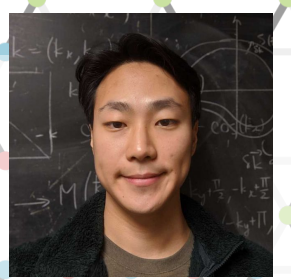
Symmetry breaking orders of kagomé metals

Leon Balents
KITP

Lectiones Amalfitanae April 2022

Collaborators



Takamori Park

Mengxing Ye

Brenden Ortiz

Stephen Wilson

PRB **104,** 035142 (2021)

B.R. Ortiz *et al*, PRL **125**, 247002 (2020)

H. Zhao *et al*, Nature **599** 216 (2021)

H. Li *et al*, Nat. Phys. **18**, 265 (2022).

Y. Xu *et al*, 2022 - unpublished

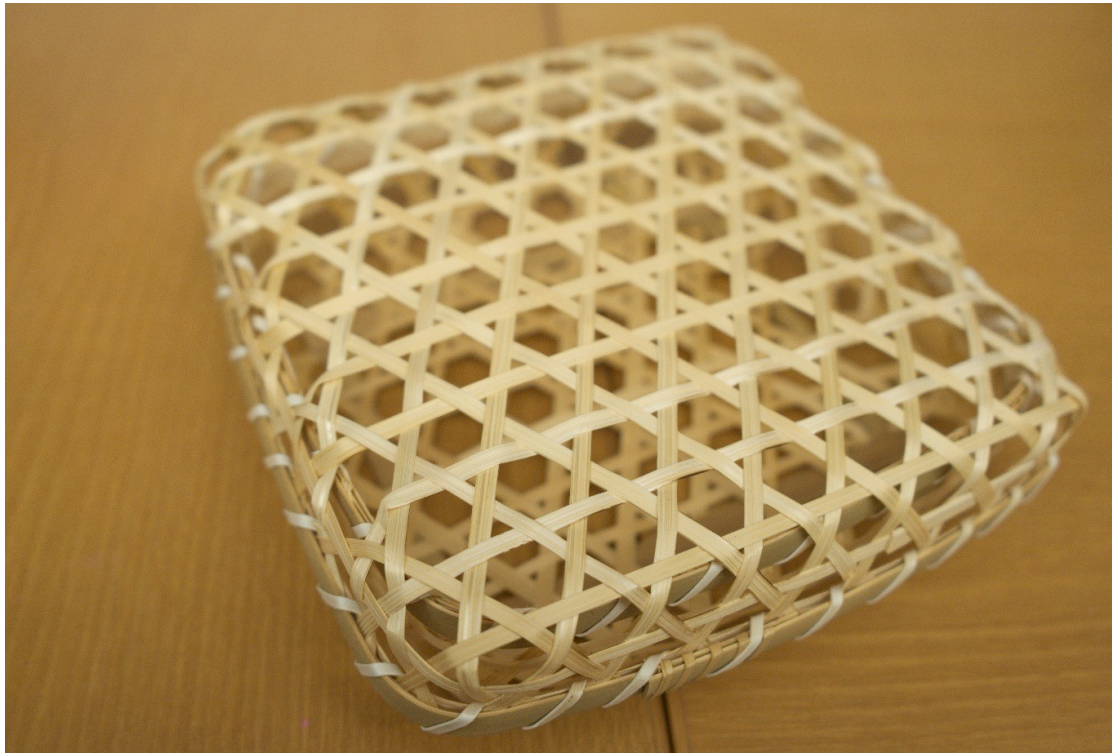
Ilija Zeljkovic, BC

Liang Wu, UPenn

outline

- Introduction: kagomé lattice and flat bands
- AV_3Sb_5 materials
- Competing orders and saddle points
- (Inverse) Occam's razor - a tour of experiments -

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.

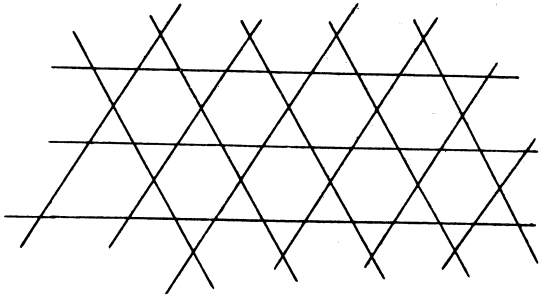
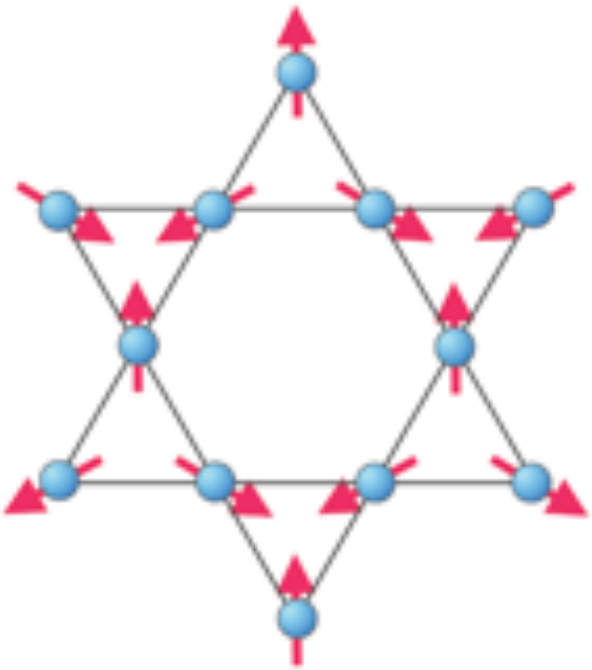


