SPICE-SPIN+X - June 2025

Magnetism in Moiré Materials

Allan MacDonald UT Austin

Acknowledgements

SIMONS FOUNDATION

Thank You!

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UNITED STATES OF AMERICA

NSF
National Science Foundation
MRSEC
MATERIALS RESEARCH SCIENCE AND ENGINEERING CENTERS

Collaborators

UT AUSTIN

Rafi Bistritzer
Fengcheng Wu

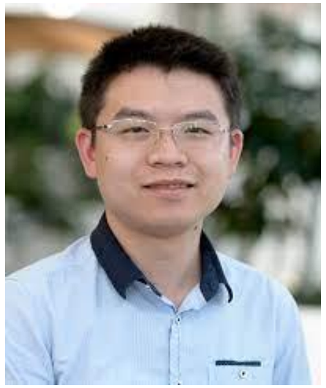
Ming Xie (Dallas)
Jihang Zhu (Maryland)
Pawel Potasz (Torun)
Naichao Hu (Leuven)
Ajesh Kumar (MIT)
Nicolas Morales-Duran (Columbia)
Nemin Wei (Yale)
Yongxin Zeng (Columbia)
Chunli Huang (Kentucky)
Toby Wolf
Bo Zou
Perry Mahon
Chao Lei

Emanuel Tutuc – Austin
Elaine Li – UT Austin
Ken Shih – UT Austin

WORLD

Dima Efetov – LMU
Brian LeRoy – Arizona
Fai Mak - Cornell
Jie Shan - Cornell
Feng Wang - Berkeley
Josh Folk – UBC
Andrea Young – UCSB
Cory Dean – Columbia
Thomas Weitz – Gottingen

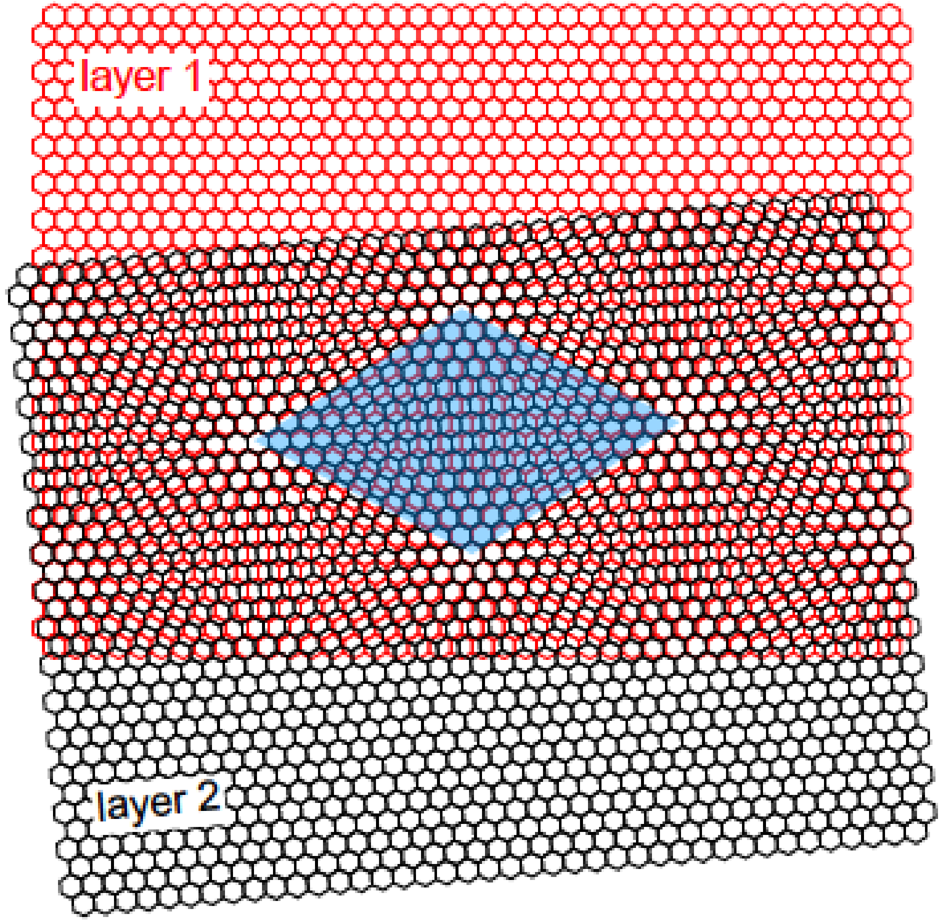
Andrei Bernevig (Princeton)
Mitch Luskin (Minnesota)
Ivar Martin (Argonne)
Jung-Jung Su (NYCU)
YC Chao (NYCU)
Alex Watson (Minnesota)
Lin Lin (Berkeley)



Fengcheng Wu
Wuhan U

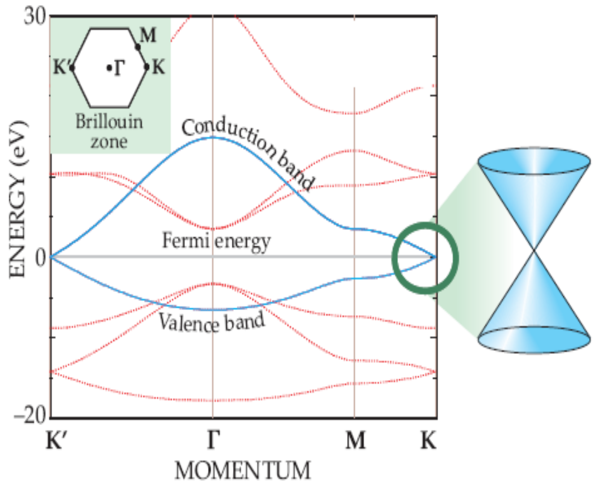
Rafi Bistritzer
Tel Aviv U

Moiré Materials

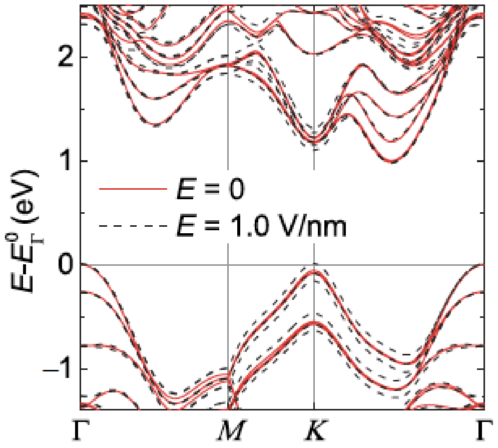

layer 1
layer 2

Moiré + Semiconductors or Semimetals = Moiré Materials

Graphene



WSe_2



Moiré Materials: Momentum Space

Quasicrystals

$$\vec{G} = n_A \vec{G}_A + n_B \vec{G}_B$$
$$\vec{G}' = n'_A \vec{G}'_A + n'_B \vec{G}'_B$$

Momentum Transfers

$$\vec{Q} = \vec{G}' - \vec{G} = n'_A \vec{G}'_A + n'_B \vec{G}'_B - n_A \vec{G}_A + n_B \vec{G}_B$$

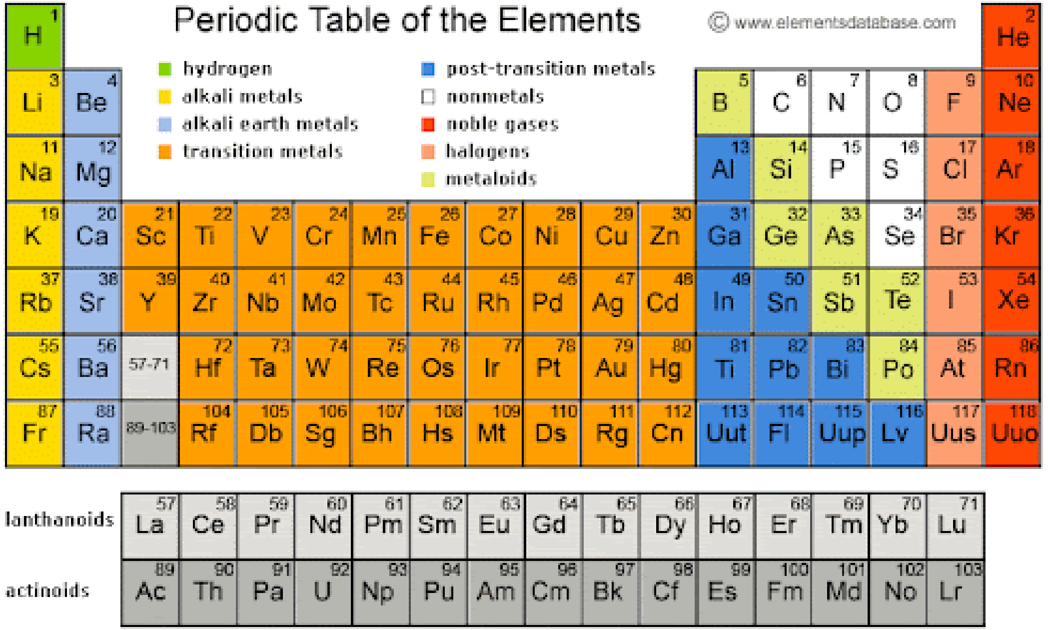
Small Momentum Transfers

$$\vec{Q} = n_A(\vec{G}_A - \vec{G}'_A) + n_B(\vec{G}_B - \vec{G}'_B)$$

Moire Reciprocal Lattice Vectors

$$\vec{Q}_{A,B} = \theta(\hat{z} \times \vec{G}_{A,B})$$

$$\Delta n\, A_{Moire} \gg 1 \gg \Delta n\, A_{Atomic}$$



Chemistry by Gating

Moiré
Materials
Magic

- I Energy Bands ✓
- II Fermi Liquids & Metals ✓
- III Insulator/Semiconductors ✓
- IV Mott Insulators/Spin Models ✓
- V Itinerant Magnetism ✓
- VI Heavy Fermions ✓
- VIII Superconductors ✓
- IX (Fractional) QHE ✓
- X Anomalous (F)QHE ✓

