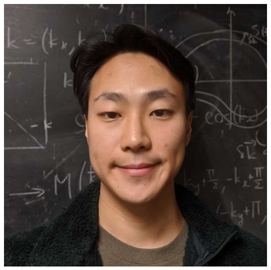
Electronic instabilities of kagomé metals and density waves in the AV_3Sb_5 materials

Leon Balents
KITP

Quantum Matter Frontiers Seminar, April 26, 2021

Collaborators



Takamori Park

Mengxing Ye

Brenden Ortiz

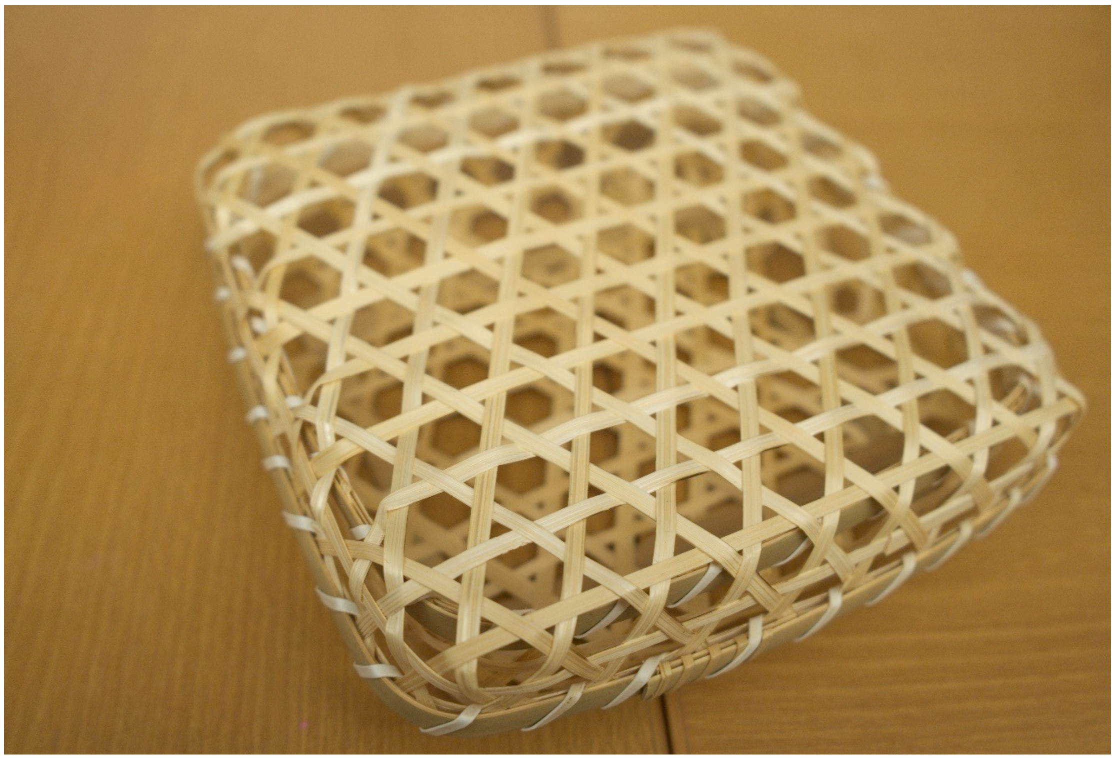
Stephen Wilson

Ilija Zeljkovic, BC

outline

- Introduction: kagomé lattice and flat bands
- AV_3Sb_5 materials
- Competing orders and saddle points
- Density wave orders and experimental evidence

Kagomé



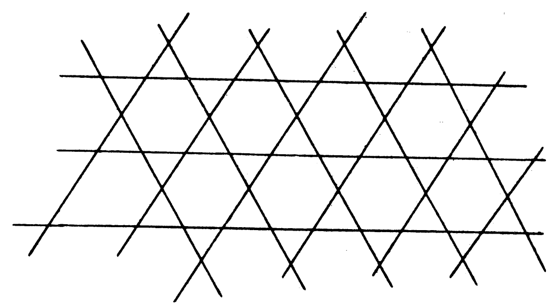
Statistics of Kagomé Lattice

Itiro SYÔZI
Department of Physics, Osaka University

(Received February 27, 1951)

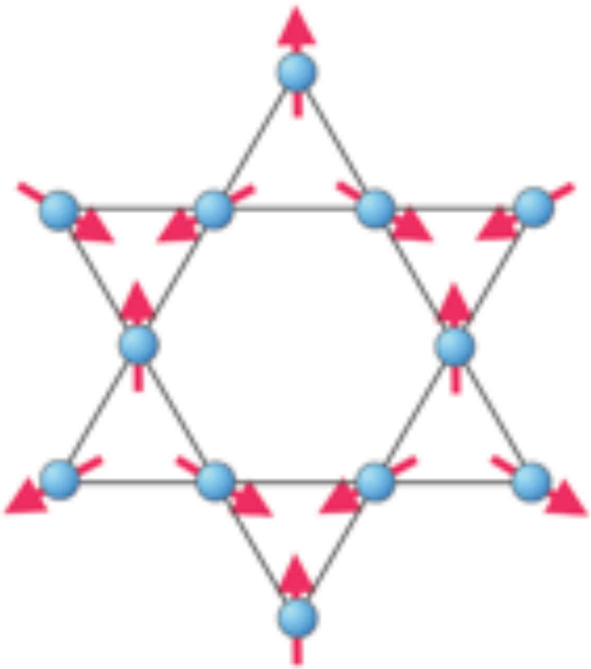
The transition temperature of the kagomé lattice with $Z=4$ is obtained and compared with that of the square lattice.

After the work of Onsager,[1] who solved exactly the problem of Ising model for the case of plane square lattice, the same problems for the honeycomb and triangular lattice were treated by several authors.[2] Other than these three types of lattices, there is left a lattice, called in Japanese kagomé (woven bomboo pattern), which consists exclusively of equivalent lattice points and equivalent bonds. Since the number of nearest neighbors of a lattice point is as many as in the square lattice, namely four, it is interesting to verify the natural conjecture that the curie point, in general, is determined solely by the relation $\mathrm{ch}2H=\sec \pi/Z$ established by Onsager for the three types of lattices.



Fig· 1. Kagomé Lattice

insulating kagomé antiferromagnets



$$H = J \sum_{\langle ij \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + \ldots$$

likely to be a QSL

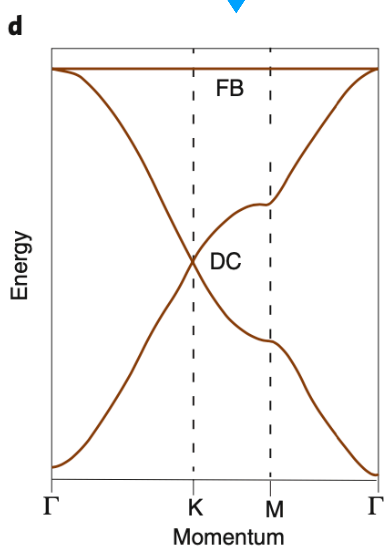
V. Elser, 1989 + many many others

Cu minerals

herbertsmithite
volborthite
kapellasite
barlowite
...

Flat bands

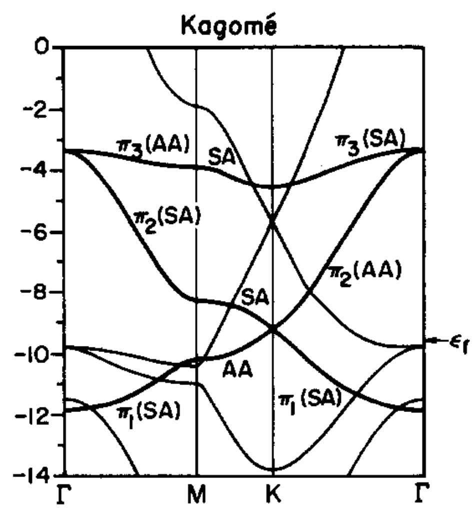
$$H = -t \sum_{\langle ij \rangle} c_i^{\dagger} c_j + \text{h.c.}$$

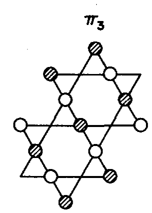


THE KAGOMÉ NET: BAND THEORETICAL AND TOPOLOGICAL ASPECTS*

ROY L. JOHNSTON† and ROALD HOFFMANN‡

Department of Chemistry and Materials Science Center, Cornell University, Ithaca, NY 14853, U.S.A.



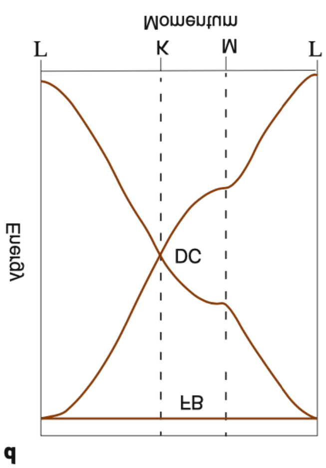


The small dispersion of the π_3-band in Kagomé boron [Fig. 1(b)] can be explained by examining the crystal orbitals in Fig. 2. At M the π_3-orbital is antibonding along chains of connected boron atoms. In a simple Hückel sense,[13] the energy of this band would be $\alpha - 2\beta$. At Γ the π_3-orbital is one of a degenerate pair, one component of which can also be represented as antibonding chains of borons, with a Hückel energy of α–2β. The energies of the bands in our extended Hückel calculation (and in reality) depart from the simple Hückel model through the inclusion of small non-nearest-neighbour interactions. The next-nearest-neighbour interactions at M are overall bonding while those at Γ are net antibonding, so the π_3-band lies at lower energy at M than the π_2/π_3 pair at Γ [see Fig. 1(b)]. At point K in the BZ, as mentioned above, the π_3-band describes a three-alternant pattern. In simple Hückel terms the energy of this crystal orbital would be $\alpha + 4(-0.5\beta) = \alpha - 2\beta$, once more. This time the next-nearest-neighbour interactions are more bonding (each atomic orbital has four next-nearest-neighbour orbitals which are in-phase) than at Γ or M, so the π_3-band shows a minimum at K. Thus, the bonding character of the π_3-band changes very little throughout the BZ. In the density of states (DOS) diagram for this net (not shown here), the flat π_3-band leads to a sharp spike. Because this band is so high above any realistic Fermi level, it is unlikely to have any consequence.

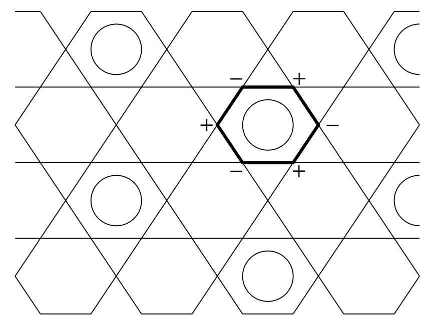
Localized magnons

Tight-binding model (with negative t) describes dispersion of magnons in ferromagnetic state. Interactions make them crystallize.