Fig. 1. Kagomé Lattice

Insulating kagomé antiferromagnets



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

likely to be a QSL

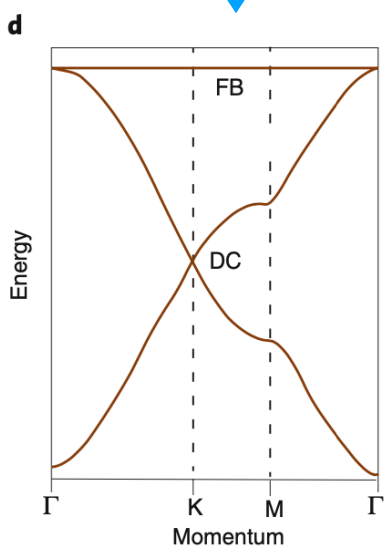
V. Elser, 1989 + many many others

Cu minerals

herbertsmithite
volborthite
kapellasite
barlowite
…

Flat bands

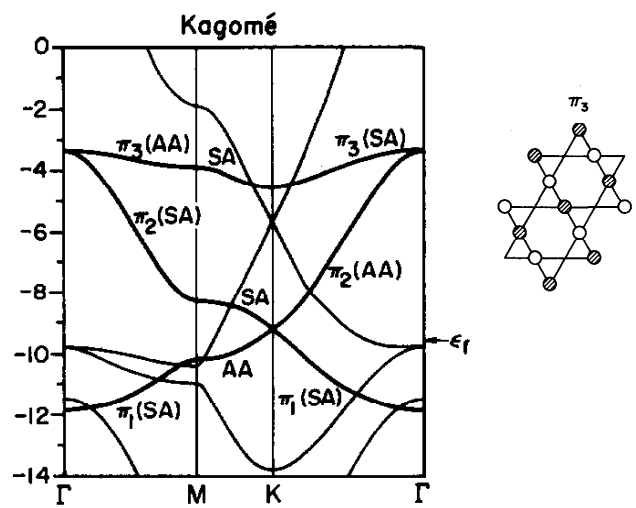
$$H = -t \sum_{\langle ij \rangle} c_i^\dagger c_j + \text{h.c.}$$



THE KAGOMÉ NET: BAND THEORETICAL AND TOPOLOGICAL ASPECTS*

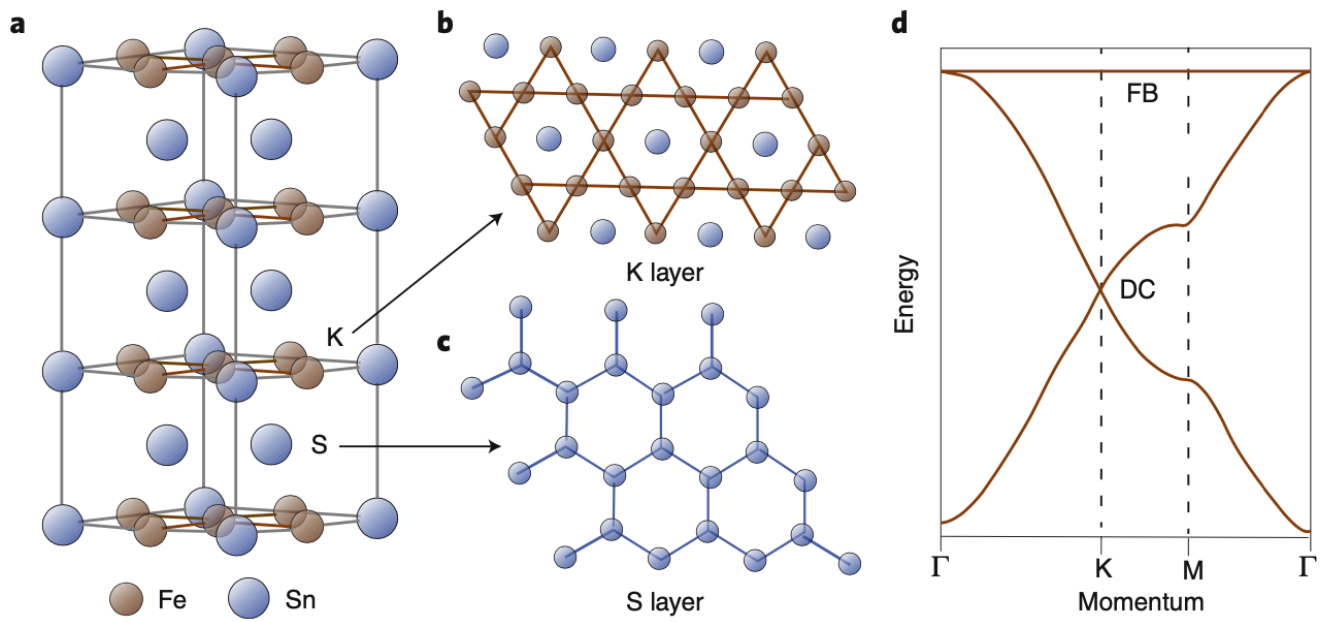
ROY L. JOHNSTON† and ROALD HOFFMANN‡

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.