Strong Coupling Stoner Instability

Interaction Strength

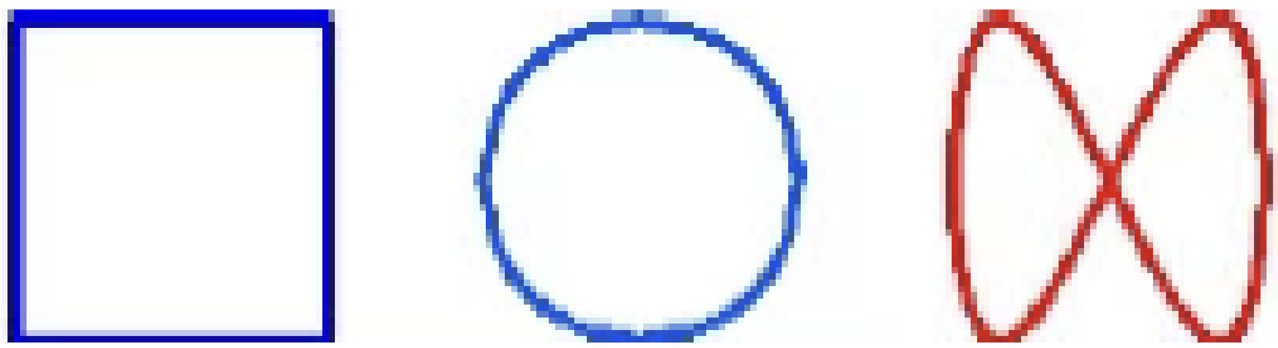
Bandwidth

$$U \sim \frac{e^2}{\varepsilon a_M} \sim \frac{10eV}{10*10} \sim 100\ meV$$

$$\mathrm{W} \sim tunable$$

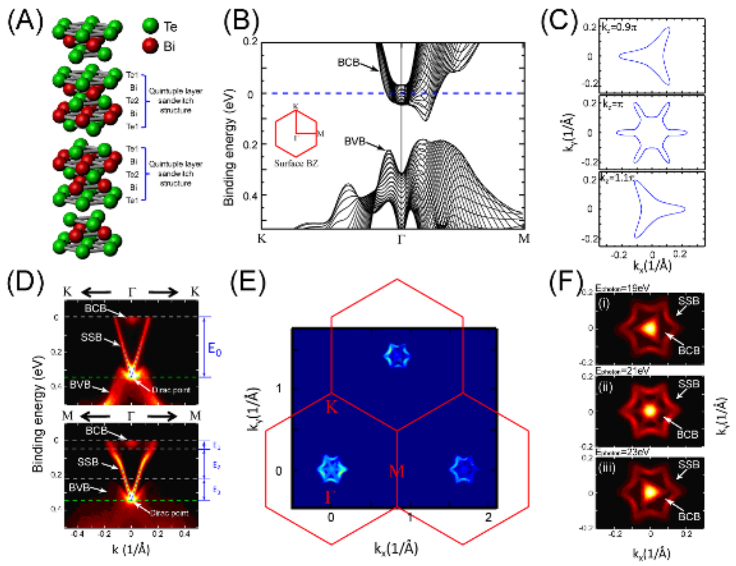
Topology in Moire Materials

Topology and Physics



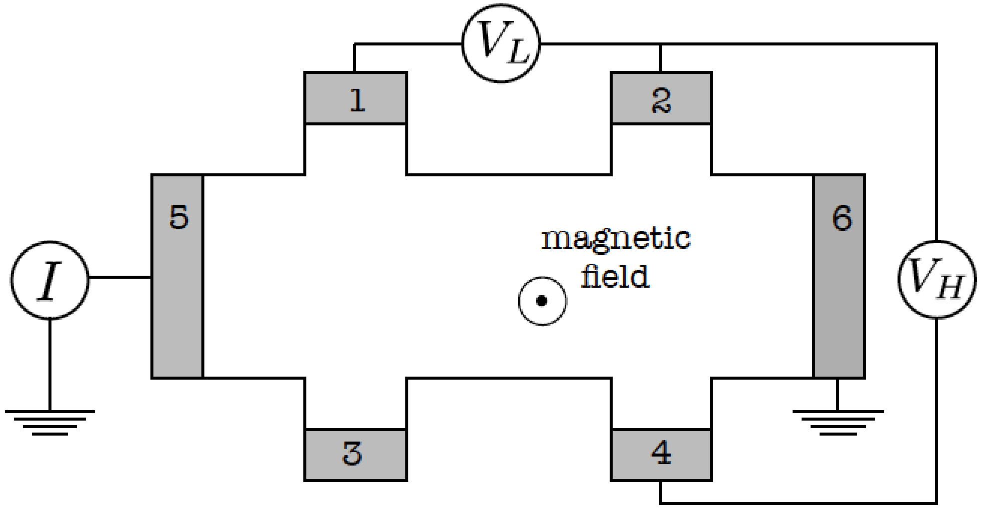
Experimental Manifestations of Non-Trivial Topology

Z X Shen Group Science (2009)

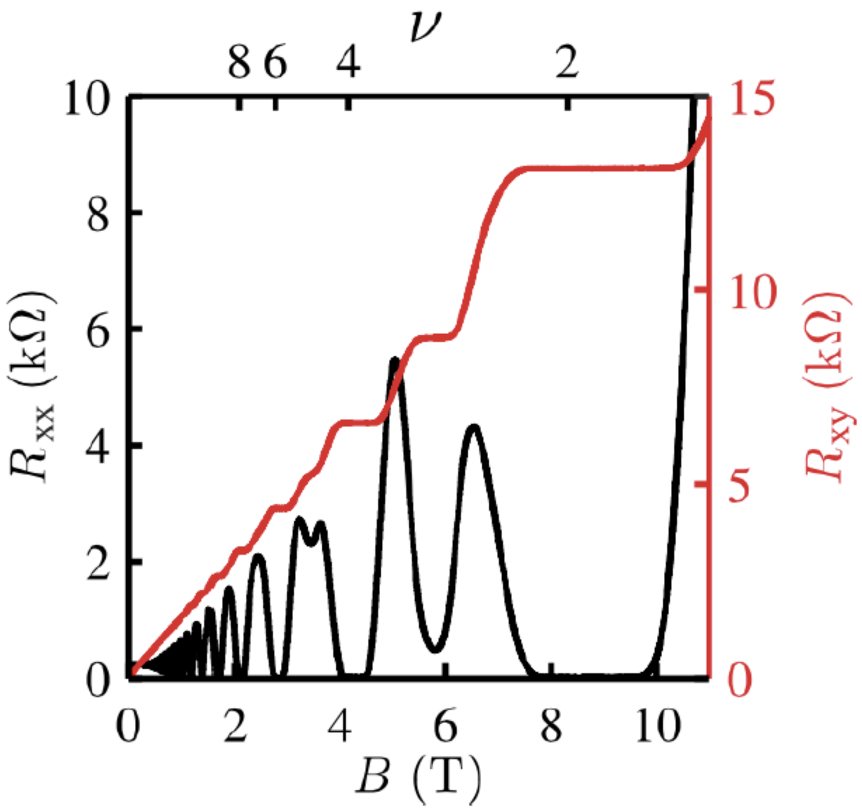


Quantum Hall Effect

Edwin Hall



Ady Stern
On-Line Lecture



Klaus von Klitzing (1980)

Topology and Band Physics

Fubini-Study Metric

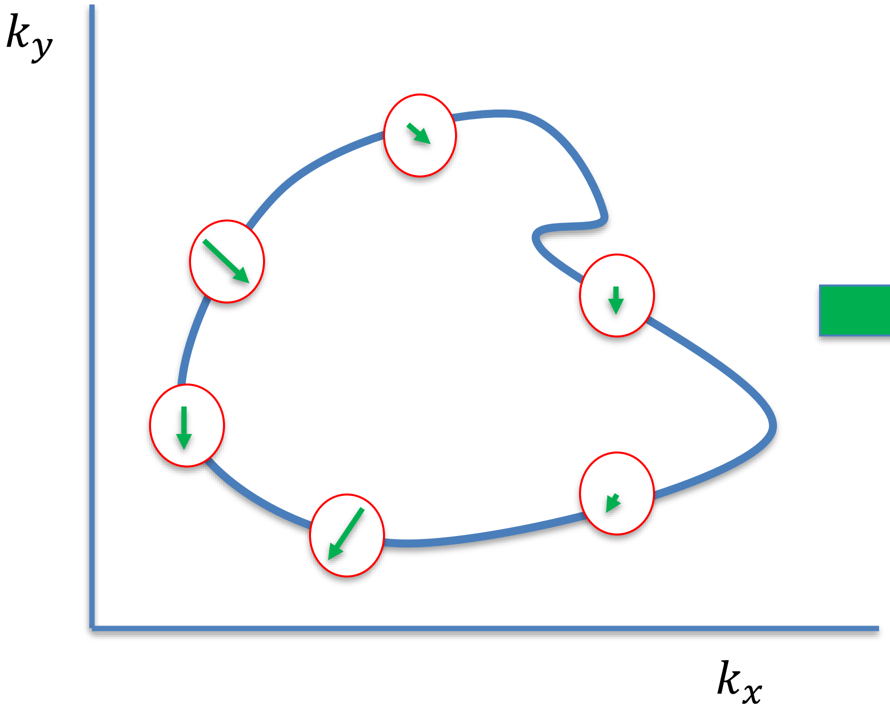
$$Q_{ij}(\boldsymbol{k}) = \langle \partial_{k_i} u_{\boldsymbol{k}} | [\mathbb{1} - |u_{\boldsymbol{k}}\rangle\langle u_{\boldsymbol{k}}|] | \partial_{k_j} u_{\boldsymbol{k}} \rangle$$

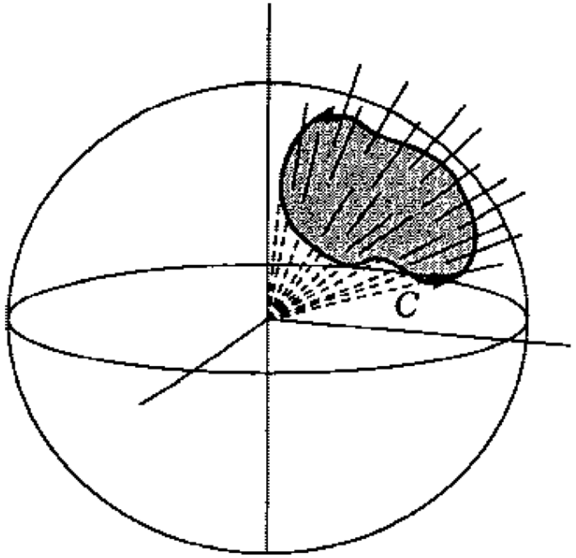
Yu et al. arXiv:2501.00098

Bloch Spheres and Berry Phases

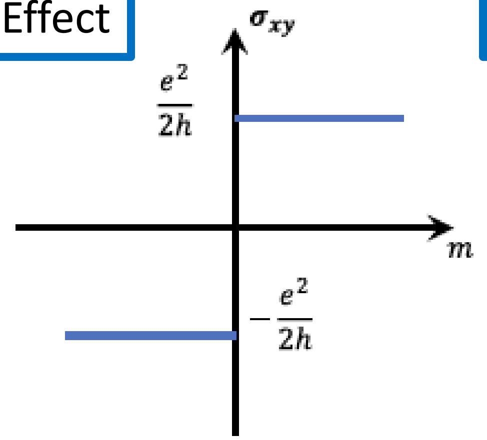
Two-Level System
Bloch Sphere

$$\Psi = \begin{pmatrix} \psi_t \\ \psi_b \end{pmatrix} = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix}$$