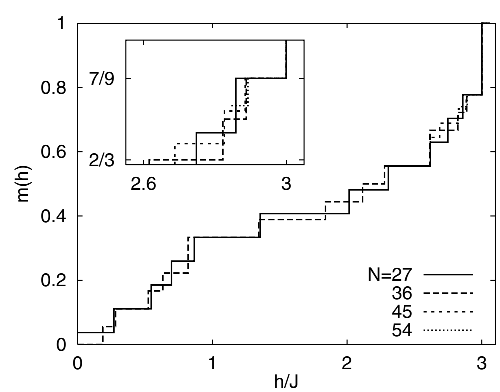
$$|\psi\rangle = \sum_i \psi_i S_i^- |FM\rangle$$



Wannier states are eigenstates within flat band

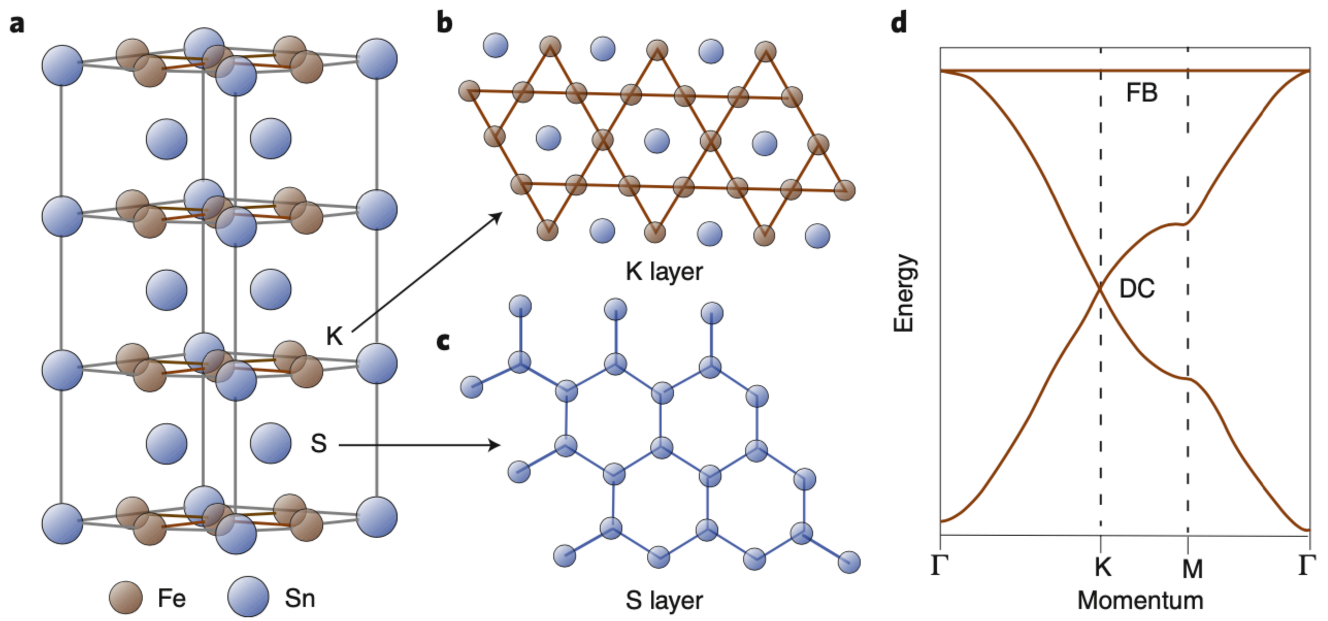


magnon crystal



Schulenburg *et al*, 2002

Kagomé metals



Mn_3Sn, Mn_3Ge, FeSn, $YbMn_6Sn_6$, CoSn, $Co_3Sn_2S_2$

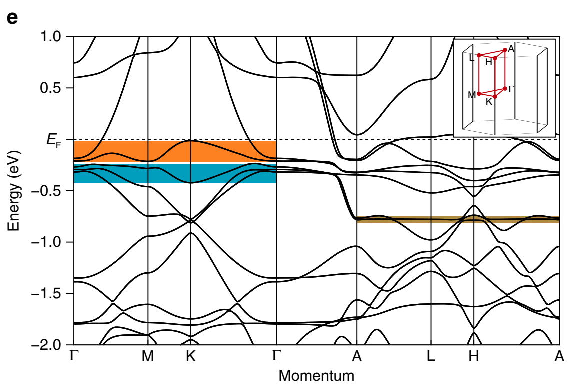
Bands and photoemission

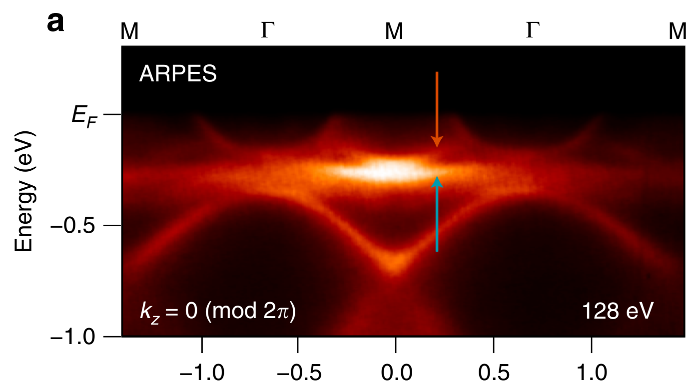
ARTICLE

https://doi.org/10.1038/s41467-020-17465-1 OPEN

Topological flat bands in frustrated kagome lattice CoSn

Mingu Kang[1], Shiang Fang[2,3,4], Linda Ye[1], Hoi Chun Po[1], Jonathan Denlinger[5], Chris Jozwiak[5], Aaron Bostwick[5], Eli Rotenberg[5], Efthimios Kaxiras[2,3], Joseph G. Checkelsky[1] & Riccardo Comin[1]✉

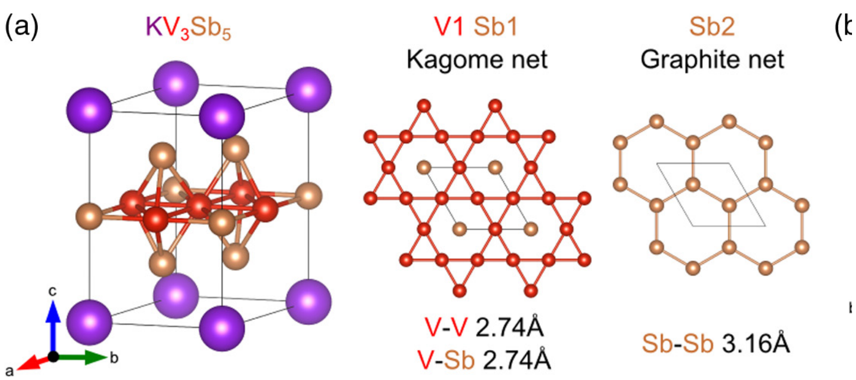




Flat bands…and??

Vanadium rush

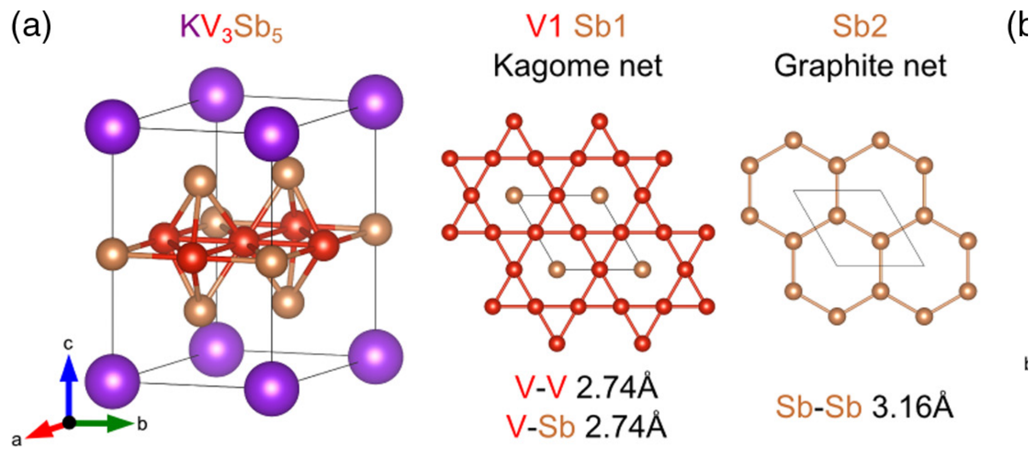
B.R. Ortiz *et al*, 2019: AV_3Sb_5

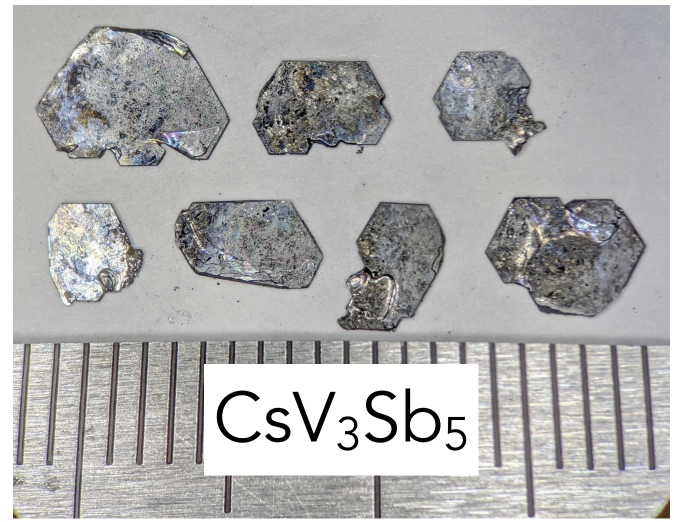


~20 papers in the last month

AV_3Sb_5

B.R. Ortiz *et al*, 2019





V kagomé layers separated by Sb honeycombs

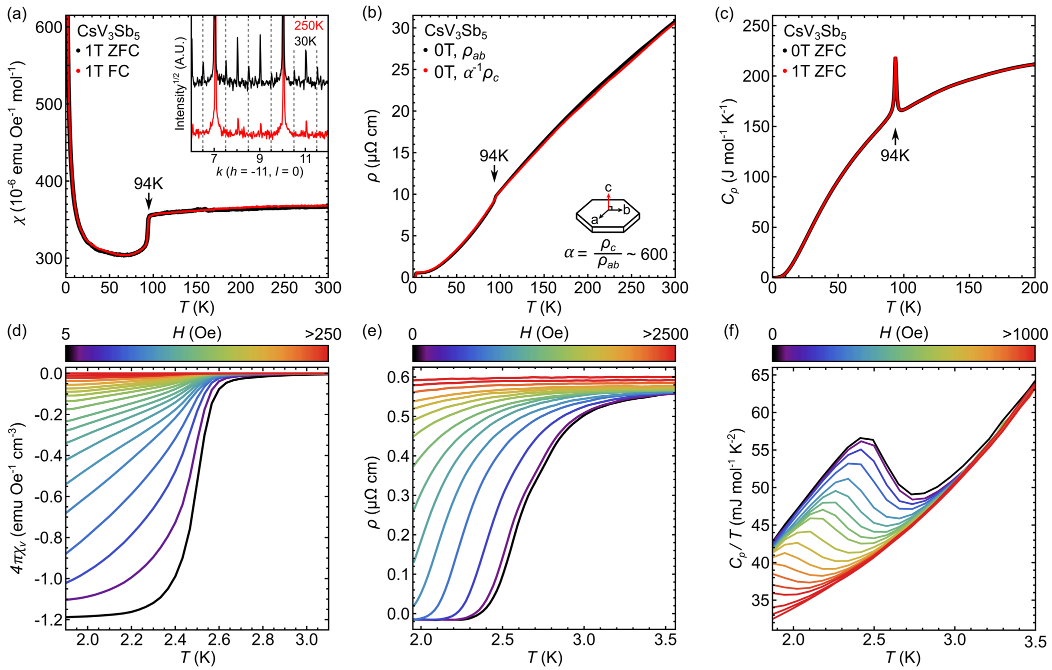
Perfect hexagonal symmetry: P6/mmm space group

Nominally $V^{14/3} = d^{1/3}$ or 1 d electron per unit cell

Very different from Fe,Mn,Co kagomés

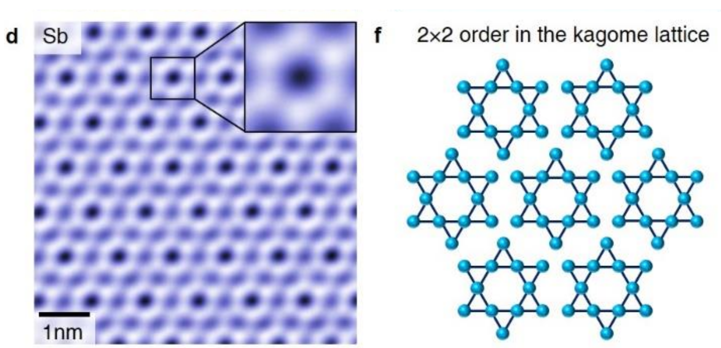
AV_3Sb_5

B.R. Ortiz *et al*, 2020



- Metallic (μΩ-cm)
- Quasi-2d: R_c/R_{ab} = 600
- Pauli paramagnetism - no local moments
- CDW transition ~90K
- SC $T_c \lesssim 3.5$K