Kagomé metals



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

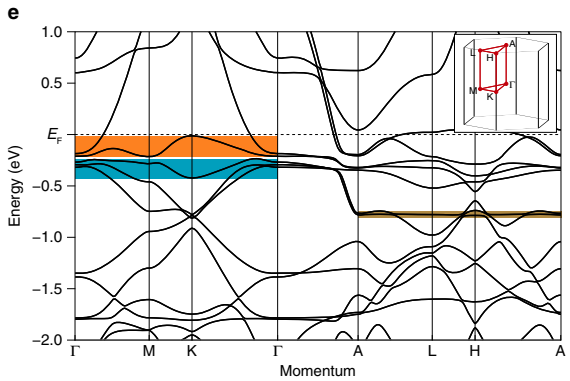
Bands and photoemission

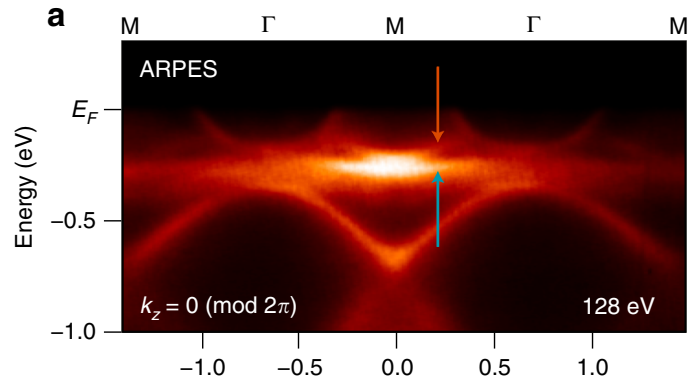
ARTICLE

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]

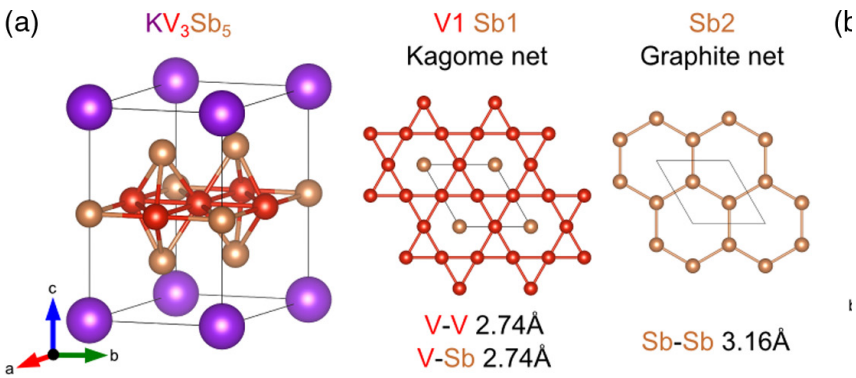




Flat bands…and??