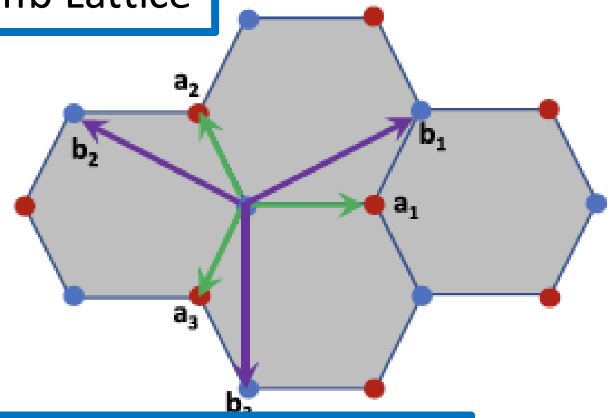


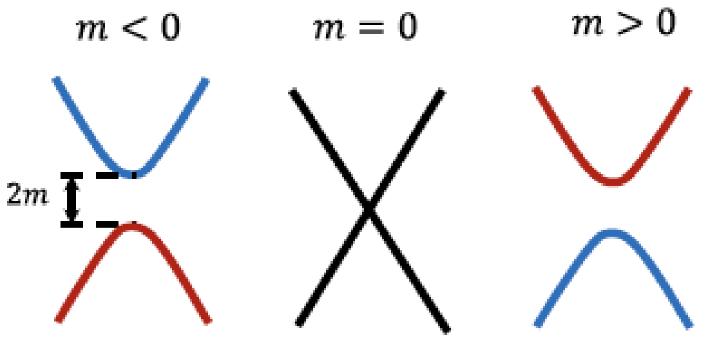


Hall Effect

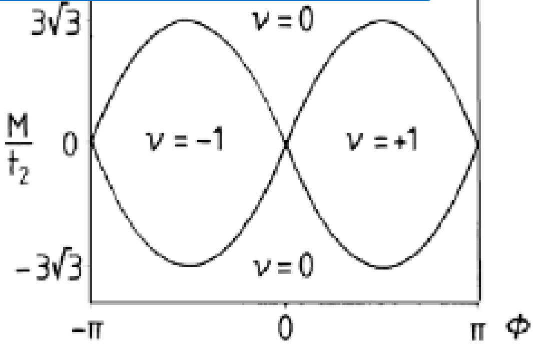


Honeycomb Lattice





Haldane Model – (1989)



Chang,Liu,AHM – RMP (2023)

Moire Material Magnetism

SU(4) vs. SU(2)

$\rho_{\alpha\beta}$ Order

N=2

$\alpha = \uparrow, \downarrow$

3 order parameters
1 eigenvalue (spin)
2 for 2 eigenvectors

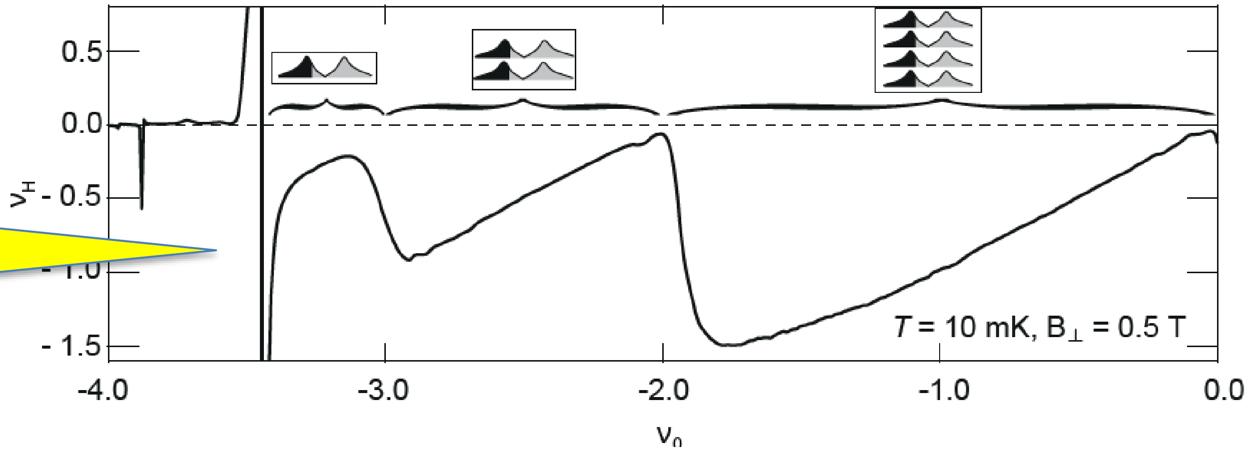
N=4

$\alpha = K\uparrow, K\downarrow, \bar{K}\uparrow, \bar{K}\downarrow$

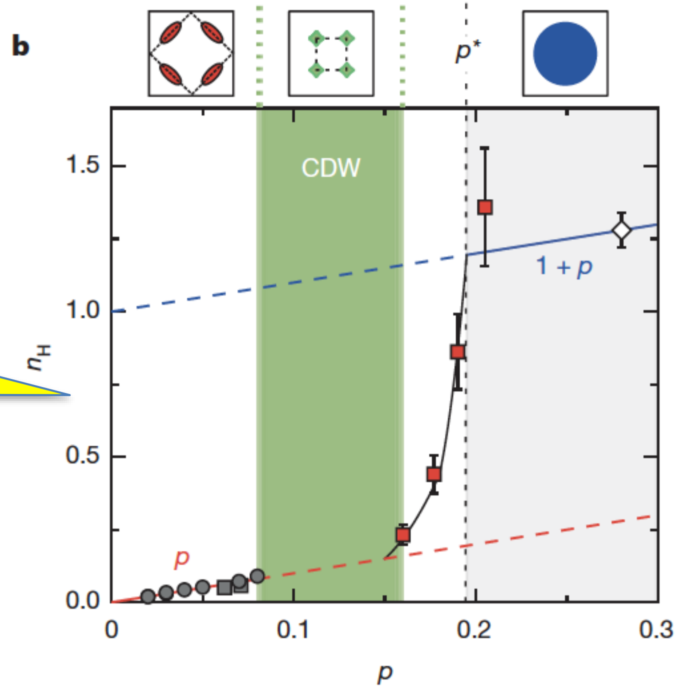
15 order parameters
3 eigenvalues (valley, spinK,spinK')
12 for 3 eigenvectors (6+4+2+0)

Fermi Surface Reconstructions are Common

Saito *et al.*
Nature (2021)

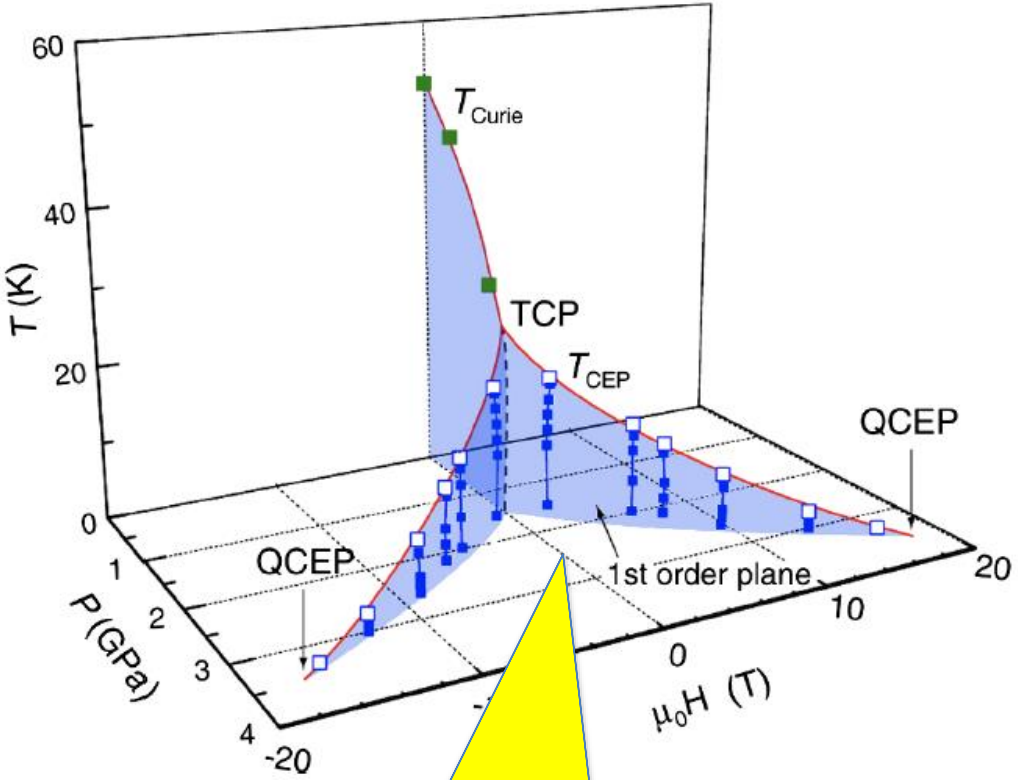


Badoux *et al.*
Nature (2016)
Putzke *et al.*
Nat. Physics (2021)