Y.-X. Jiang *et al*, 2020/21



"3Q" CDW quadruples 2d unit cell

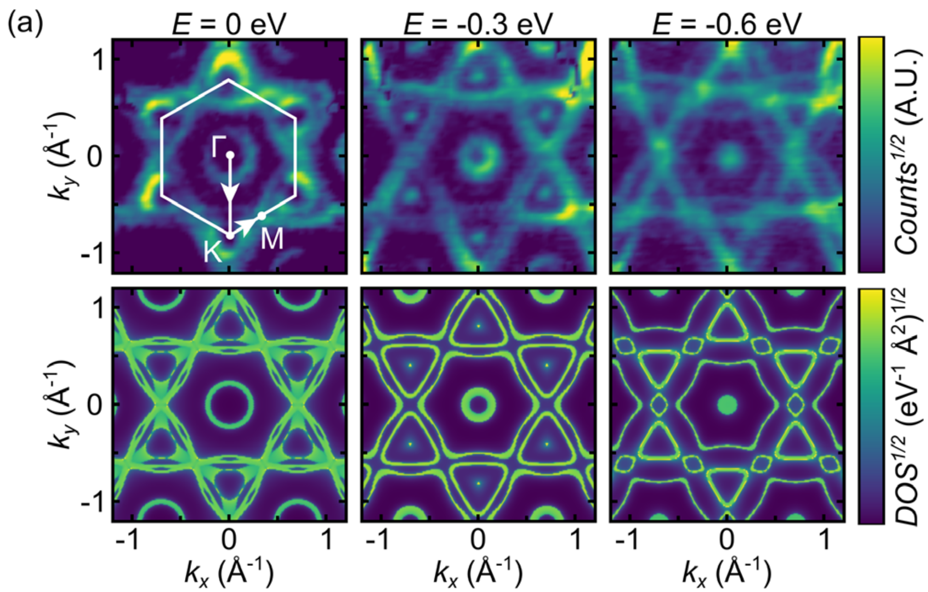
AV_3Sb_5

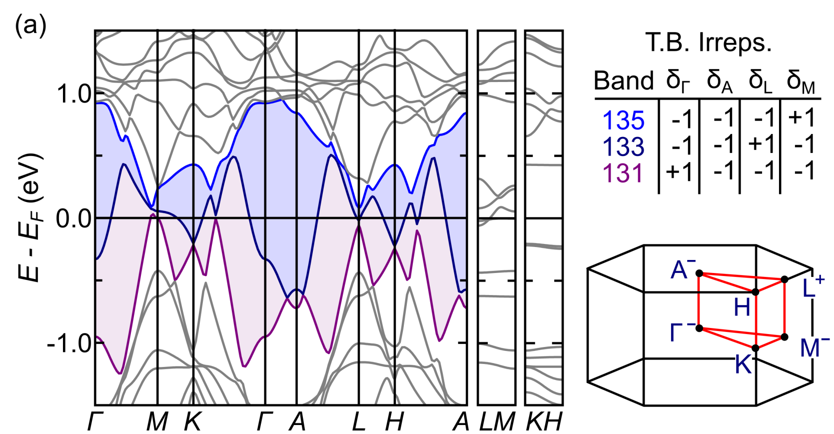
Band structure

B.R. Ortiz *et al*, 2020

ARPES

DFT



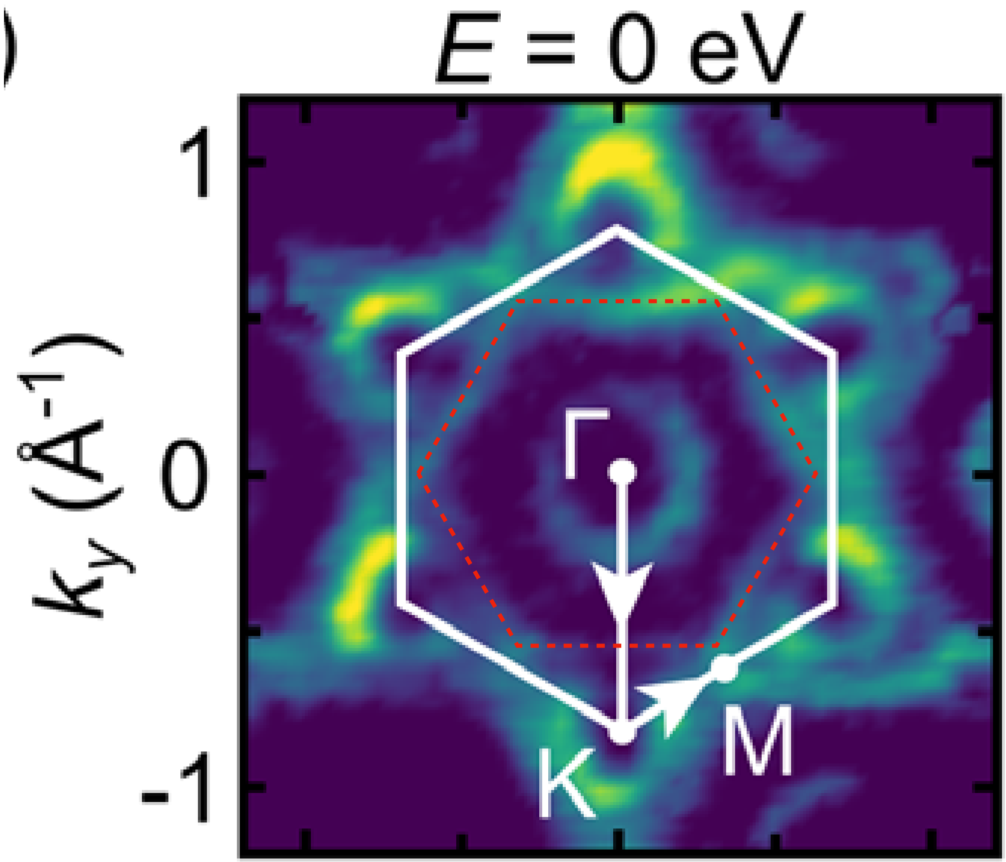


- Clearly many bands, mostly V but also Sb
- Several quasi-2d Fermi surfaces (*very* far from the ionic picture)

AV_3Sb_5

Band structure

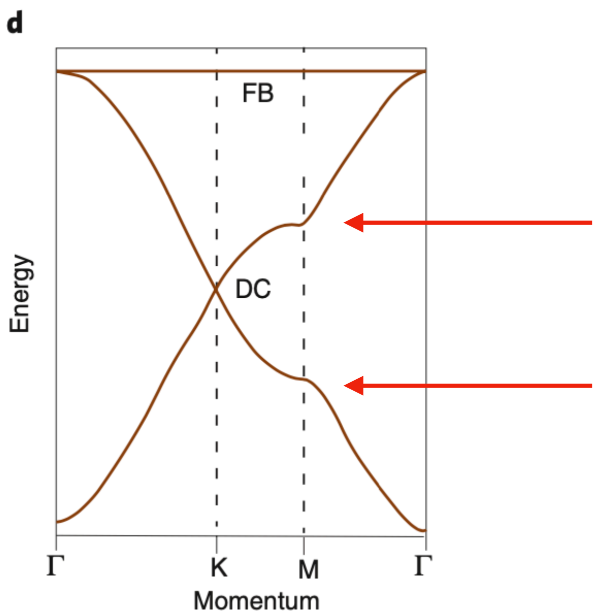
B.R. Ortiz *et al*, 2020



approximately hexagonal Fermi surface "inscribed" in Brillouin zone

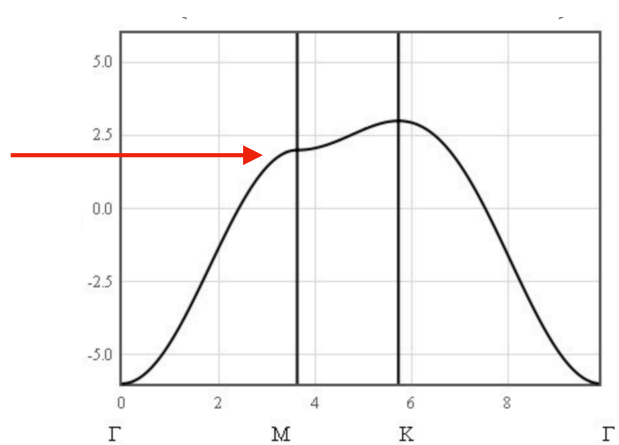
FS corners are located at M points

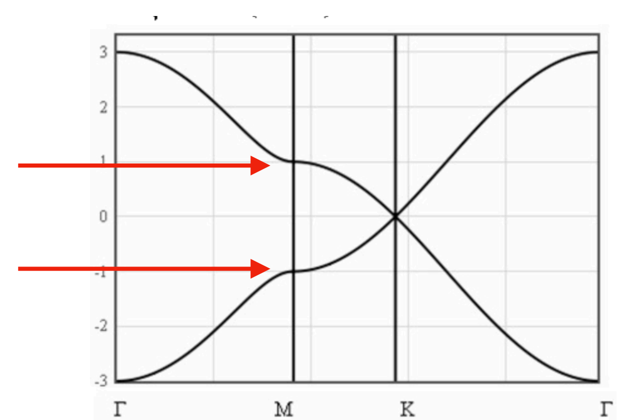
Saddle points



M-point saddles are very common in hexagonal systems

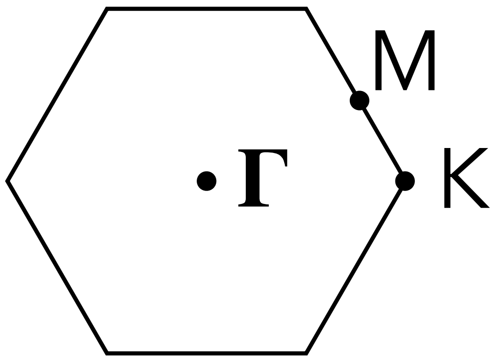
saddle points





Saddle points

Why?



M point is always a critical point:

$$\boldsymbol{\nabla}\epsilon(\boldsymbol{k})|_{\boldsymbol{k}=M} = 0$$

Morse theory: for a "sufficiently smooth" function on a closed 2d manifold

$$n_{\max} - n_{\rm sp} + n_{\min} = \chi_E$$ = 0 for torus

2 - 3 + 1 = 0
(K) (M) ($\mathbf{\Gamma}$)

Square lattice

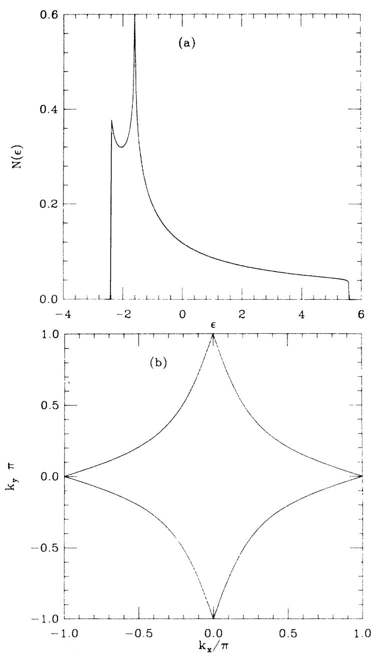
Enhanced superconductivity

VOLUME 56, NUMBER 25 PHYSICAL REVIEW LETTERS 23 JUNE 1986

Enhanced Superconductivity in Quasi Two-Dimensional Systems

J. E. Hirsch
Department of Physics, University of California, San Diego, La Jolla, California 92093
and
D. J. Scalapino
Department of Physics, University of California, Santa Barbara, Santa Barbara, California 93106
(Received 11 September 1985)

We show that the tendency for superconductivity of a weakly coupled 2D electron system can be significantly enhanced if the Fermi energy is close to a logarithmic Van Hove singularity in the density of states. Using results from perturbation theory, supported by quantum Monte Carlo simulations, we calculate T_c and explore the effects of the quasiparticle lifetime and higher-order interactions on this enhancement. This mechanism suggests possible new directions in the search for 2D excitonic superconductivity.



