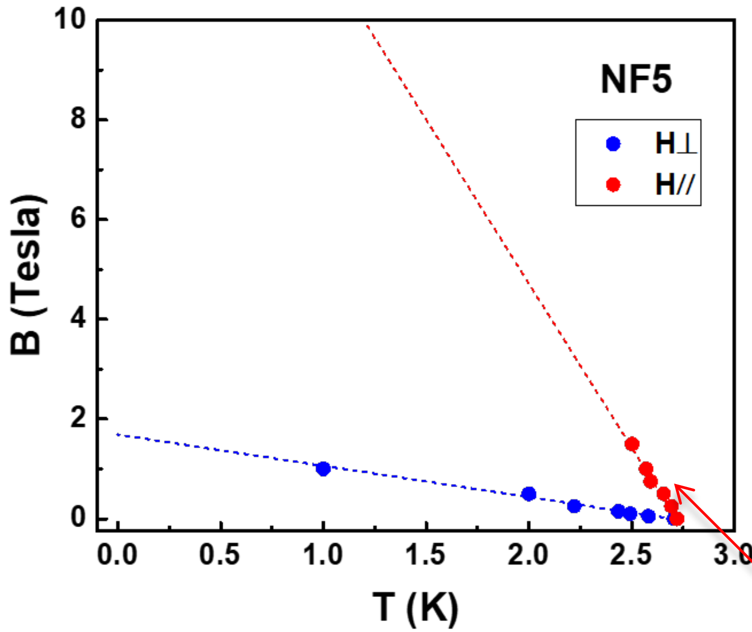
Transition temperatures: theory versus expt

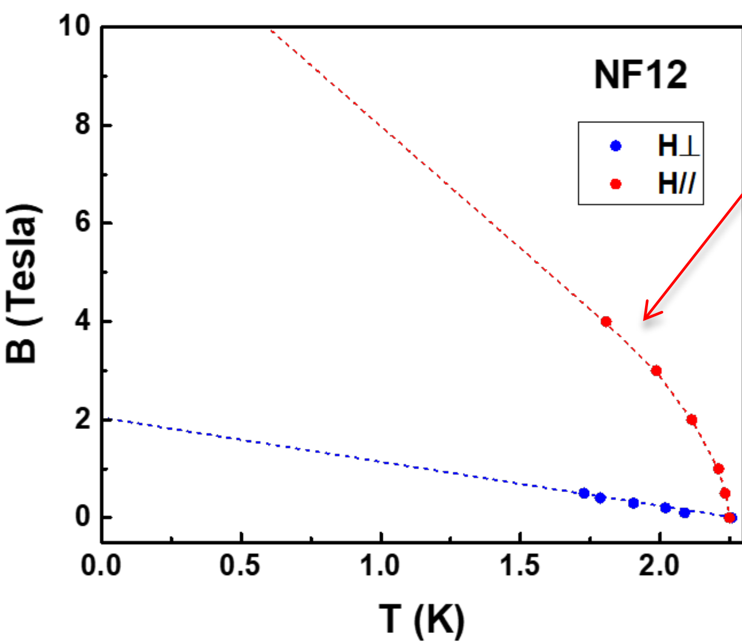


$$1 \text{ quintuple layer} \approx 1nm$$

The Debye temperature: 180K, the speed of phonon: $v_p = 2$ km/s , the decay length ξ_d about 1.2nm, the mass of ions: 124.7u, and the charge of ions being taken to be average of 3e and 4e, i.e., 3.53e.