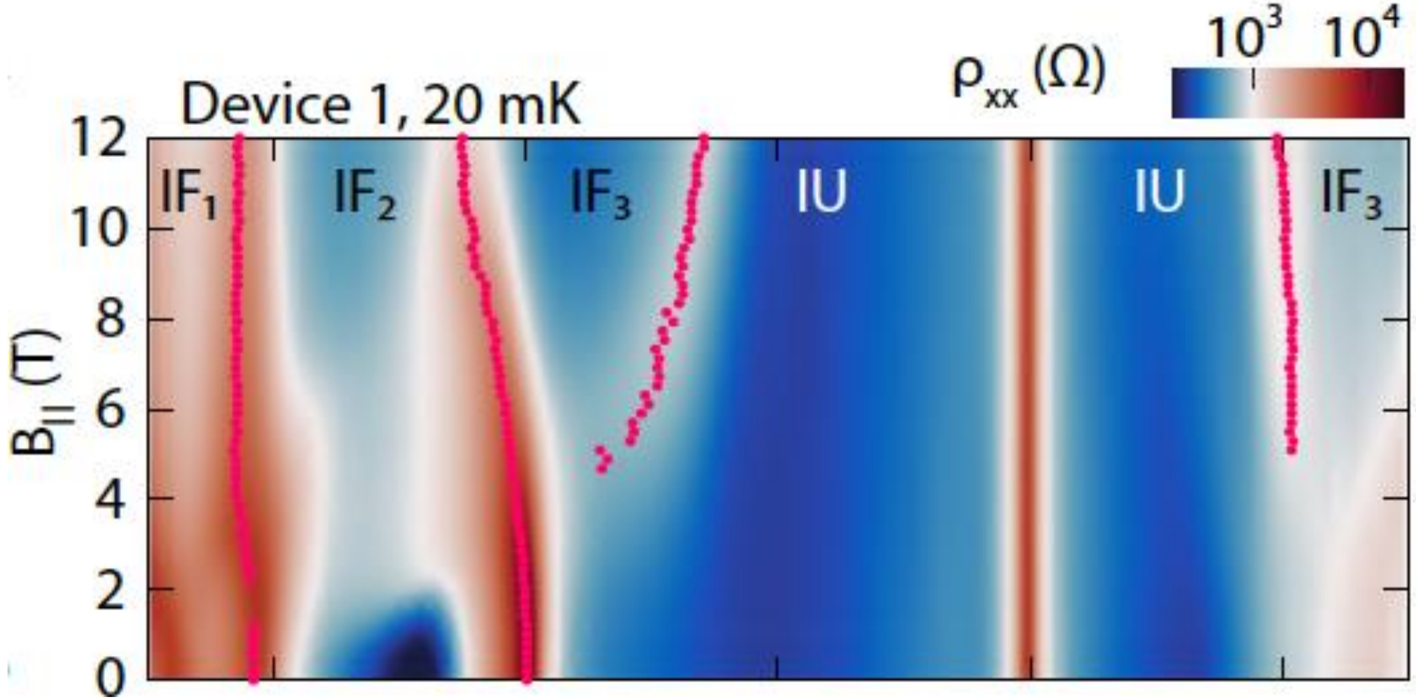
Non-Analytic Corrections
Magnetic Metal Case

Lonzarich Taillefer JPC (1985)
Chitov and Millis PRL,PRB (2001)
Kirkpatrick Belitz PRB (2003)
Chubukov Maslov PRB (2003,4)



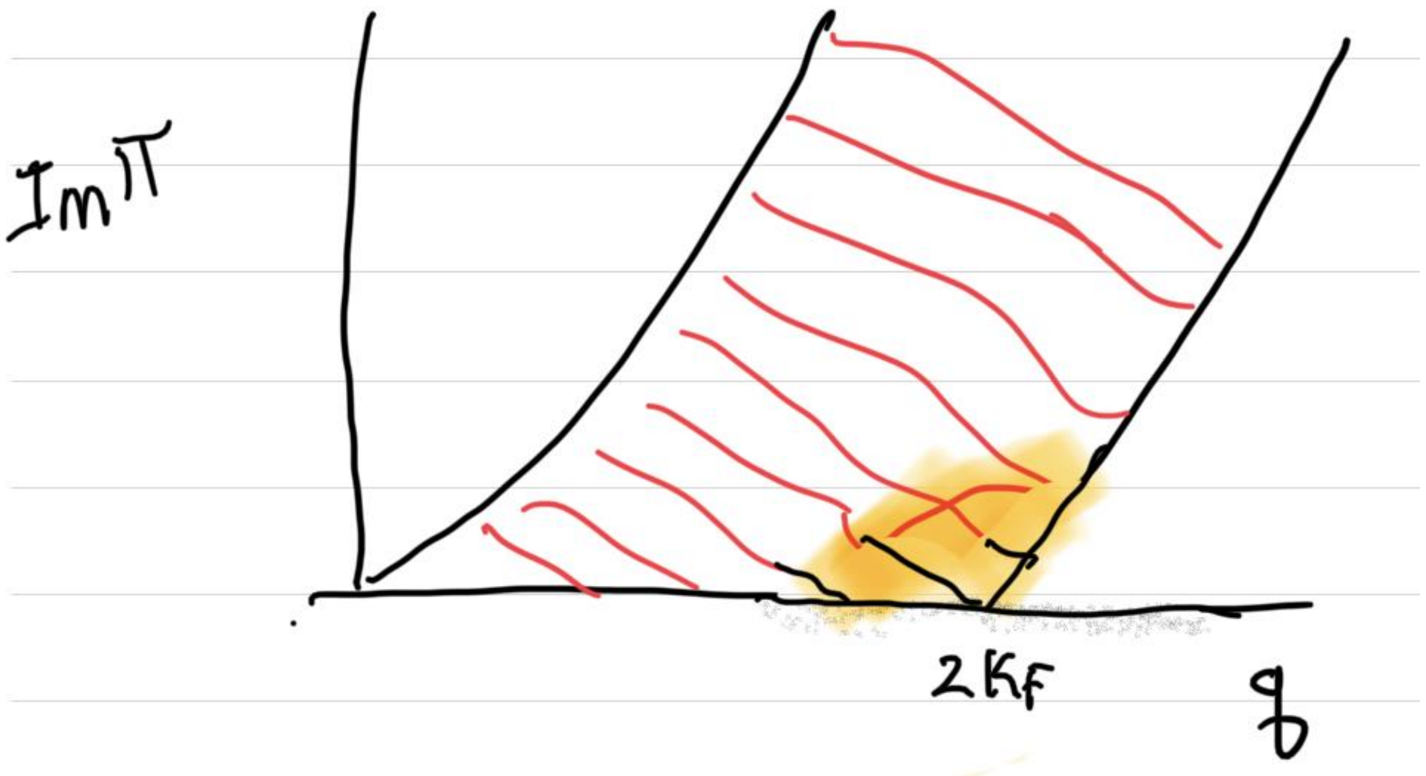
Brando *et al.* RMP (2016)

MAtBG Phase Diagram - Expt



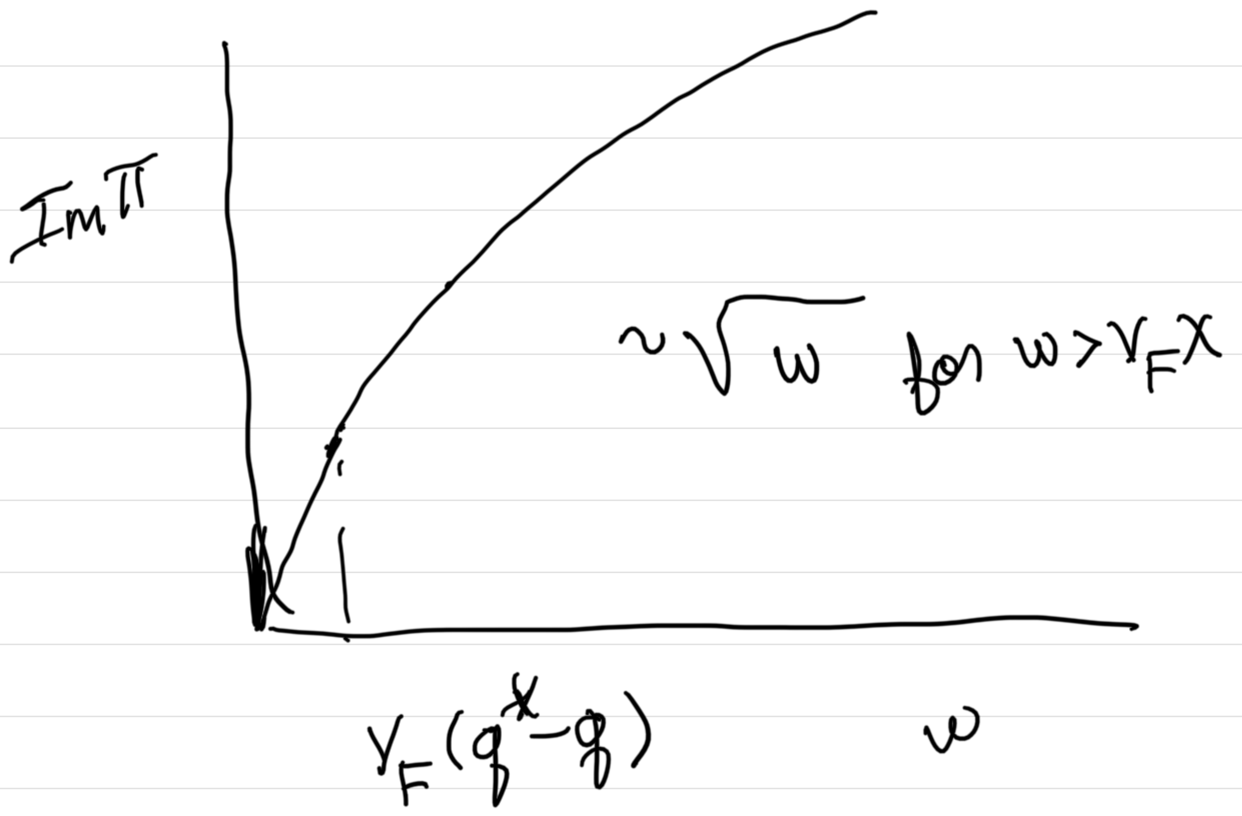
Rozen *et al.* arXiv:2009.01836
Saito et al. Nature (2021)

NAC to FLT - Why?



Xie, Qin, and AHM – arXiv:soon

NAC to FLT - Why?