...

$$P_0(q)=\frac{1}{N}\sum\frac{1-f(\epsilon_{p+q})-f(\epsilon_p)}{\epsilon_{p+q}+\epsilon_p}.$$

$$P_0=A\ln^2(t/T)+B\ln(t/T)+C,$$

Renormalization Group (RG)

describes competition of SC with antiferromagnetism

Superconductivity and Antiferromagnetism in the Two-Dimensional Hubbard Model: Scaling Theory.

H. J. SCHULZ
Laboratoire de Physique des Solides, Université Paris-Sud - 91405 Orsay, France

(received 16 June 1987; accepted 14 July 1987)

Antiferromagnetism and superconductivity in a quasi two-dimensional electron gas. Scaling theory of a generic Hubbard model

P. Lederer+, G. Montambaux++ and D. Poilblanc+++

Laboratoire de Physique des Solides*, Bât. 510, Université Paris-Sud, Centre d'Orsay, 91405 Orsay Cedex, France

(Reçu le 8 juillet 1987, accepté le 27 juillet 1987)

$$\left.\begin{aligned} G_1' &= 2G_1\left(G_4-G_1\right)l_o \\ G_2' &= -2\left(G_2^2+G_3^2\right)l \\ G_3' &= -4G_2G_3l+2G_3\left(2G_4-G_1\right)l_o \\ G_4' &= \left(G_3^2+G_4^2\right)l_o \end{aligned}\right\} \quad (7)$$

Square lattice

Enhanced superconductivity

VOLUME 56, NUMBER 25 PHYSICAL REVIEW LETTERS 23 JUNE 1986

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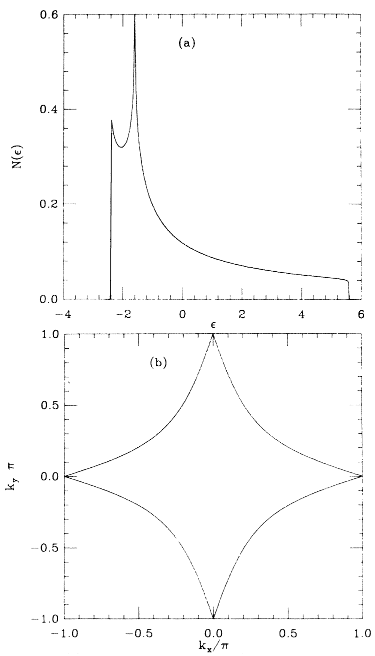


$$P_0(q) = \frac{1}{N}\sum \frac{1-f(\epsilon_{p+q})-f(\epsilon_p)}{\epsilon_{p+q}+\epsilon_p}.$$

$$P_0 = A\ln^2(t/T) + B\ln(t/T) + C,$$

Renormalization Group (RG)

VOLUME 81, NUMBER 15 PHYSICAL REVIEW LETTERS 12 OCTOBER 1998

Truncation of a Two-Dimensional Fermi Surface due to Quasiparticle Gap Formation at the Saddle Points

Nobuo Furukawa* and T. M. Rice
Institute for Theoretical Physics, ETH-Hönggerberg, CH-8093 Zurich, Switzerland
Manfred Salmhofer
Mathematik, ETH Zentrum, CH-8092 Zürich, Switzerland
(Received 12 June 1998)

$$\dot{g}_1 = 2d_1 g_1(g_2 - g_1) + 2d_2 g_1 g_4 - 2d_3 g_1 g_2, \quad (4)$$

$$\dot{g}_2 = d_1(g_2^2 + g_3^2) + 2d_2(g_1 - g_2)g_4 - d_3(g_1^2 + g_2^2), \quad (5)$$

$$\dot{g}_3 = -2g_3 g_4 + 2d_1 g_3(2g_2 - g_1), \quad (6)$$

$$\dot{g}_4 = -(g_3^2 + g_4^2) + d_2(g_1^2 + 2g_1 g_2 - 2g_2^2 + g_4^2). \quad (7)$$

Here, we introduced the normalization $g_i \to h g_i$, to give dimensionless couplings, and $\dot{g}_i \equiv (dg_i)/(dy)$, where $y \equiv \ln^2(\omega/E_0) \propto \chi_0^{\mathrm{pp}}(\omega)$. We define functions which de-

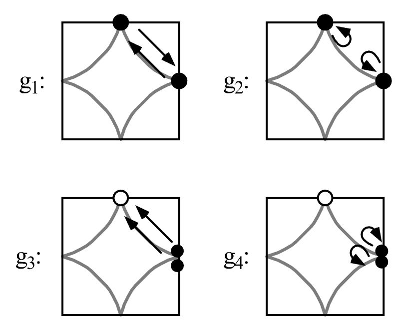


FIG. 2. The definitions of vertices for the two-patch model.

Hexagonal systems

PRL **101,** 156402 (2008) PHYSICAL REVIEW LETTERS week ending 10 OCTOBER 2008

Itinerant Electron-Driven Chiral Magnetic Ordering and Spontaneous Quantum Hall Effect in Triangular Lattice Models

Ivar Martin and C. D. Batista
Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA
(Received 24 July 2008; published 9 October 2008)

instabilities driven by saddle points:
3Q spin density wave

ARTICLES
PUBLISHED ONLINE: 22 JANUARY 2012 | DOI: 10.1038/NPHYS2208
nature physics

Chiral superconductivity from repulsive interactions in doped graphene

Rahul Nandkishore[1], L. S. Levitov[1] and A. V. Chubukov[2]*

PHYSICAL REVIEW B **86**, 115426 (2012)

Interplay of superconductivity and spin-density-wave order in doped graphene

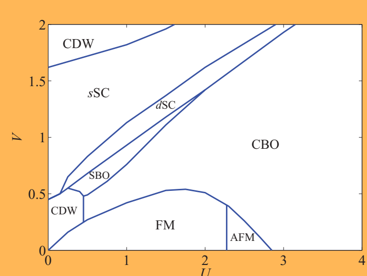
Rahul Nandkishore[1,2] and Andrey V. Chubukov[3]
[1]*Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*
[2]*Princeton Center for Theoretical Science, Princeton University, Princeton, NJ 08540, USA*
[3]*Department of Physics, University of Wisconsin-Madison, Madison, Wisconsin 53706, USA*
(Received 24 July 2012; published 19 September 2012)

RG analysis:
d+id and spin density wave on honeycomb lattice

PHYSICAL REVIEW B **87**, 115135 (2013)

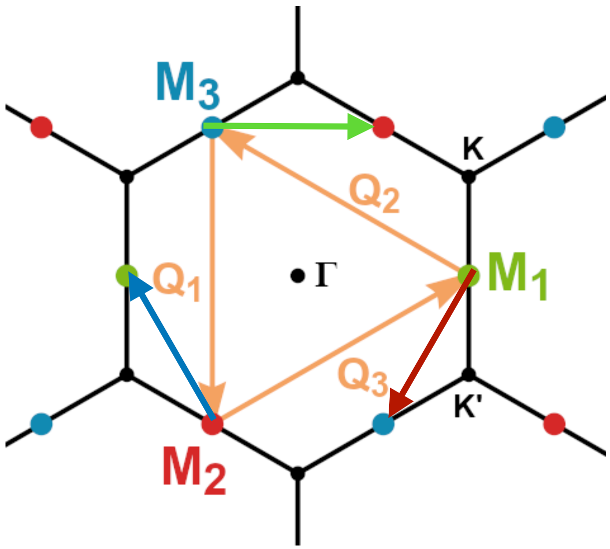
Competing electronic orders on kagome lattices at van Hove filling

Wan-Sheng Wang, Zheng-Zhao Li, Yuan-Yuan Xiang, and Qiang-Hua Wang
National Laboratory of Solid State Microstructures, Nanjing University, Nanjing, 210093, China
(Received 4 September 2012; published 25 March 2013)



functional RG analysis of single orbital model:
CDW and SC orderings

M-point orders



M_1=M_2-M_3 etc.
(up to RLVs)

these are the CDW wavevectors in experiment

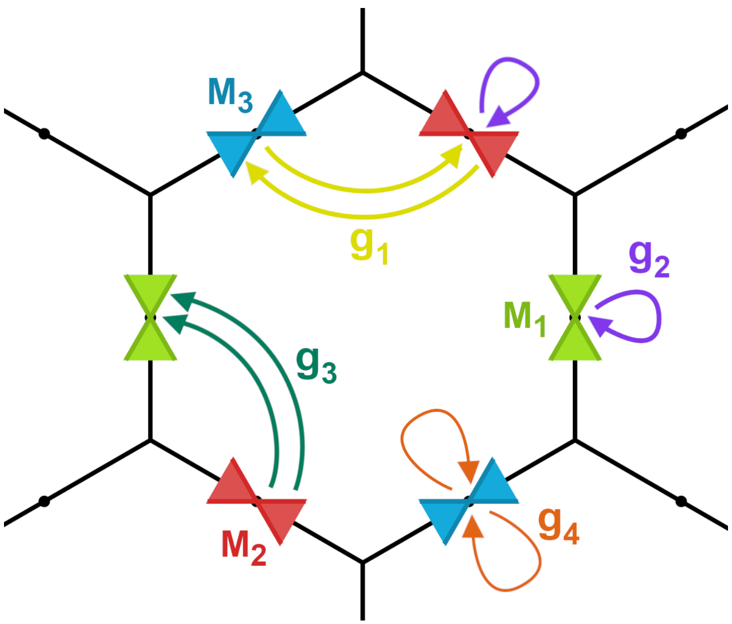
Order parameters:

- particle/hole: $c^{\dagger}_{a\sigma}c_{b\sigma'}$
- particle-particle: $c_{a\sigma}c_{b\sigma'}$

OP	Definition
rCDW	$N_\alpha = G_{\mathrm{rCDW}} \frac{\lvert\epsilon_{\alpha\beta\gamma}\rvert}{2\mathcal{N}} \sum_{\boldsymbol{q}} \left\langle c^{\dagger}_{\beta\boldsymbol{q}} c_{\gamma\boldsymbol{q}} \right\rangle$
iCDW	$\phi_\alpha = G_{\mathrm{iCDW}} \frac{\epsilon_{\alpha\beta\gamma}}{2i\mathcal{N}} \sum_{\boldsymbol{q}} \left\langle c^{\dagger}_{\beta\boldsymbol{q}} c_{\gamma\boldsymbol{q}} \right\rangle$
rSDW	$\boldsymbol{S}_\alpha = G_{\mathrm{rSDW}} \frac{\lvert\epsilon_{\alpha\beta\gamma}\rvert}{2\mathcal{N}} \sum_{\boldsymbol{q}} \left\langle c^{\dagger}_{\beta\boldsymbol{q}} \frac{\boldsymbol{\sigma}}{2} c_{\gamma\boldsymbol{q}} \right\rangle$
iSDW	$\boldsymbol{\psi}_\alpha = G_{\mathrm{iSDW}} \frac{\epsilon_{\alpha\beta\gamma}}{2i\mathcal{N}} \sum_{\boldsymbol{q}} \left\langle c^{\dagger}_{\beta\boldsymbol{q}} \frac{\boldsymbol{\sigma}}{2} c_{\gamma\boldsymbol{q}} \right\rangle$
sSC	$\Delta_s = G_{\mathrm{sSC}} \frac{1}{\sqrt{3}\mathcal{N}} \sum_{\boldsymbol{q}} \langle c_{\alpha\boldsymbol{q}\downarrow} c_{\alpha-\boldsymbol{q}\uparrow} \rangle$
dSC	$\Delta_{xy} = G_{\mathrm{dSC}} \frac{1}{\mathcal{N}} \times \sum_{\boldsymbol{q}} \langle c_{\boldsymbol{q}\downarrow} D_{xy} c_{-\boldsymbol{q}\uparrow} \rangle$ $\Delta_{x^2-y^2} = G_{\mathrm{dSC}} \frac{1}{\mathcal{N}} \times \sum_{\boldsymbol{q}} \langle c_{\boldsymbol{q}\downarrow} D_{x^2-y^2} c_{-\boldsymbol{q}\uparrow} \rangle$