Vanadium rush

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



1-2 papers a week

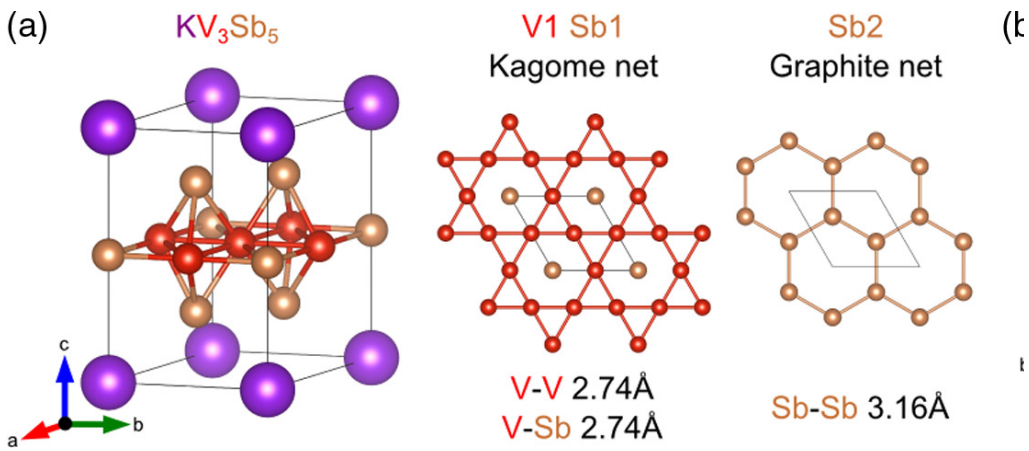
A review

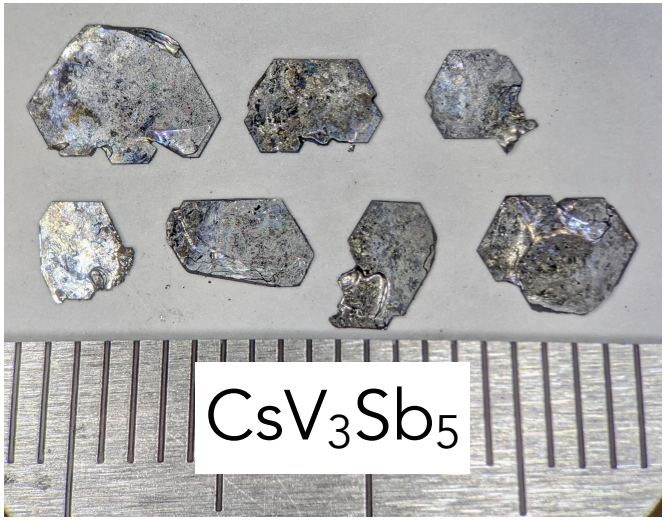
Charge order and superconductivity in kagome materials

Titus Neupert[1], M. Michael Denner[1], Jia-Xin Yin[2], Ronny Thomale[3,4] and M. Zahid Hasan[2,5,6,7]

AV_3Sb_5

B.R. Ortiz *et al*, 2019





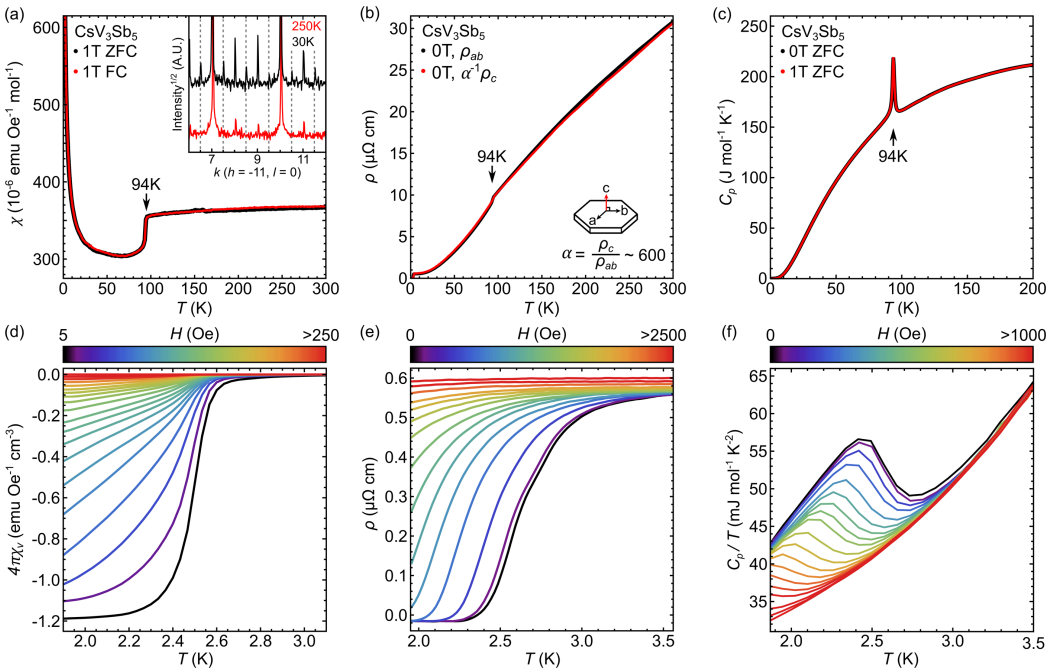
V kagomé layers separated by Sb honeycombs