Xie, Qin, and AHM - arXiv:soon

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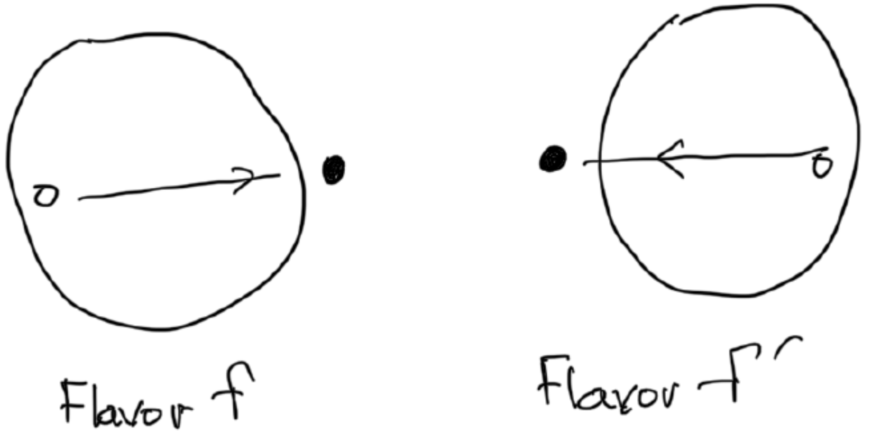
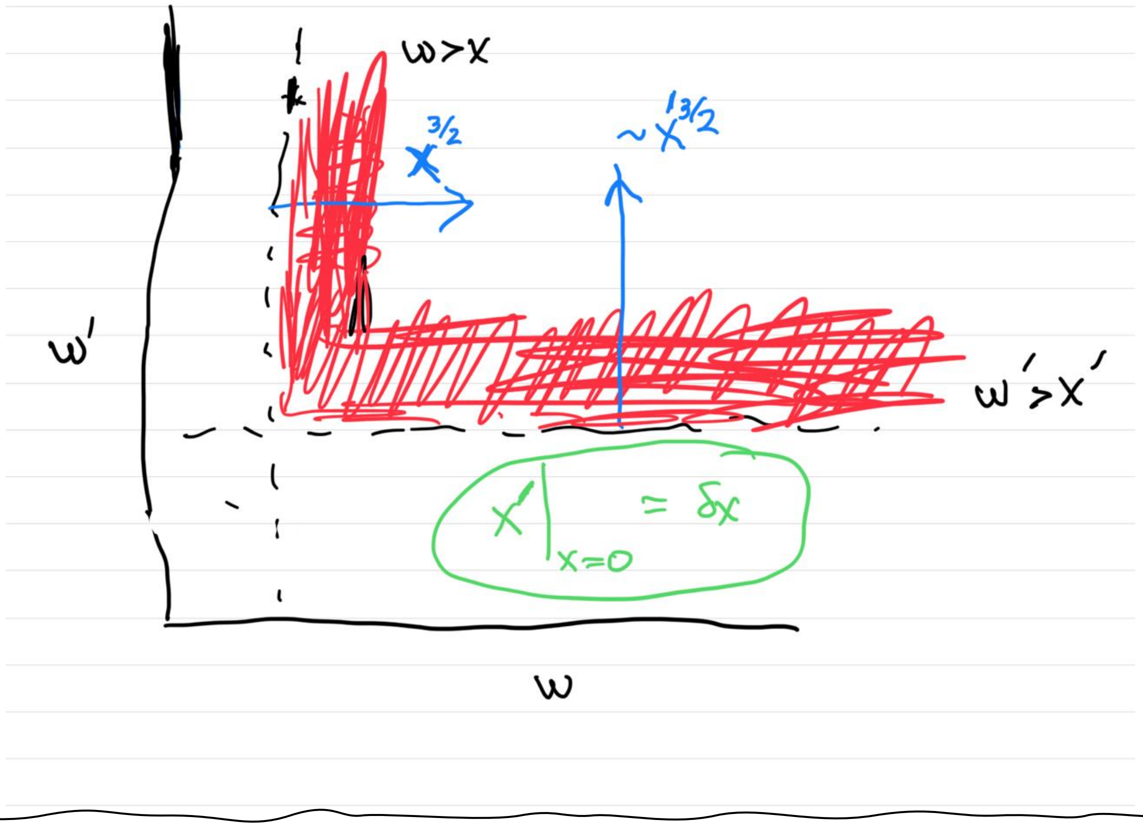


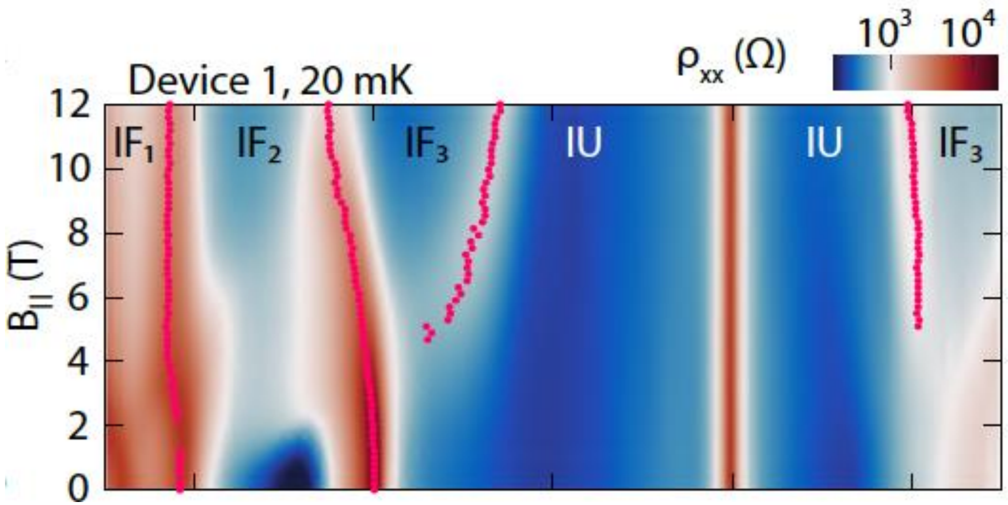
$$-\bar{V}^2 \int d\omega \int d\omega' \frac{\Pi^{I}(\omega, \vec{q})\, \Pi^{I'}(\omega', -\vec{q})}{\omega + \omega'}$$

NAC to FLT - Why?