M-point RG

Saddle point RG: determines behavior for very weak interactions, such that log² is dominant even over log



$$y = \Pi_{pp}(0, E) \sim \ln^2(\Lambda/E)$$

inter-valley exchange $\frac{\mathrm{d}g_1}{\mathrm{d}y} = 2d_1 g_1(g_2 - g_1),$

inter-valley density $\frac{\mathrm{d}g_2}{\mathrm{d}y} = d_1(g_2^2 + g_3^2),$

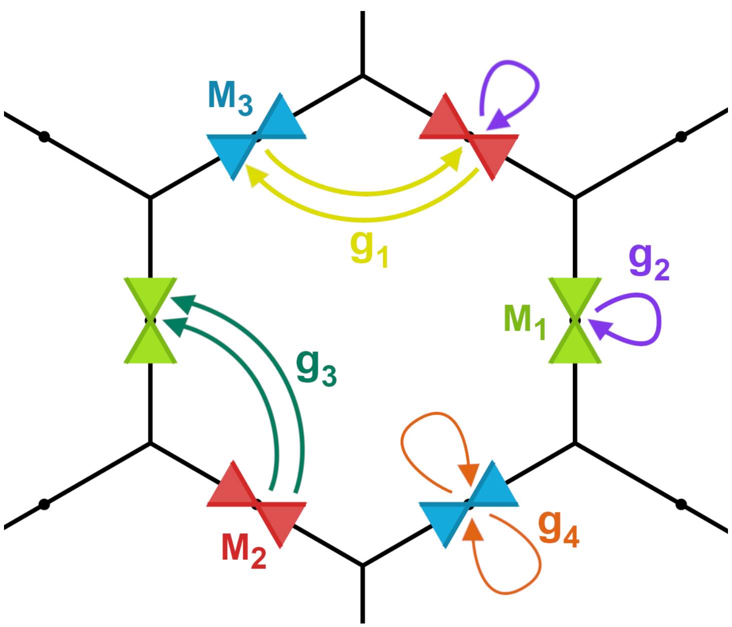
umklapp $\frac{\mathrm{d}g_3}{\mathrm{d}y} = -g_3^2 - 2g_3 g_4 + 2d_1 g_3(2g_2 - g_1),$

intra-valley $\frac{\mathrm{d}g_4}{\mathrm{d}y} = -2g_3^2 - g_4^2,$

- Sign of g_1 preserved: $g_1>0$ favors singlet/charge while $g_1<0$ favors triplet/spin
- Sign of g_3 preserved: $g_3>0$ prefers imaginary density wave while $g_3<0$ favors real density wave

M-point RG

Saddle point RG: determines behavior for very weak interactions, such that log² is dominant even over log



$$y = \Pi_{pp}(0, E) \sim \ln^2(\Lambda/E)$$

inter-valley exchange $\frac{\mathrm{d}g_1}{\mathrm{d}y} = 2d_1 g_1(g_2 - g_1),$

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umklapp $\frac{\mathrm{d}g_3}{\mathrm{d}y} = -g_3^2 - 2g_3 g_4 + 2d_1 g_3(2g_2 - g_1),$

intra-valley $\frac{\mathrm{d}g_4}{\mathrm{d}y} = -2g_3^2 - g_4^2,$

PHYSICAL REVIEW B VOLUME 53, NUMBER 18 1 MAY 1996-II

Weak-coupling phase diagram of the two-chain Hubbard model

Leon Balents and Matthew P. A. Fisher

Institute for Theoretical Physics, University of California, Santa Barbara, California 93106-4030

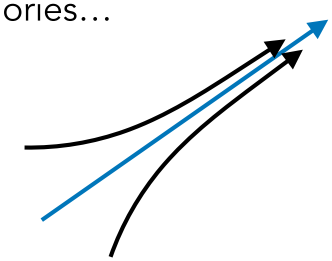
(Received 30 August 1995; revised manuscript received 9 November 1995)

memories…

Analysis:

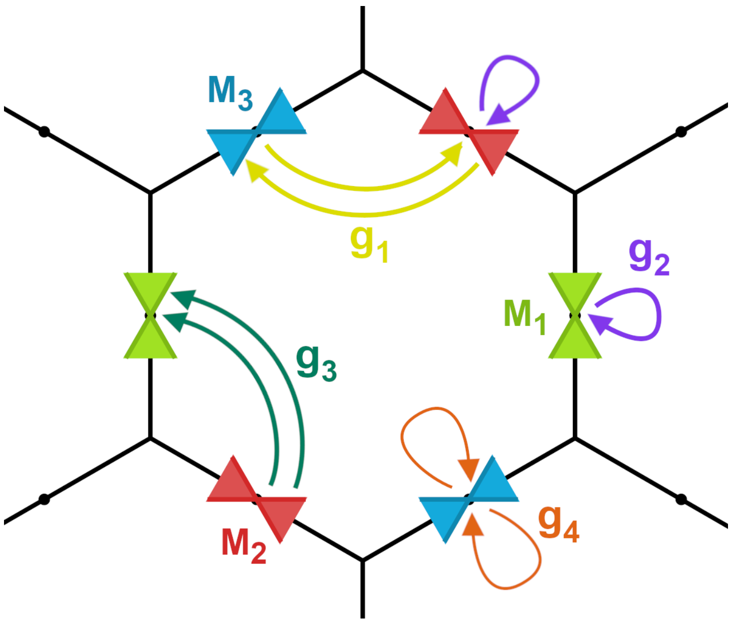
- 4 instability pathways

$$g_i \sim \frac{G_i}{y_c - y}$$

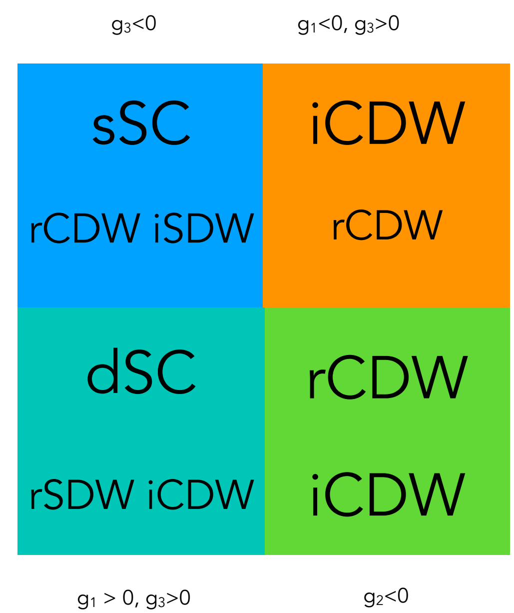


M-point RG

Saddle point RG: determines behavior for very weak interactions, such that $\log^2$ is dominant even over log



OP	Definition	Interaction strength (G)
rCDW	$N_\alpha = G_{\text{rCDW}} \frac{\lvert\epsilon_{\alpha\beta\gamma}\rvert}{2\mathcal{N}} \sum_{\boldsymbol{q}} \left\langle c^\dagger_{\beta\boldsymbol{q}} c_{\gamma\boldsymbol{q}} \right\rangle$	$-2g_1 + g_2 - g_3$
iCDW	$\phi_\alpha = G_{\text{iCDW}} \frac{\epsilon_{\alpha\beta\gamma}}{2i\mathcal{N}} \sum_{\boldsymbol{q}} \left\langle c^\dagger_{\beta\boldsymbol{q}} c_{\gamma\boldsymbol{q}} \right\rangle$	$-2g_1 + g_2 + g_3$
rSDW	$\boldsymbol{S}_\alpha = G_{\text{rSDW}} \frac{\lvert\epsilon_{\alpha\beta\gamma}\rvert}{2\mathcal{N}} \sum_{\boldsymbol{q}} \left\langle c^\dagger_{\beta\boldsymbol{q}} \frac{\boldsymbol{\sigma}}{2} c_{\gamma\boldsymbol{q}} \right\rangle$	$g_2 + g_3$
iSDW	$\boldsymbol{\psi}_\alpha = G_{\text{iSDW}} \frac{\epsilon_{\alpha\beta\gamma}}{2i\mathcal{N}} \sum_{\boldsymbol{q}} \left\langle c^\dagger_{\beta\boldsymbol{q}} \frac{\boldsymbol{\sigma}}{2} c_{\gamma\boldsymbol{q}} \right\rangle$	$g_2 - g_3$
sSC	$\Delta_s = G_{\text{sSC}} \frac{1}{\sqrt{3}\mathcal{N}} \sum_{\boldsymbol{q}} \langle c_{\alpha\boldsymbol{q}\downarrow} c_{\alpha-\boldsymbol{q}\uparrow} \rangle$	$-2g_3 - g_4$
dSC	$\Delta_{xy} = G_{\text{dSC}} \frac{1}{\mathcal{N}} \times \sum_{\boldsymbol{q}} \langle c_{\boldsymbol{q}\downarrow} D_{xy} c_{-\boldsymbol{q}\uparrow} \rangle$ $\Delta_{x^2-y^2} = G_{\text{dSC}} \frac{1}{\mathcal{N}} \times \sum_{\boldsymbol{q}} \langle c_{\boldsymbol{q}\downarrow} D_{x^2-y^2} c_{-\boldsymbol{q}\uparrow} \rangle$	$g_3 - g_4$



Analysis:

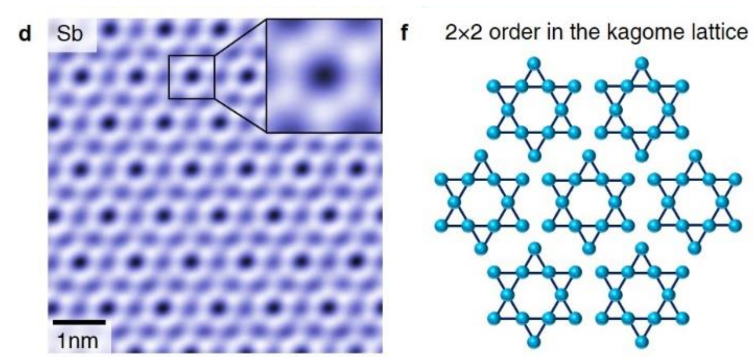
- 4 instability pathways

if bare couplings are comparable, larger order dominates

Density waves

Return to experiment: what can we say about density wave orders?

sSC rCDW iSDW	iCDW rCDW
dSC rSDW iCDW	rCDW iCDW



rCDW order

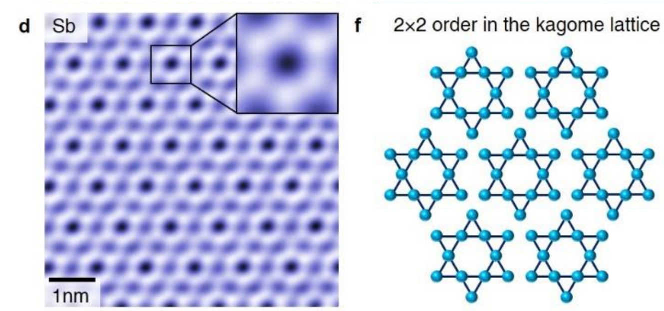
- Several possible order parameters with the observed in-plane periodicity of charge modulation
- Is rCDW the primary order? Or could this be due to other iCDW,rSDW orders?

rCDW

General plan: apply Landau/symmetry analysis

$$N_1 \sim \langle c_{2\sigma}^\dagger c_{3\sigma} \rangle = \langle c_{3\sigma}^\dagger c_{2\sigma} \rangle$$