Perfect hexagonal symmetry: P6/mmm space group

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

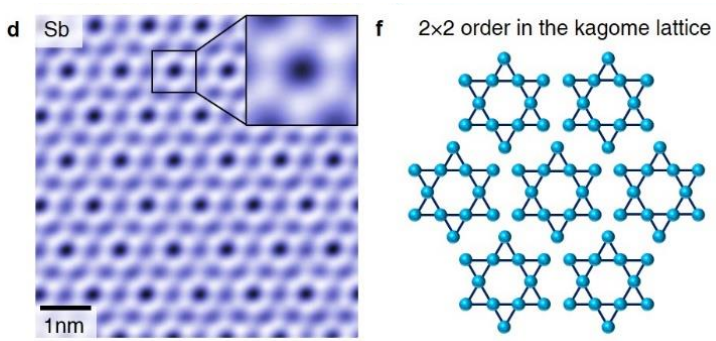
AV_3Sb_5

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

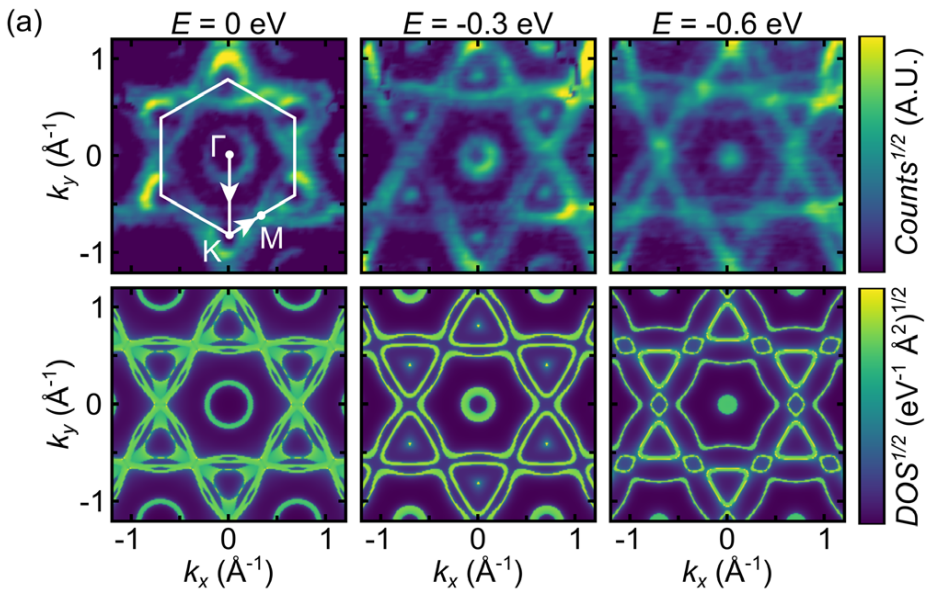
AV_3Sb_5

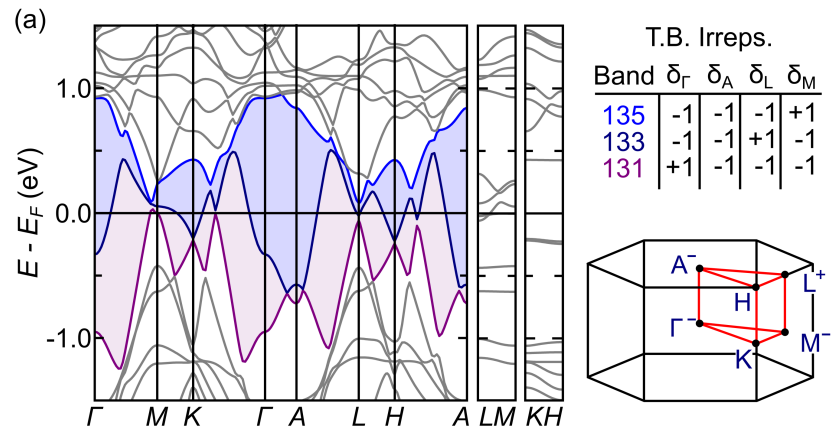
Band structure

B.R. Ortiz *et al*, 2020

ARPES

DFT



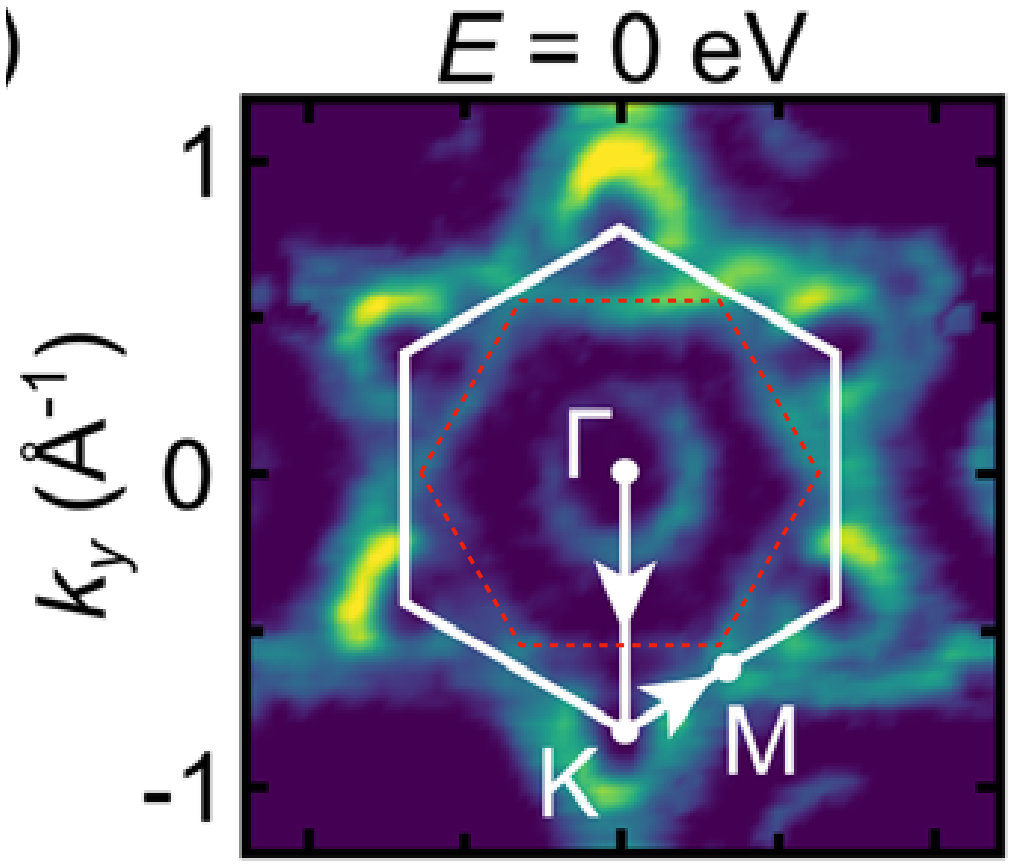


- Clearly many bands, mostly V but also Sb
- Several quasi-2d Fermi surfaces (*very* far from the ionic picture)