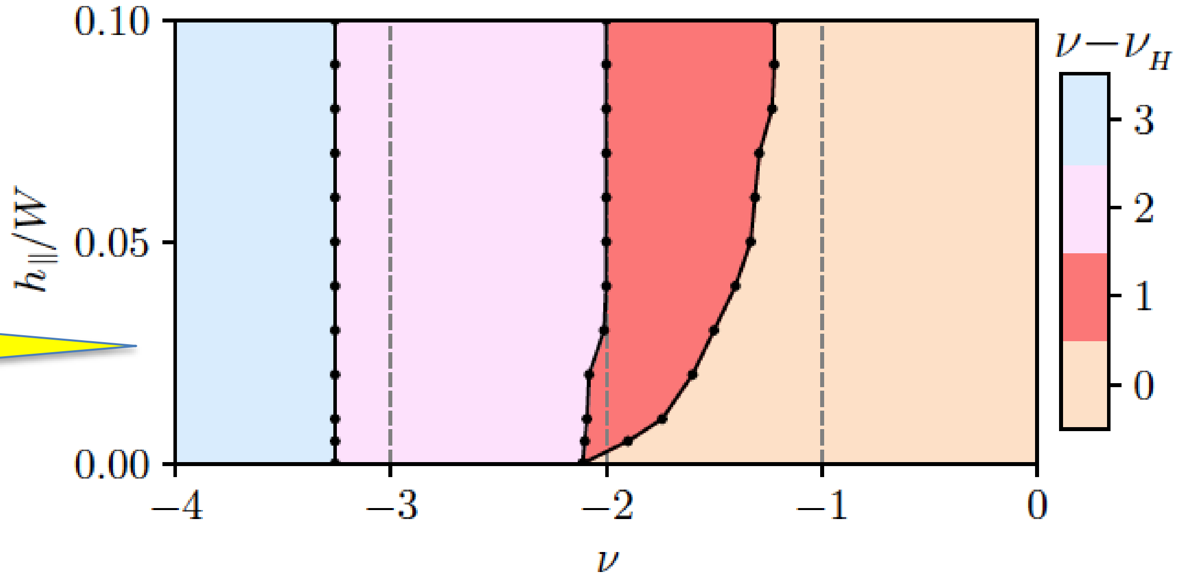


$$E_c = \alpha\, m^2 + \beta\, m^4 - \gamma\, |m|^3$$

MAtBG Phase Diagram



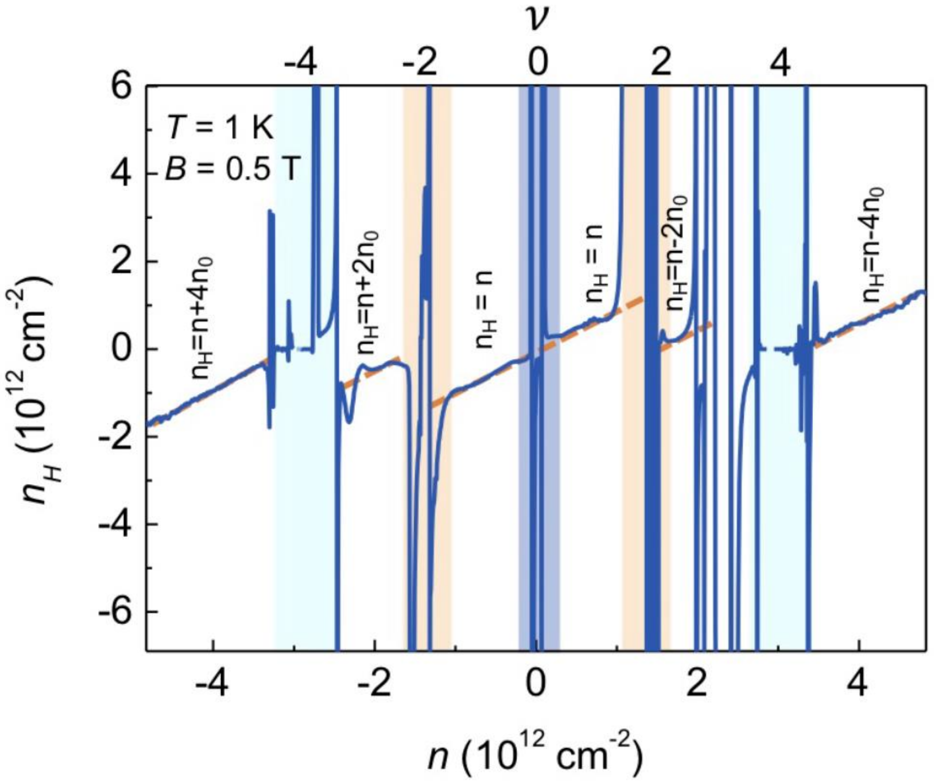
Expt

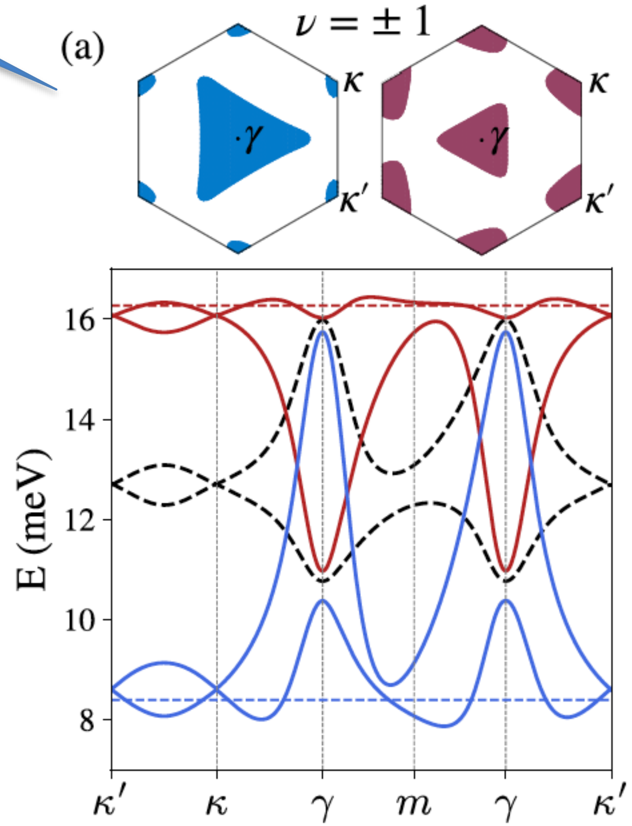


Theory

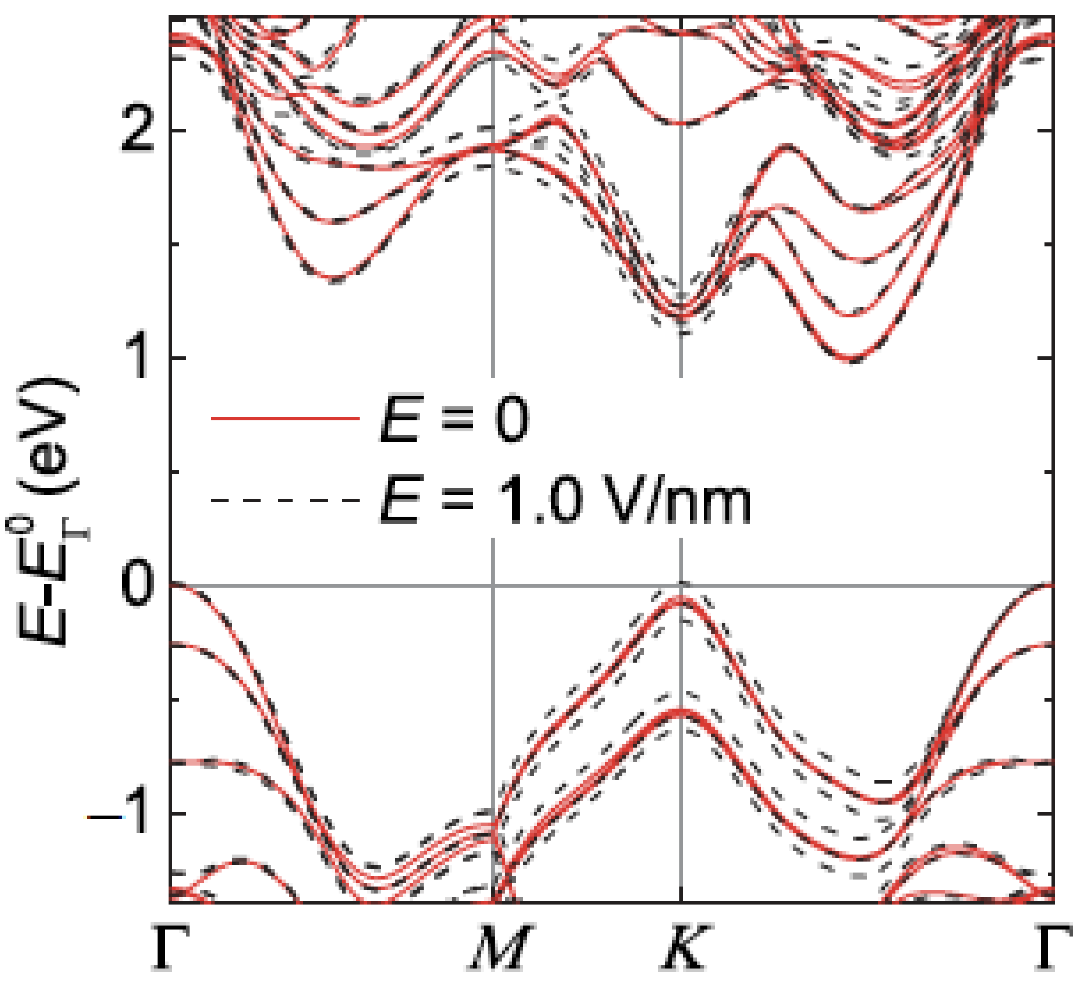
Fermi Surfaces

Zhu et al. PRB (2024)





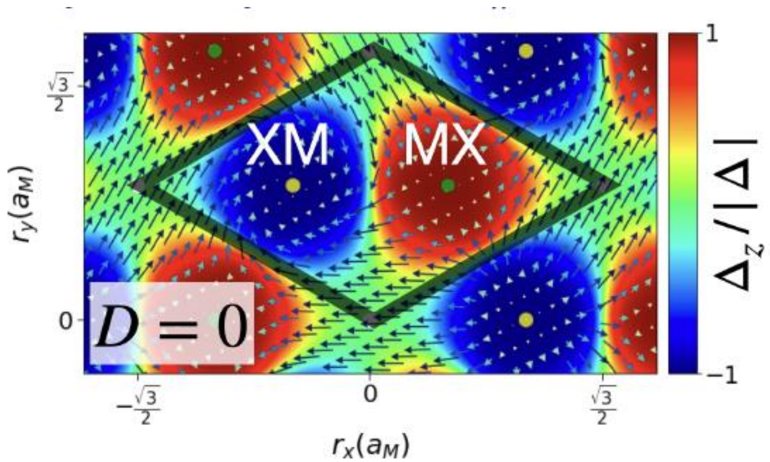
	MoS_2	$MoSe_2$	$MoTe_2$	WS_2	WSe_2
MoS_2	Homo Gamma				
$MoSe_2$	(S,Se)	Homo Gamma			
$MoTe_2$	(S,Te)	(Se,Te)	Homo K		
WS_2	(Mo,W)	(S,Se)	(Se,Te)	Homo Gamma	
WSe_2	(Se,Se) ? (S,Se)	(Mo,W)	(Se,Te)	(S,Se)	Homo K



Layer Pseudospins in TMD Homo/Heterobilayers

Surprise!

A Skyrmion Lattice

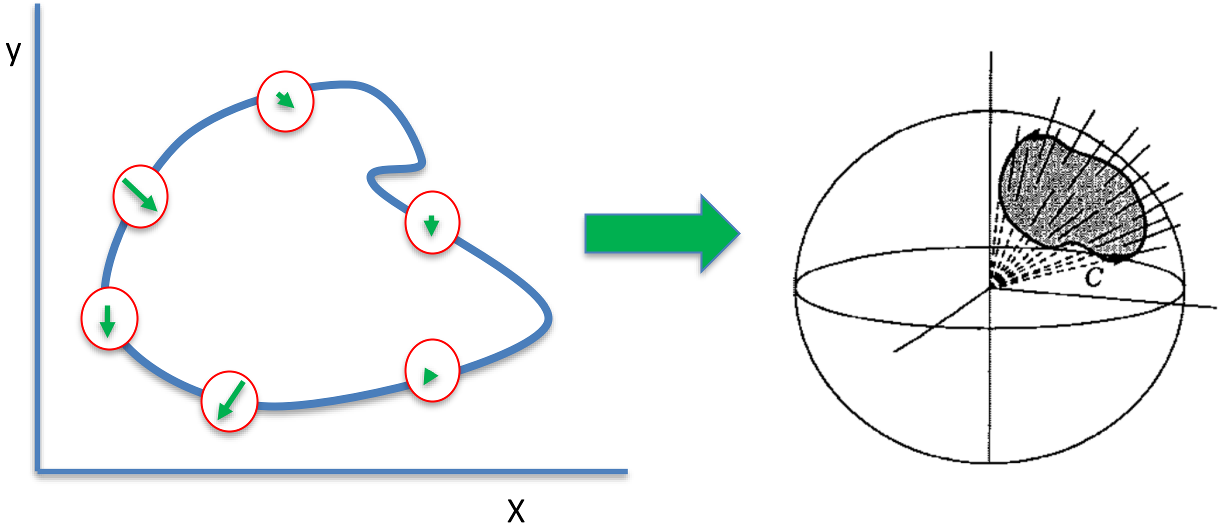


TMD AA Homobilayer Theory – Wu et al. - PRL (2019)

Bloch Spheres and Berry Phases

Layer Spinor
Bloch Sphere

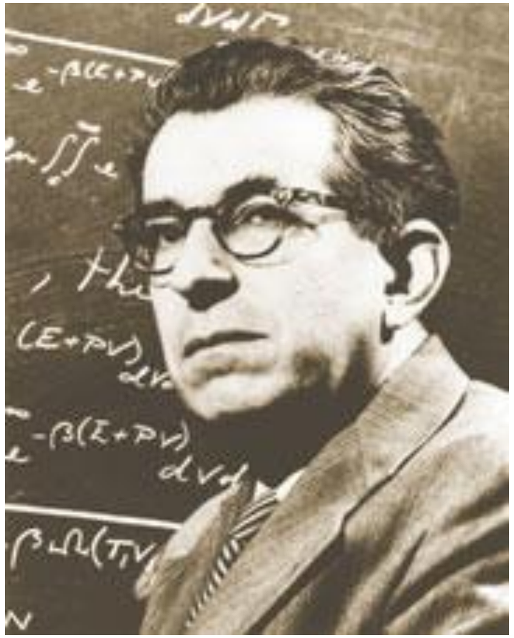
$$\Psi = \begin{pmatrix} \psi_t \\ \psi_b \end{pmatrix} = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix}$$