+ cyclic permutations



invariant under time-reversal

point group symmetries ~ tetrahedral T_d

$$f_{\mathrm{rCDW}} = \left(\frac{1}{2G_{\mathrm{rCDW}}} + K_1 \right) \sum_\alpha N_\alpha^2 + K_2 N_1 N_2 N_3$$
$$+ K_4 \left(\sum_\alpha N_\alpha^2 \right)^2 + (K_3 - 2K_4) \sum_{\alpha<\beta} N_\alpha^2 N_\beta^2 + \mathcal{O}(N^5)$$

cubic term: dominant near T_c and generically fixes 3Q order

$$K_2 \approx -\frac{16}{\pi^2 t \Lambda^2 k_B T} H_2(\mu/k_B T),$$

$$K_3 \approx \frac{8}{3\pi^2 \Lambda^2 (k_B T)^2} H_3(\mu/k_B T), \qquad \text{(D9)}$$

$$K_4 \approx \frac{1}{12\sqrt{3}\pi^2 t \Lambda^2 (k_B T)^2} H_4(\mu/k_B T) \ln\left(t\Lambda^2/k_B T\right), \qquad \text{(D10)}$$

$$H_2(z) = \int_0^\infty \mathrm{d}x \int_0^{x/\sqrt{3}} \mathrm{d}y \Bigg(\frac{F(\tilde\varepsilon_1(x,y)-z)}{(\tilde\varepsilon_1(x,y)-\tilde\varepsilon_2(x,y))(\tilde\varepsilon_1(x,y)-\tilde\varepsilon_3(x,y))} - \frac{F(\tilde\varepsilon_2(x,y)-z)}{(\tilde\varepsilon_1(x,y)-\tilde\varepsilon_2(x,y))(\tilde\varepsilon_2(x,y)-\tilde\varepsilon_3(x,y))} + \frac{F(\tilde\varepsilon_3(x,y)-z)}{(\tilde\varepsilon_1(x,y)-\tilde\varepsilon_3(x,y))(\tilde\varepsilon_2(x,y)-\tilde\varepsilon_3(x,y))} \Bigg),$$

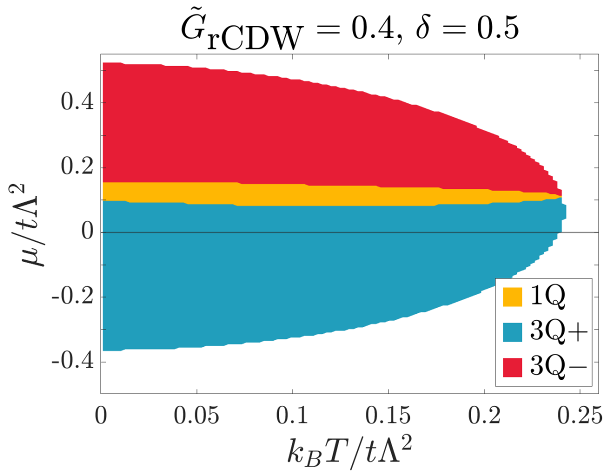
$$H_3(z) = \int_0^\infty \mathrm{d}x \int_0^{x/\sqrt{3}} \mathrm{d}y \Bigg(\frac{F'(\tilde\varepsilon_1(x,y)-z)}{(\tilde\varepsilon_1(x,y)-\tilde\varepsilon_2(x,y))(\tilde\varepsilon_1(x,y)-\tilde\varepsilon_3(x,y))} - \frac{F'(\tilde\varepsilon_2(x,y)-z)}{(\tilde\varepsilon_1(x,y)-\tilde\varepsilon_2(x,y))(\tilde\varepsilon_2(x,y)-\tilde\varepsilon_3(x,y))} + \frac{F'(\tilde\varepsilon_3(x,y)-z)}{(\tilde\varepsilon_1(x,y)-\tilde\varepsilon_3(x,y))(\tilde\varepsilon_2(x,y)-\tilde\varepsilon_3(x,y))} \Bigg),$$

$$H_4(z) = \int_0^\infty \mathrm{d}v \left(\frac{-F(v-z)+F(-v-z)}{v^3} + \frac{F'(v-z)+F'(-v-z)}{z^2} \right).$$

sorry Taka…

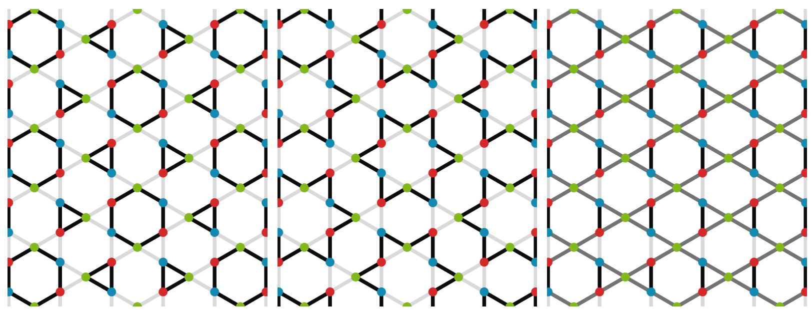
rCDW

Can also analyze via microscopic MFT w/o Landau expansion



generic example:
3Q order dominates, with
1Q CDW intervening

1st order transition in MFT



primarily bond order (due to compatibility irrep of M_a points with site irreps)

iCDW*

Time-reversal odd $\phi_a \sim i\epsilon_{abc}\langle c^\dagger_{a\sigma} c_{b\sigma}\rangle$

Discovery of topological charge order in kagome superconductor KV_3Sb_5

Authors: Yu-Xiao Jiang[1]*, Jia-Xin Yin[1]*†, M. Michael Denner[2]*, Nana Shumiya[1]*, Brenden R. Ortiz[3]*, Junyi He[4], Xiaoxiong Liu[2], Songtian S. Zhang[1], Guoqing Chang[5], Ilya Belopolski[1], Qi Zhang[1], Md Shafayat Hossain[1], Tyler A. Cochran[1], Daniel Multer[1], Maksim Litskevich[1], Zi-Jia Cheng[1], Xian P. Yang[1], Zurab Guguchia[6], Gang Xu[4], Ziqiang Wang[7], Titus Neupert[2], Stephen D. Wilson[3], M. Zahid Hasan[1,8]†

Analysis of charge order in the kagome metal AV_3Sb_5 (A =K,Rb,Cs)

M. Michael Denner,[1] Ronny Thomale,[2,3] and Titus Neupert[1]

[1] *Department of Physics, University of Zurich, Winterthurerstrasse 190, 8057 Zurich, Switzerland*
[2] *Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany*
[3] *Department of Physics, Indian Institute of Technology Madras, Chennai 600036, India*

(Dated: March 29, 2021)

Complex charge density waves at Van Hove singularity on hexagonal lattices: Haldane-model phase diagram and potential realization in kagome metals AV_3Sb_5

Yu-Ping Lin[1] and Rahul M. Nandkishore[1,2]

[1] *Department of Physics, University of Colorado, Boulder, Colorado 80309, USA*
[2] *Center for Theory of Quantum Matter, University of Colorado, Boulder, Colorado 80309, USA*

(Dated: April 21, 2021)

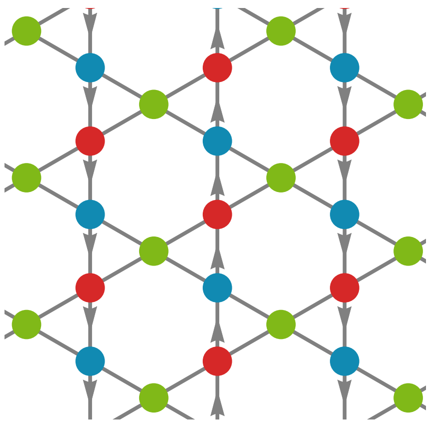
Theorists like it odd

iCDW*

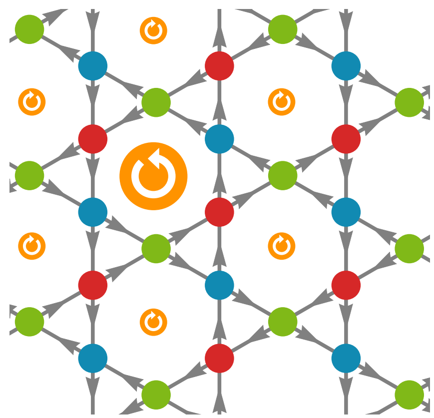
Time-reversal odd $\phi_a \sim i\epsilon_{abc}\langle c^\dagger_{a\sigma} c_{b\sigma}\rangle$

Physics: represents modulated *current* at Q_a

*probably we should not call it a CDW at all. Not our fault!



1Q iCDW



3Q iCDW

circulating orbital moments

macroscopically breaks TR

$\Phi = \phi_1\phi_2\phi_3$ transforms like M_z

iCDW

Does it induce rCDW?

Landau theory: point-group + TR = O_h symmetry

$$
\begin{aligned}
f_{\mathrm{CDW}} &= r_\phi \sum_{\alpha=1}^{3} \phi_\alpha^2 + r_N \sum_{\alpha=1}^{3} N_\alpha^2 \\
&+ K_2 \left(N_1 N_2 N_3 - \phi_2 \phi_3 N_1 - \phi_1 \phi_3 N_2 - \phi_2 \phi_1 N_3\right) \\
&+ K_4 \left(\sum_{\alpha=1}^{3} \phi_\alpha^2 + N_\alpha^2\right)^2 \\
&+ (K_3 - 2K_4) \sum_{\alpha<\beta} (\phi_\alpha^2 + N_\alpha^2)(\phi_\beta^2 + N_\beta^2) + \mathcal{O}(\phi^6, N^5).
\end{aligned}
$$

3Q iCDW induces 3Q rCDW

no cubic term: 3Q and 1Q possible even near T_c

3Q iCDW induces rCDW

Conceivably iCDW order may be "hidden" behind rCDW

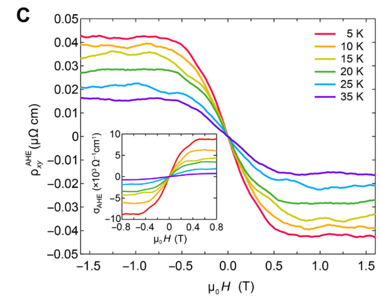
Evidence for TR breaking?

Anomalous Hall Effect

PHYSICS Sci. Adv. 2020

Giant, unconventional anomalous Hall effect in the metallic frustrated magnet candidate, KV_3Sb_5

Shuo-Ying Yang[1]*, Yaojia Wang[1]*, Brenden R. Ortiz[2], Defa Liu[1], Jacob Gayles[3,4], Elena Derunova[1], Rafael Gonzalez-Hernandez[5,6], Libor Šmejkal[6,7,8], Yulin Chen[9], Stuart S. P. Parkin[1], Stephen D. Wilson[2], Eric S. Toberer[10], Tyrel McQueen[11], Mazhar N. Ali[1†]

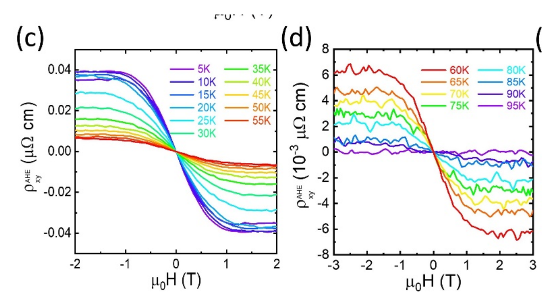


KV_3Sb_5

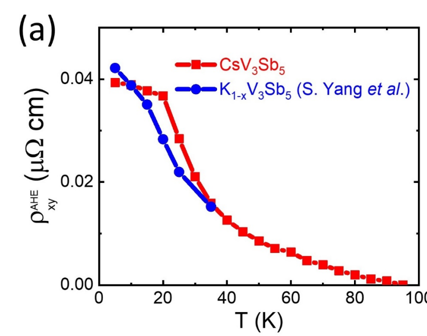
arXiv:2102.10987

Concurrence of anomalous Hall effect and charge density wave in a superconducting topological kagome metal

F. H. Yu[1], T. Wu[1], Z. Y. Wang[1], B. Lei[1], W. Z. Zhuo[1], J. J. Ying[1*], and X. H. Chen[1,2,3†]



CsV_3Sb_5



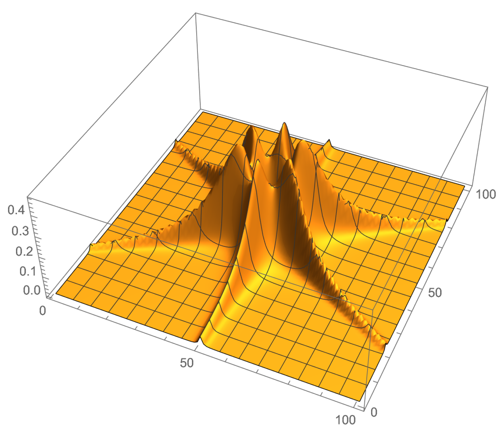
Chern physics?