AV_3Sb_5

Band structure

B.R. Ortiz *et al*, 2020



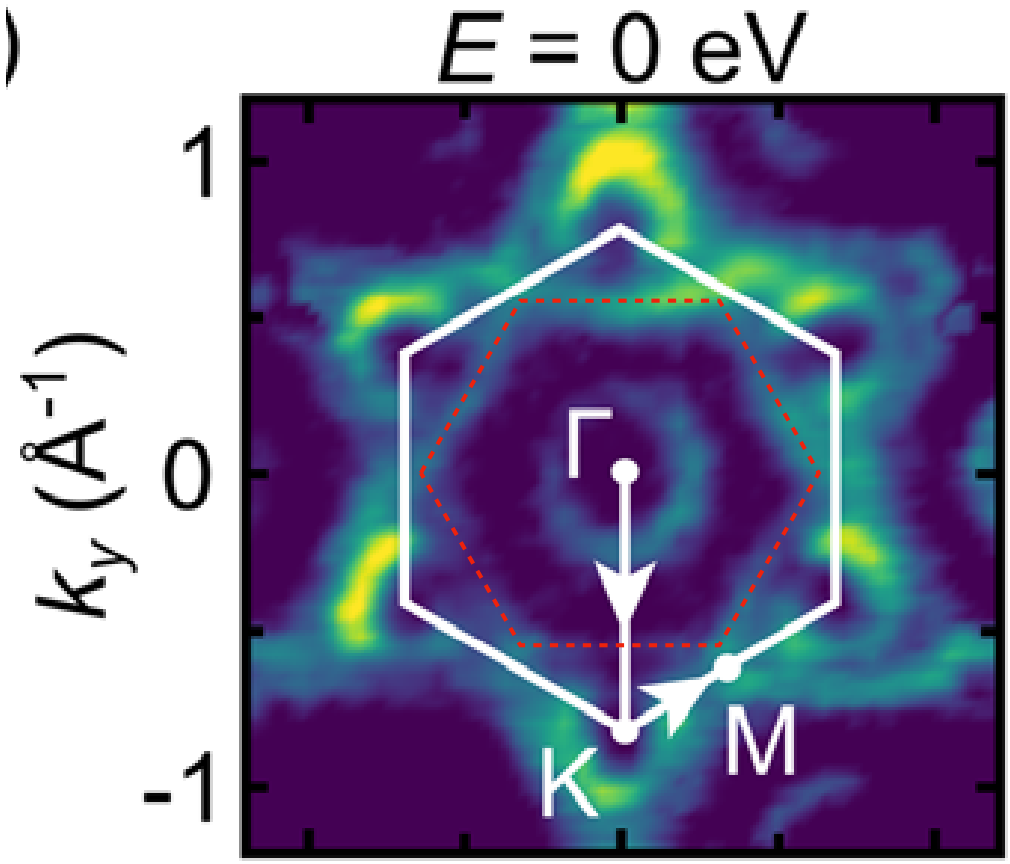
approximately hexagonal Fermi surface "inscribed" in Brillouin zone