On the Problem of the Molecular Theory of Superconductivity*

F. London
Duke University, Durham, North Carolina
(Received April 25, 1948)

Werner Heisenberg



Fritz London

$$I_{kl} = 4\pi h^2 e^2 / V |p_k - p_l|^2$$

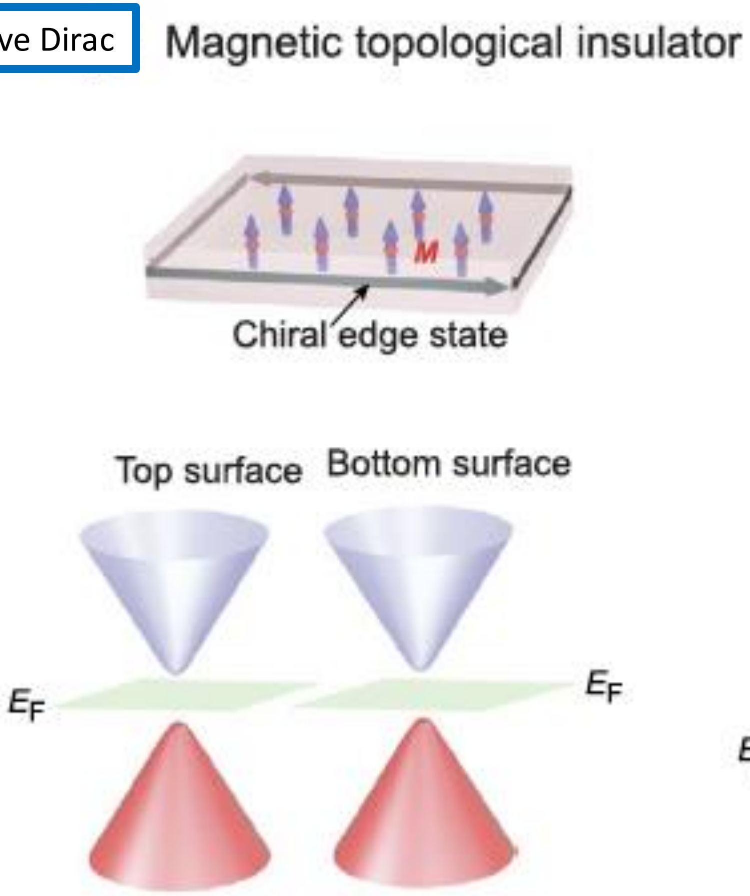
We assembled indications which suggest that it is most probably the exchange interaction associated with the Coulomb field of the electrons which is responsible for this "condensation in momentum space." Ferromagnetism and superconductivity would then be considered as two opposite limiting cases of the same effect, depending on whether the exchange interaction competing with the zero-point energy promotes parallel orientation of the electronic spins or a coordination of the translational momentum in a state of vanishing total spin.

F. London Phys. Rev. **74** (1948)

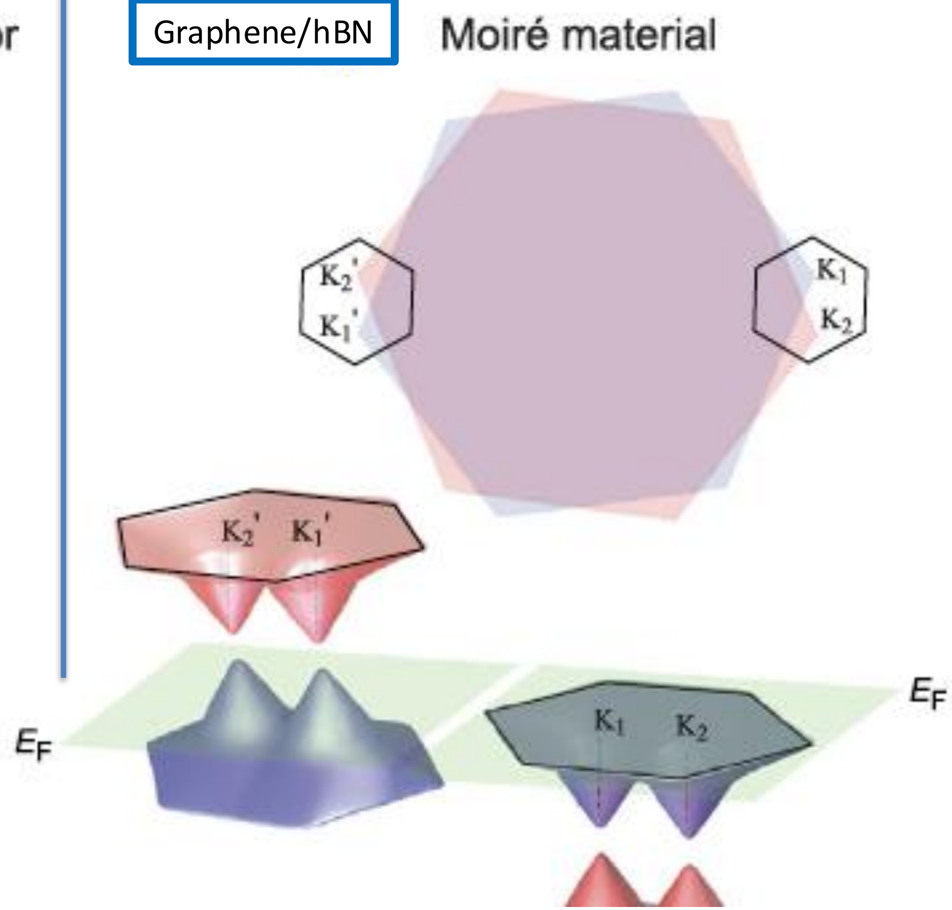
Spin Magnetism

Orbital Magnetism

Masive Dirac



Graphene/hBN



CZ Chang, CX Liu, AHM – RMP (2023)

Orbital vs. Spin Magnetization

$$H = \left[\sum_{i=1}^{N}\left(\frac{-\hbar^2}{2m}\left(-i\vec{\nabla}_i + \frac{e}{\hbar c}\vec{A}_i\right)^2 + V_i\right) + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{|\vec{r}_i - \vec{r}_j|}\right] - g\mu_B B_s \sum_{i=1}^{n}\vec{s}_i \cdot \hat{z}$$

$$\vec{A} = \frac{B_{orb}}{2}(-y, x, 0)$$

$$M_{orb} = \left\langle \frac{\partial H}{\partial B_{orb}} \right\rangle = \left\langle \frac{1}{c}\int d\vec{r}\,(\vec{r} \times \vec{j}) \right\rangle$$

Typically Zero at B=0

$$M_s = \left\langle \frac{\partial H}{\partial B_s} \right\rangle = g\mu_B \left\langle \sum_{i=1}^{n} s_{iz} \right\rangle$$