Nested Fermi surface + iCDW = Chern band

Y-P Lin + R. Nandkishore, 2021 and probably elsewhere?

$$H(\boldsymbol{k}) = \begin{pmatrix} \epsilon_1(\boldsymbol{k}) & i\phi_3 & -i\phi_2 \\ -i\phi_3 & \epsilon_2(\boldsymbol{k}) & i\phi_1 \\ i\phi_2 & -i\phi_1 & \epsilon_3(\boldsymbol{k}) \end{pmatrix}$$

→ Berry curvature and orbital moments peak near avoided crossings



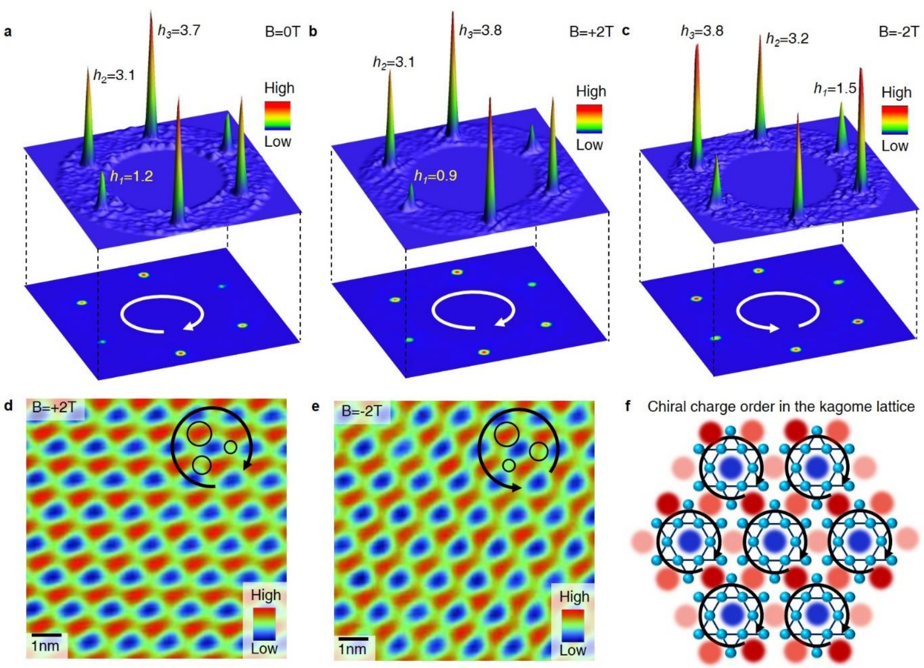
orbital moment is O(1) for electrons within iCDW gap of the M points

Evidence for TR breaking?

STM

Discovery of topological charge order in kagome superconductor KV_3Sb_5 arXiv:2012.15709v2

Authors: Yu-Xiao Jiang[1]*, Jia-Xin Yin[1]*†, M. Michael Denner[2]*, Nana Shumiya[1]*, Brenden R. Ortiz[3]*, Junyi He[4], Xiaoxiong Liu[2], Songtian S. Zhang[1], Guoqing Chang[5], Ilya Belopolski[1], Qi Zhang[1], Md Shafayat Hossain[1], Tyler A. Cochran[1], Daniel Multer[1], Maksim Litskevich[1], Zi-Jia Cheng[1], Xian P. Yang[1], Zurab Guguchia[6], Gang Xu[4], Ziqiang Wang[7], Titus Neupert[2], Stephen D. Wilson[3], M. Zahid Hasan[1,8]†



Claim: "chiral charge order:

- 3Q state has 3 different amplitudes $N_a > N_b > N_c$
- Order is switched by applied field

Comments:

- First statement not related to TR
- Peak heights are approximately 2-fold symmetric: 2 large and 1 small
- Any change in charge order odd in field and achieved with such small fields is remarkable!

rSDW

$\boldsymbol{S}_a \sim c^\dagger_{b\alpha}\boldsymbol{\sigma}_{\alpha\beta}c_{c\beta}$ Generally breaks TR

This is the favored DW for purely repulsive interactions

Landau theory

$$f_{\text{rSDW}} = \left(\frac{1}{2G_{\text{rSDW}}} + \frac{K_1}{4}\right)\sum_\alpha |\boldsymbol{S}_\alpha|^2 + \frac{K_2}{4}\left(N_1\boldsymbol{S}_2\cdot\boldsymbol{S}_3 + N_2\boldsymbol{S}_3\cdot\boldsymbol{S}_1 + N_3\boldsymbol{S}_1\cdot\boldsymbol{S}_2\right) + \frac{K_3}{16}\sum_{\alpha<\beta}|\boldsymbol{S}_\alpha|^2|\boldsymbol{S}_\beta|^2 + \frac{K_4}{16}\sum_\alpha|\boldsymbol{S}_\alpha|^4 + + K_5\sum_{\alpha<\beta}|\boldsymbol{S}_\alpha\cdot\boldsymbol{S}_\beta|^2 + K_6\left(\boldsymbol{S}_1\cdot\boldsymbol{S}_2\times\boldsymbol{S}_3\right)^2 + \cdots$$

rSDW can induce 3Q rCDW

Collinear 3Q SDW: $\boldsymbol{S}_a = \boldsymbol{S}$ — generates 3Q rCDW but no Berry curvature

Tetrahedral 3Q state: $\boldsymbol{S}_a = S\hat{\boldsymbol{x}}_a$ — does not induce rCDW but has Berry curvature

I. Martin + C. Batista, 2008

So to summarize

Observed rCDW order could be primary or induced by iCDW or rSDW. How do we differentiate?

- Measure spontaneous local moments in iCDW/rSDW — moments may be tiny
- Measure macroscopic TR breaking in iCDW state — may be spoiled by domains
- Simpler tests arise from 3d effects. These tests can already be compared to existing experiments and favor primary rCDW order

3d order

Assumption: inter-layer coupling is weak compared to intra-layer interactions, and generally decays with distance in c direction

Inter-layer free energy:

rapidly decreasing with δ

$$f_\perp = \sum_{z=0}^{\infty} \sum_{\delta=1}^{\infty} \left(K_{\perp,\delta} N_{a,z} N_{a,z+\delta} + L_{\perp,\delta} \phi_{a,z} \phi_{a,z+\delta} + J_{\perp,\delta} \boldsymbol{S}_{a,z} \cdot \boldsymbol{S}_{a,z+\delta} \right)$$

3d order

Assumption: inter-layer coupling is weak compared to intra-layer interactions, and generally decays with distance in c direction

rapidly decreasing with δ

Inter-layer free energy:

$$f_\perp = \sum_{z=0}^{\infty} \sum_{\delta=1}^{\infty} \left(K_{\perp,\delta} N_{a,z} N_{a,z+\delta} + L_{\perp,\delta} \phi_{a,z} \phi_{a,z+\delta} + J_{\perp,\delta} \boldsymbol{S}_{a,z} \cdot \boldsymbol{S}_{a,z+\delta} \right)$$

$$\phi_{a,z} = \pm \phi_{a,z+1} \qquad \boldsymbol{S}_{a,z} = \pm \boldsymbol{S}_{a,z+1}$$

This is allowed because of TR.

Primary iCDW/rSDW order has k_z=0,½

***Induced* rCDW ~ (ϕ/S)^2 order has k_z=0**

3d order

Assumption: inter-layer coupling is weak compared to intra-layer interactions, and generally decays with distance in c direction

Inter-layer free energy:

rapidly decreasing with δ

$$f_\perp = \sum_{z=0}^{\infty}\sum_{\delta=1}^{\infty}\left(K_{\perp,\delta}N_{a,z}N_{a,z+\delta} + L_{\perp,\delta}\phi_{a,z}\phi_{a,z+\delta} + J_{\perp,\delta}\boldsymbol{S}_{a,z}\cdot\boldsymbol{S}_{a,z+\delta}\right)$$

If $K_{\perp,1}>0$, want $N_{a,z}=-N_{a,z+1}$ *but this cannot be satisfied*

Single-layer minima have $N_1N_2N_3$ fixed (= +1 for example)

Inter-layer correlation forces only $N_{a,z} \neq N_{a,z+1}$ for some a.

3d order

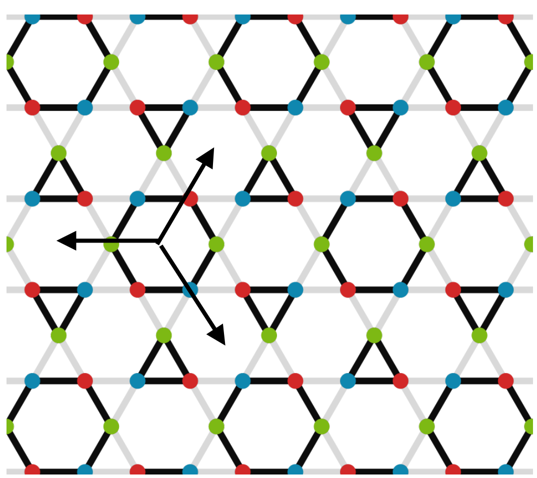
Assumption: inter-layer coupling is weak compared to intra-layer interactions, and generally decays with distance in c direction

rapidly decreasing with δ

Inter-layer free energy:

$$f_\perp = \sum_{z=0}^{\infty}\sum_{\delta=1}^{\infty}\left(K_{\perp,\delta}N_{a,z}N_{a,z+\delta} + L_{\perp,\delta}\phi_{a,z}\phi_{a,z+\delta} + J_{\perp,\delta}\boldsymbol{S}_{a,z}\cdot\boldsymbol{S}_{a,z+\delta}\right)$$

inter-layer displacement in 3 possible directions



3d order

Mapping to Potts model:

$$(111), (1\bar{1}\bar{1}), (\bar{1}1\bar{1}), (\bar{1}\bar{1}1) \to \sigma = 1, 2, 3, 4$$

1d Potts chain

$$f_\perp = \sum_{z=0}^{\infty} \sum_{\delta=1}^{\infty} K_{\perp,\delta} N_0^2 \left(4\delta_{\sigma_z, \sigma_{z+\delta}} - 1\right)$$

generally has complex even aperiodic ground states

When $|K_{\perp,1}| \gg |K_{\perp,2}| \gg |K_{\perp,3}| \cdots$

can show that ground states have k_z=0,½,⅓,¼

3d order

Upshot: iCDW and rSDW should have k_z=0 rCDW order

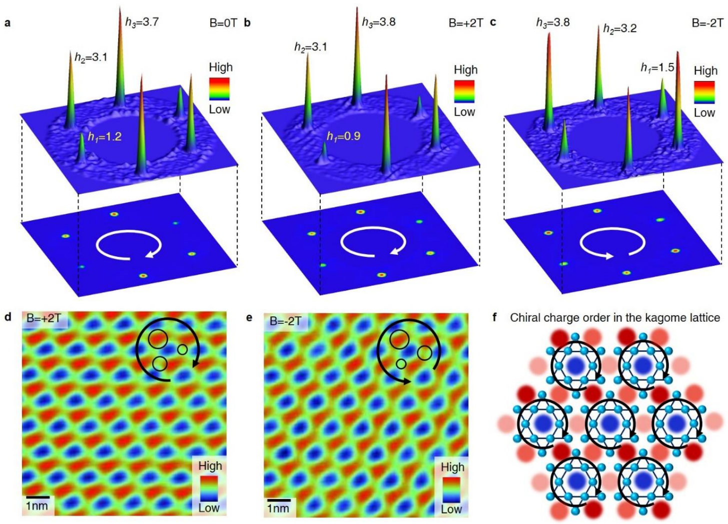
Experiments (x-rays):

A	k_z
Cs	¼
K	½
Rb	½

consistent with primary rCDW

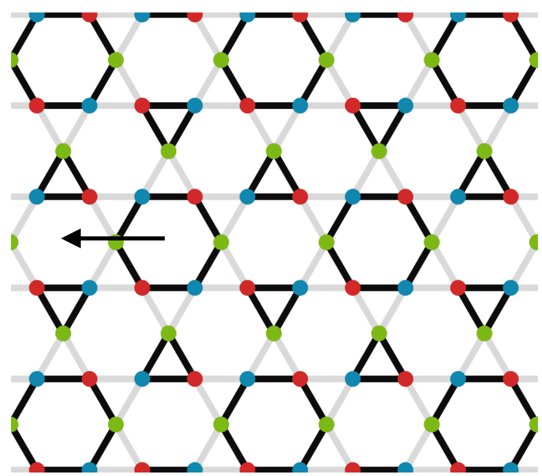
Chiral charge order?