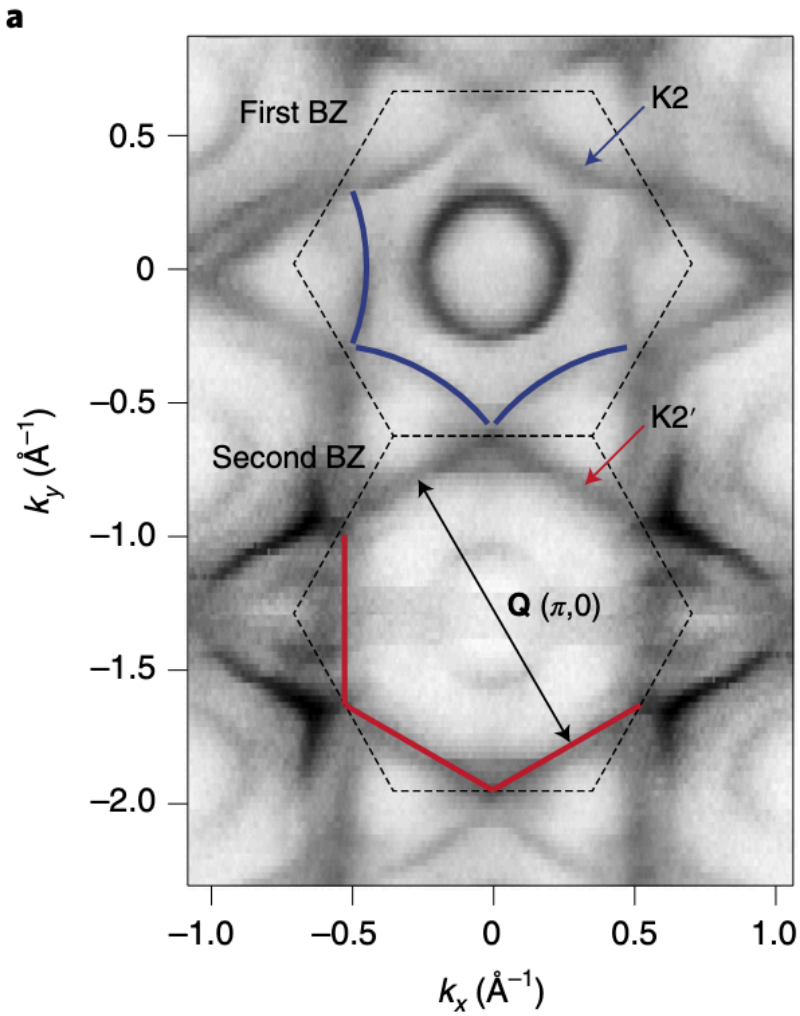
FS corners are located at M points

AV_3Sb_5

Band structure

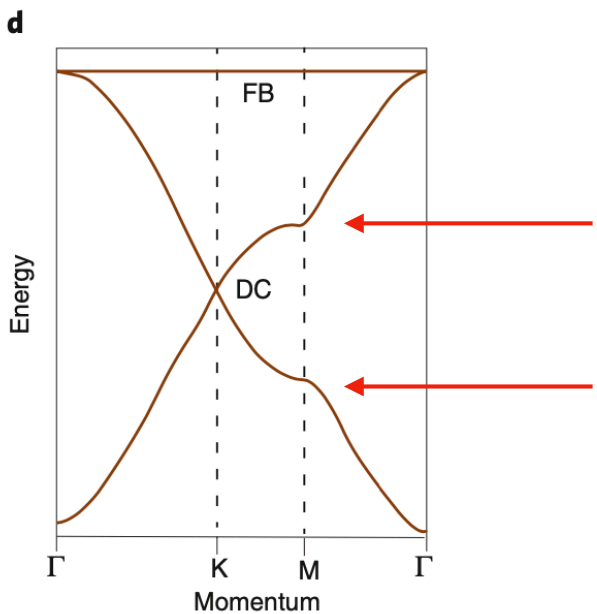
B.R. Ortiz *et al*, 2020





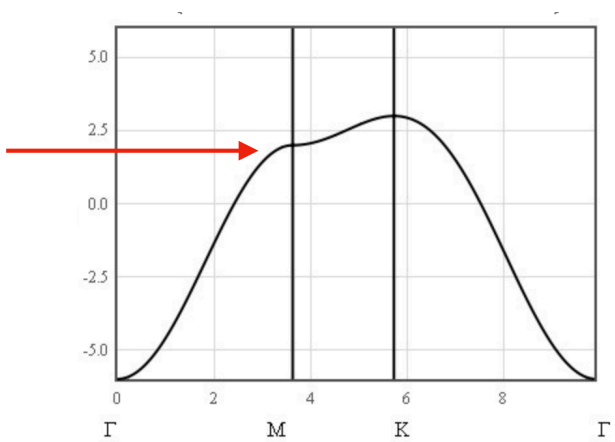
M. Kang *et al*, 2022

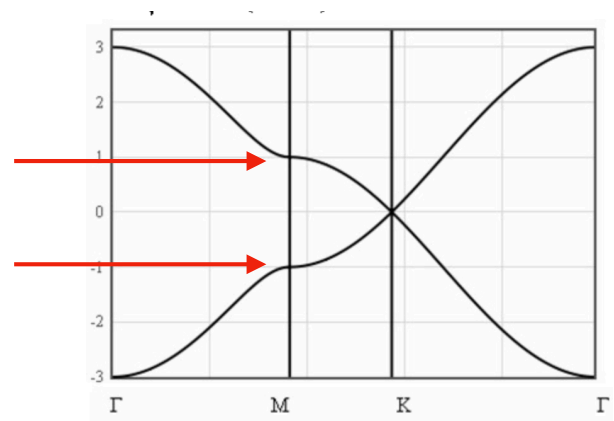
Saddle points



saddle points

M-point saddles are very common in hexagonal systems





van Hove singularity

The Occurrence of Singularities in the Elastic Frequency Distribution of a Crystal

LÉON VAN HOVE
Institute for Advanced Study, Princeton, New Jersey
(Received December 5, 1952)

It is shown that for a crystal, under the assumption of harmonicity for the interatomic forces and as a consequence of the periodic structure, the frequency distribution function of elastic vibrations has analytic singularities. In the general case, the nature of the singularities depends only on the number of dimensions of the crystal. For a two-dimensional crystal, the distribution function has logarithmically infinite peaks. In the three-dimensional case, the distribution function itself is continuous whereas its first derivative exhibits infinite discontinuities. These results are elementary consequences of a theorem of Morse on the existence of saddle points for functions defined on a torus.