Non-zero in Typical Ferromagnets

Cousins of Orbital Magnetization

Orbital Magnetization

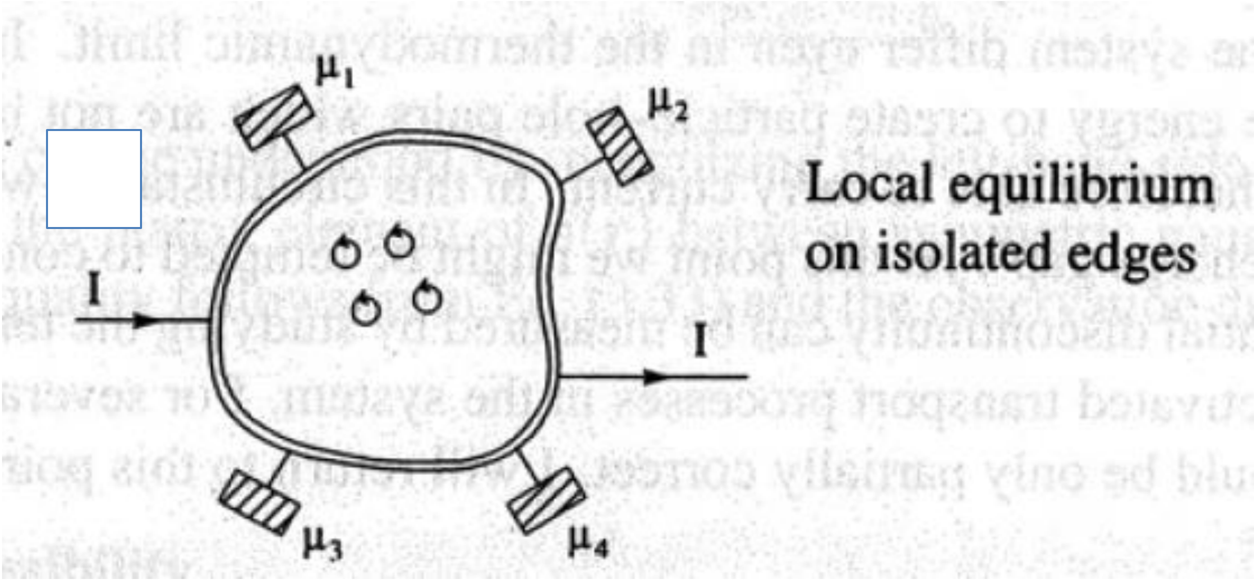
Anomalous Hall Effect

Kerr/Faraday Effect

Require
Broken `Orbital'
Time Reversal
+

Edge States, Orbital Magnetization, and QHE

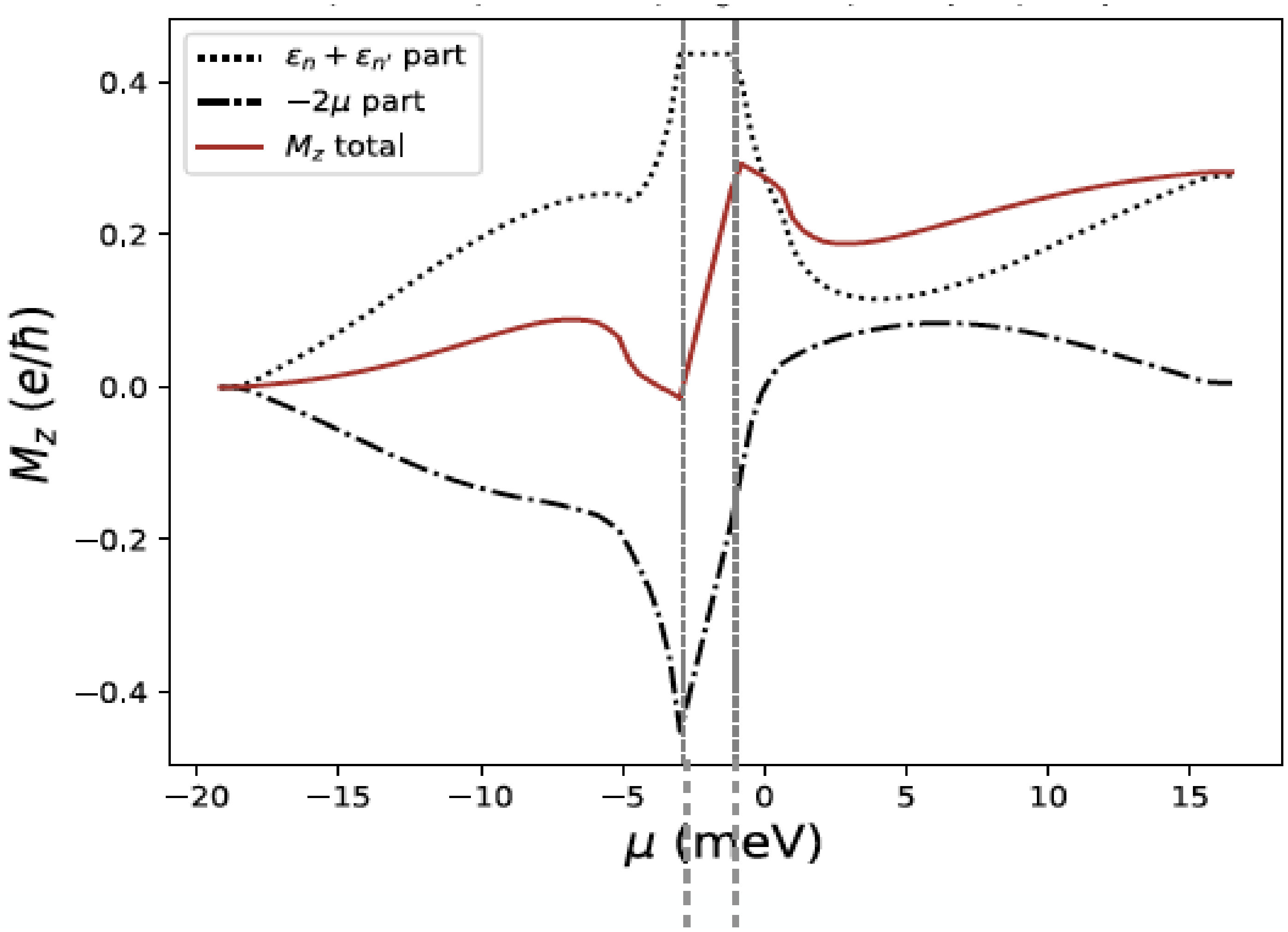
$$I=\frac{c}{A}\frac{\partial M}{\partial \mu}\delta\mu = \frac{c}{A}\frac{\partial N}{\partial B}\delta\mu$$



Purely Orbital Ferromagnetism occurs in MATBG

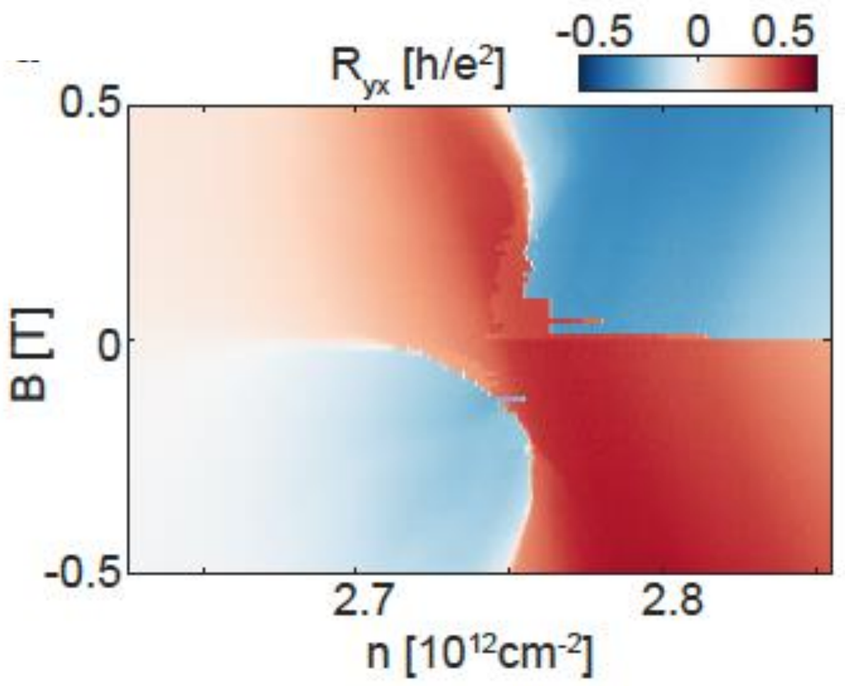
$$\frac{\Delta M}{\mu_B N_{uc}} = \frac{C m A_{uc} E_{gap}}{\pi \hbar^2}$$

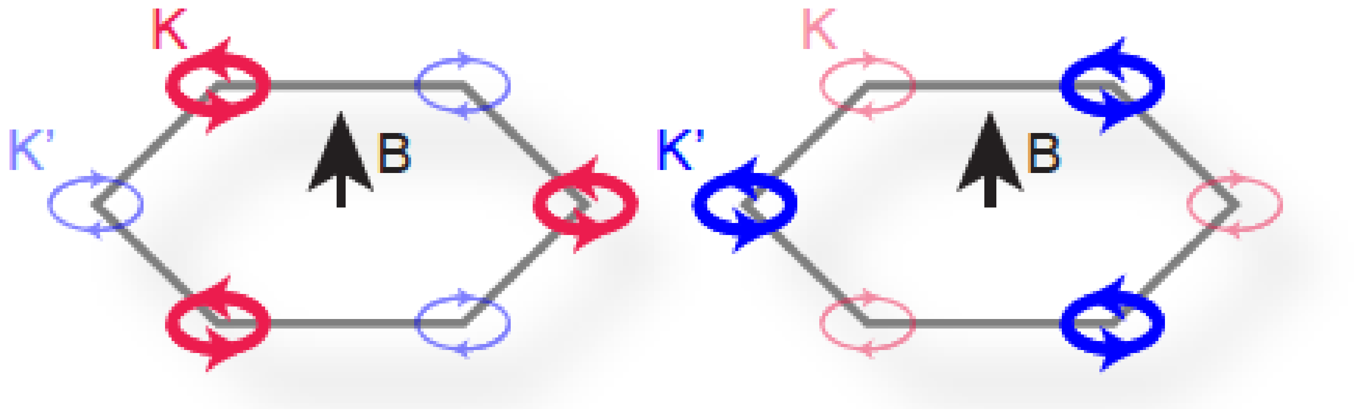
MATBG/hBN Magnetization



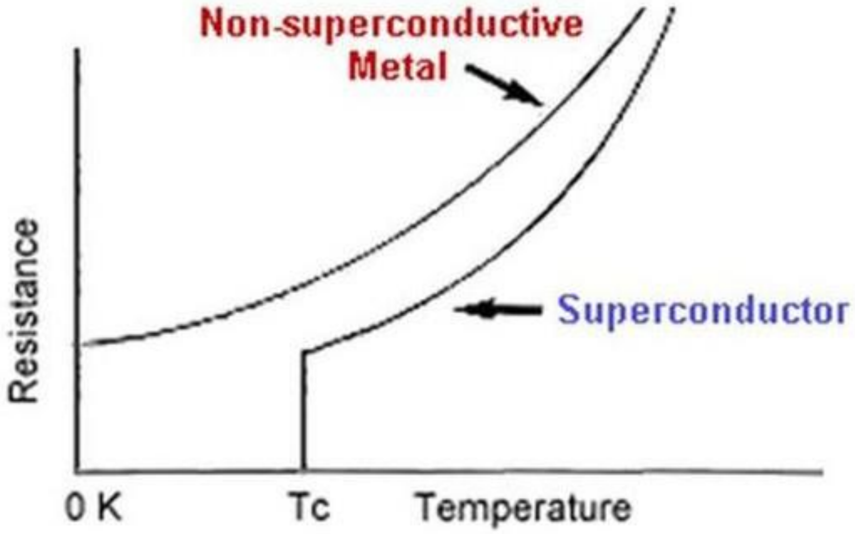
Zhu et al. - PRL (2020)

Electrical Magnetization Reversal

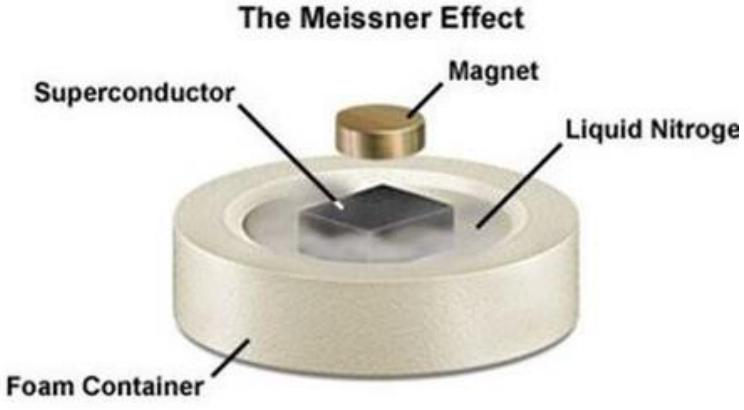


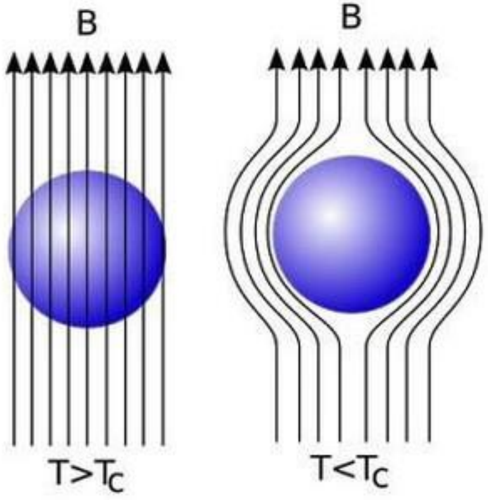


Polshyn et al. Nature (2020)



◆Zero resistivity
◆Perfect diamagnetism





$$\vec{j} = -\frac{n_s e^2}{mc} \vec{A}$$

From: https://vajiramias.com/current-affairs/superconductivity/5cea6a021d5def3dd9b17c7b/


… and why is the Hall conductance 25812.807 Ohms
It is a simple number that everyone will remember

… and why are they superconductors
Nobody knows

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Magnetism in Moiré Materials

Allan MacDonald UT Austin