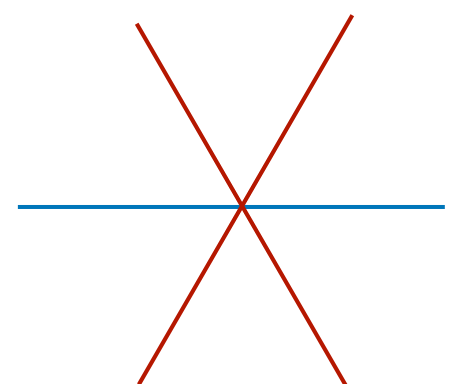
arXiv:2012.15709v2



Does 3d order shed any light?

A: Yes. 3d order breaks rotational symmetry in the top layer

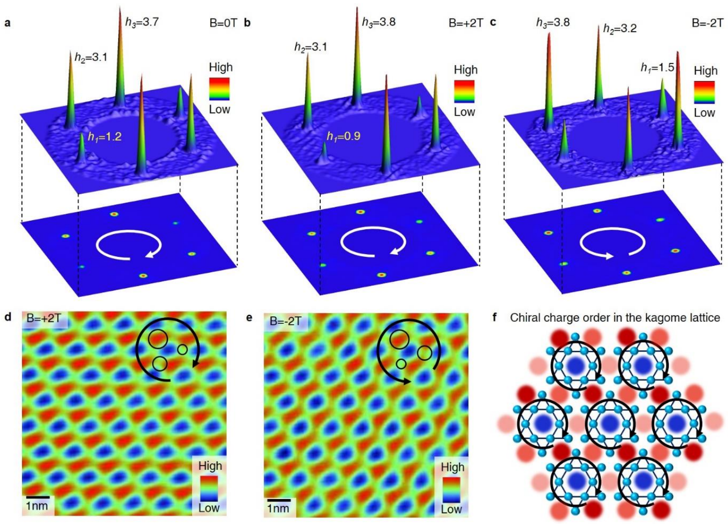




Can show charge peaks split into $|N_a|=|N_b|\neq|N_c|$

Chiral charge order?

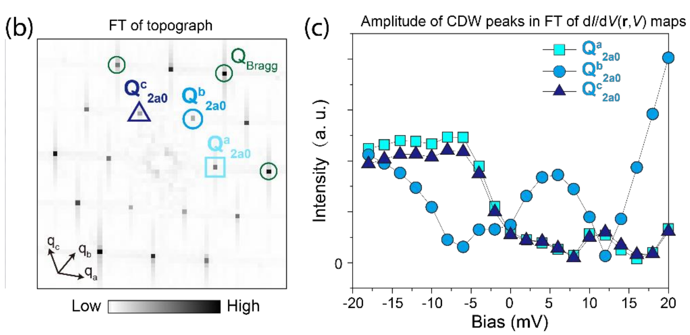
arXiv:2012.15709v2

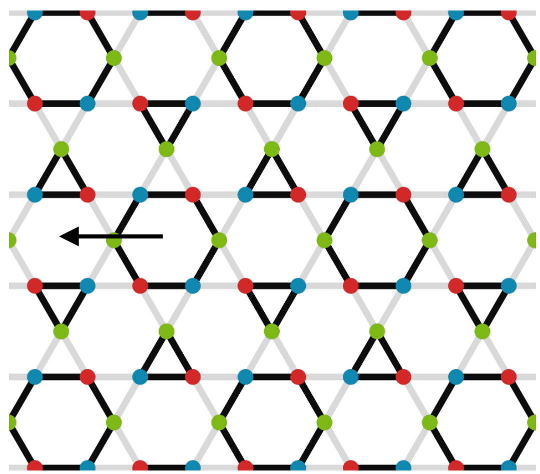


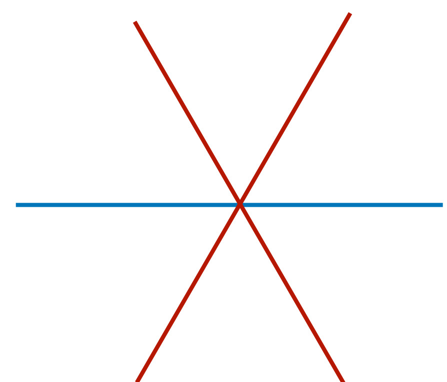
Does 3d order shed any light?

A: Yes. 3d order breaks rotational symmetry in the top layer

arXiv:2104.08209

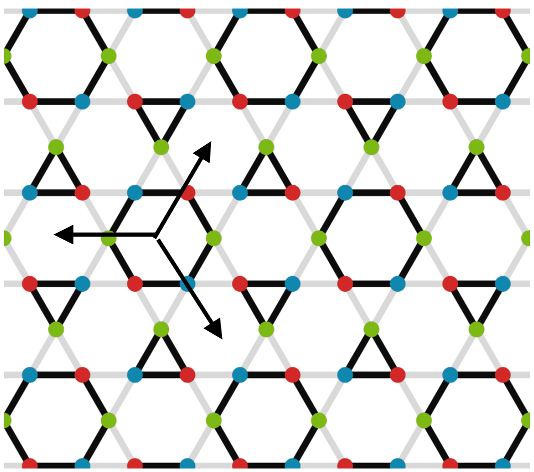






Can show charge peaks split into $|N_a|=|N_b|\neq|N_c|$

Bulk rotational symmetry breaking



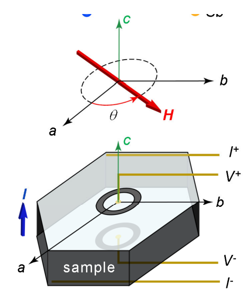
Only way to prevent bulk rotational symmetry breaking is to have a screw axis

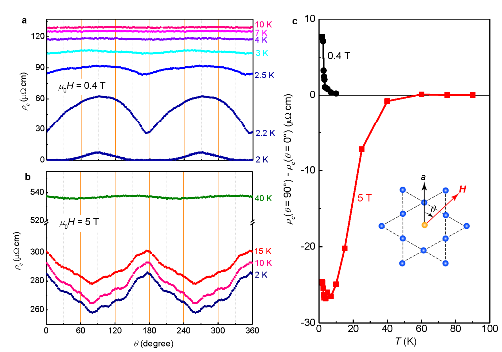
$k_z = 0, \frac{1}{2}, \frac{1}{3}, \frac{1}{4}$

break C_3 symmetry in bulk
(applies to all 3 materials)

Nematic electronic state and twofold symmetry of superconductivity in the topological kagome metal CsV_3Sb_5

Ying Xiang[1†], Qing Li[1†], Yongkai Li[2,3†], Wei Xie[1], Huan Yang[1*], Zhiwei Wang[2,3*], Yugui Yao[2,3], and Hai-Hu Wen[1*]





may not be useful to use "nematicity" as constraint on superconductivity

Explanation for AHE?

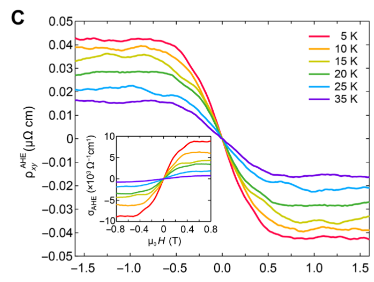
All these aspects seem to strongly support primary rCDW order

And yet…

PHYSICS Sci. Adv. 2020

Giant, unconventional anomalous Hall effect in the metallic frustrated magnet candidate, KV_3Sb_5

Shuo-Ying Yang[1]*, Yaojia Wang[1]*, Brenden R. Ortiz[2], Defa Liu[1], Jacob Gayles[3,4], Elena Derunova[1], Rafael Gonzalez-Hernandez[5,6], Libor Šmejkal[6,7,8], Yulin Chen[9], Stuart S. P. Parkin[1], Stephen D. Wilson[2], Eric S. Toberer[10], Tyrel McQueen[11], Mazhar N. Ali[1]†



KV_3Sb_5

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Concurrence of anomalous Hall effect and charge density wave in a superconducting topological kagome metal

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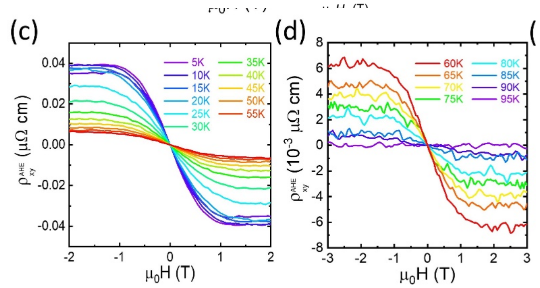
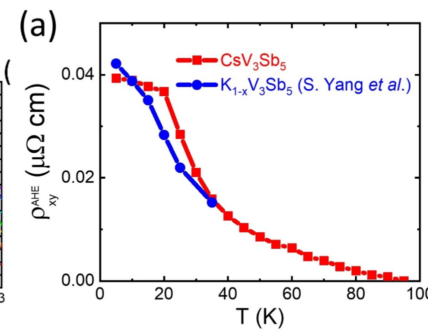
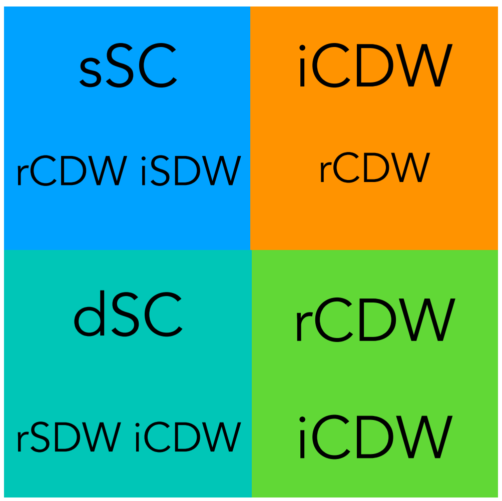




CsV_3Sb_5

- Extraneous origin
- TRS breaking order emerges at $T_c' < T_c$
- TRS breaking induced by applied field

Proximate iCDW order?



iCDW and rCDW
nearly degenerate
(differentiated by
umklapp g_3)

<u>an obviously oversimplified theory</u>

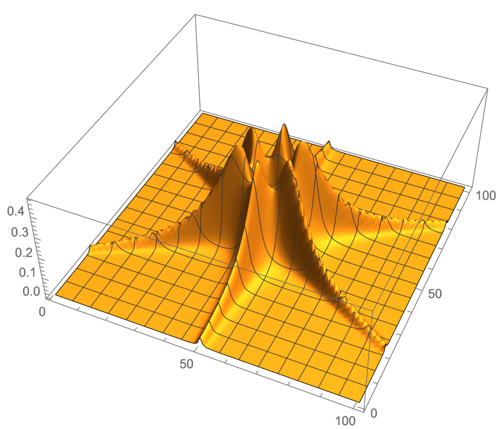
$$\Delta_a = N_a + i\phi_a = |\Delta| e^{i\theta}$$

difference of condensation energies of rCDW and iCDW

$$\mathcal{E} = -m|\Delta|^2 (1 + \lambda \cos\theta) - \mu h m |\Delta| \sin\theta$$

$$\tan\theta = \frac{\mu h}{\lambda |\Delta|}$$

orbital moment in iCDW: gains energy linear in field



Could iCDW may be induced by modest fields?

Summary

- AV_3Sb_5 kagomé metals may realize van Hove scenario of electronic instabilities
- Substantial evidence for primary 3Q real CDW order
- Tantalizing hints of topology and time-reversal symmetry breaking
- Q: is the mechanism for CDW really electronic?
    - We believe e-ph coupling helps to stabilize the CDW. Calculation shows that coupling to M-point optical moes provides suitable attractive channels.
- Q: What does this all imply for superconductivity at lower T?
    - Not clear. Current experimental studies are quite controversial. Presumably a good understanding of the normal state will help.

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