Evidence of triplet pairing





$$\text{clean: } H_{c_2}^{\text{orb}}(0) = -0.73 \left.\frac{dH_{c_2}}{dT}\right|_{T=T_c} \times T_c$$

$$\text{dirty: } H_{c_2}^{\text{orb}}(0) = -0.69 \left.\frac{dH_{c_2}}{dT}\right|_{T=T_c} \times T_c$$

$H_{c_2}^{\square}(0)$ dominated by orbital effects

(Paramagnetic limiting is absent)

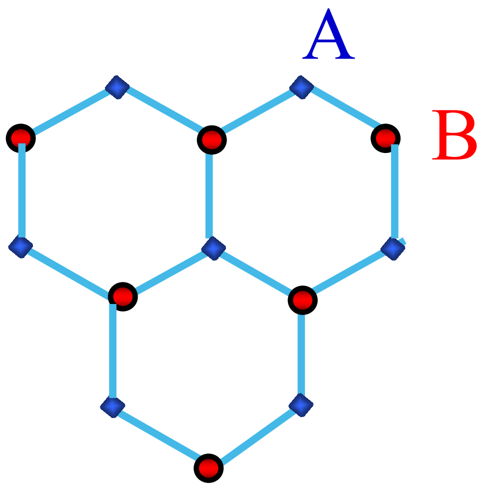
Estimated $H_{C_2}^{\text{orb}}(0) = 34 - 36$ Tesla

$$H_{c_2}^{\square}(0) \approx 12T << \text{Estimated } H_{C_2}^{\text{orb}}(0)$$

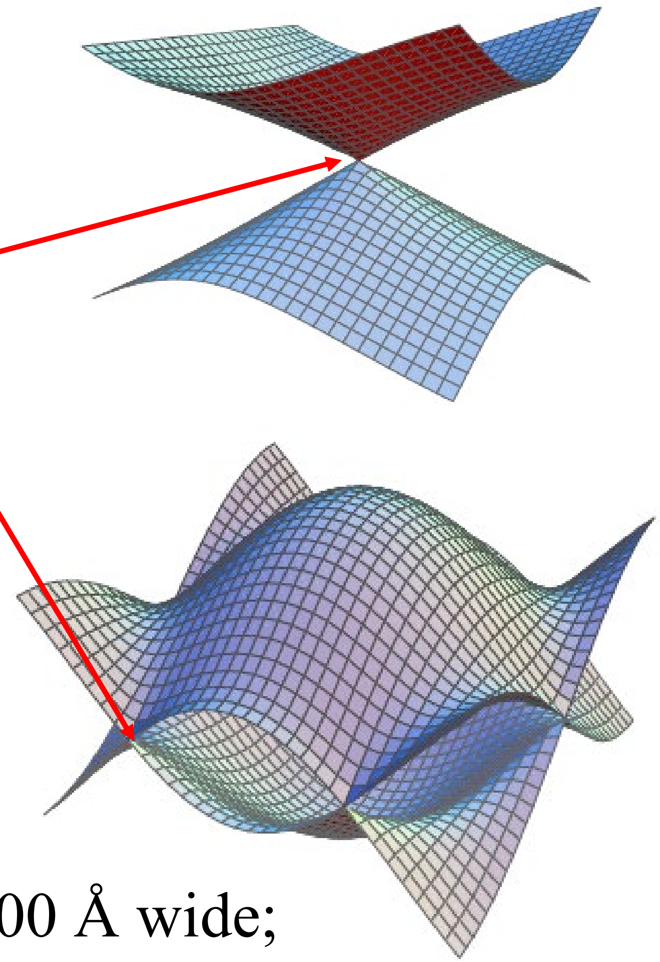
$$H_{c_2}^{\square}(0) = \text{ Pauli limit}$$

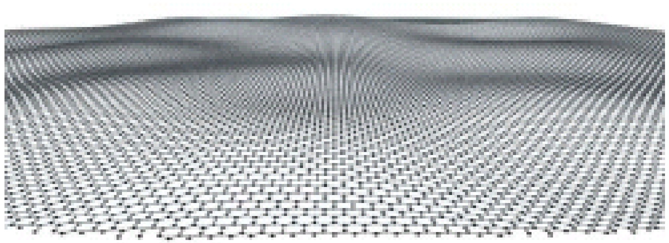
$\Rightarrow$ singlet pairing dominates

2D Dirac Fermions in Graphene



Dirac points





Ripples are of order 2–20 Å high and 20–200 Å wide;
Meyer et al., Nature 446, 60, (2007);
Fasolinao et al., Nature Materials 6, 858 (2007)