As noticed by Smollett, the logarithmic peaks obtained for the two-dimensional lattices considered are a simple consequence of the existence of saddle points for the function $\nu(\mathbf{q})$ expressing the frequency of an elastic plane wave in terms of its wave vector. The

For $l=2$, the two-dimensional torus has Betti numbers $R_0=1$, $R_1=2$, $R_2=1$. If a branch of $\nu(\mathbf{q})$ satisfies the above conditions, it has therefore at least one maximum, two saddle points and one minimum. The corresponding singularities in $g(\nu)$ were listed in Sec. II. By reason of symmetry the two saddle points may often correspond to the same value of $\nu(\mathbf{q})$; they will then produce one single logarithmic peak in $g(\nu)$.

Two-Dimensional Crystal

$(M, i=0) \quad \epsilon_1=\epsilon_2=-1,$

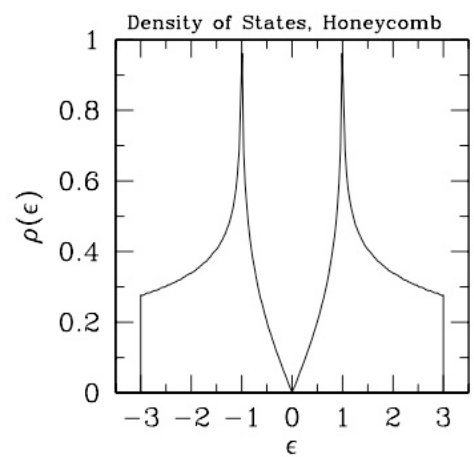
$$g(\nu)=\begin{cases} C+(\pi v_0/Zla)+0(\nu-\nu_c) & \text{for} \quad \nu<\nu_c \\ C+0(\nu-\nu_c) & \text{for} \quad \nu>\nu_c \end{cases}$$

$(S, i=1) \quad \epsilon_1=-\epsilon_2=\pm 1,$

$$g(\nu)=C-\frac{v_0}{Zla}\log\left|1-\frac{\nu}{\nu_c}\right|+0(\nu-\nu_c)$$

$(m, i=2) \quad \epsilon_1=\epsilon_2=1,$

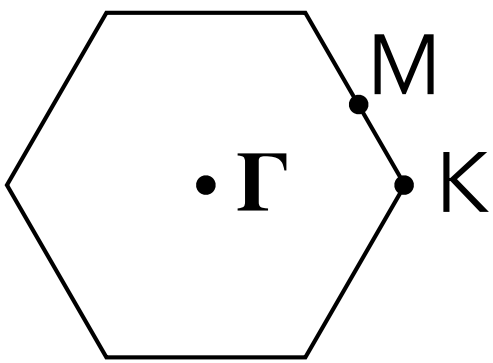
$$g(\nu)=\begin{cases} C+0(\nu-\nu_c) & \text{for} \quad \nu<\nu_c \\ C+(\pi v_0/Zla)+0(\nu-\nu_c) & \text{for} \quad \nu>\nu_c. \end{cases}$$



from stack exchange, not vH's paper

Saddle points

Why?



M point is always a critical point:

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

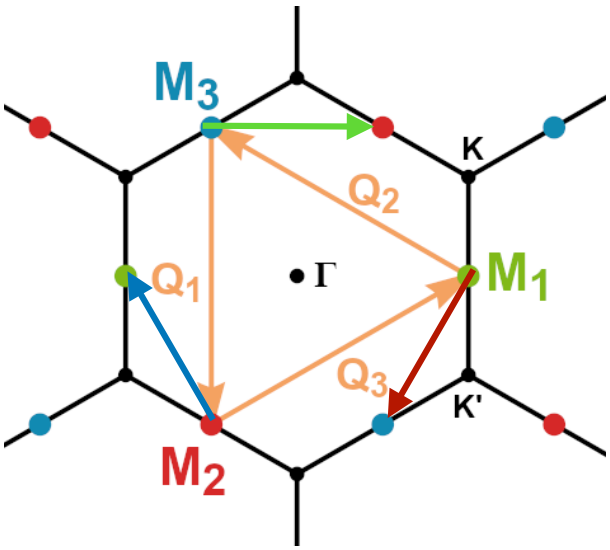
Morse theory: for a "sufficiently smooth" function on a closed 2d manifold

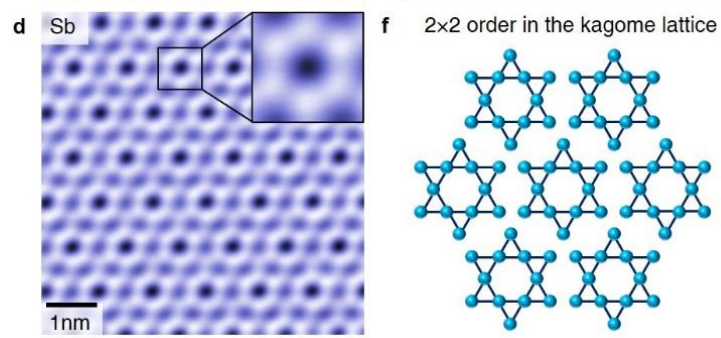
$$n_{\max} - n_{\mathrm{sp}} + n_{\min} = \chi_E$$ = 0 for torus

2 - 3 + 1 = 0

(K) (M) ($\boldsymbol{\Gamma}$)

Connection to AVS



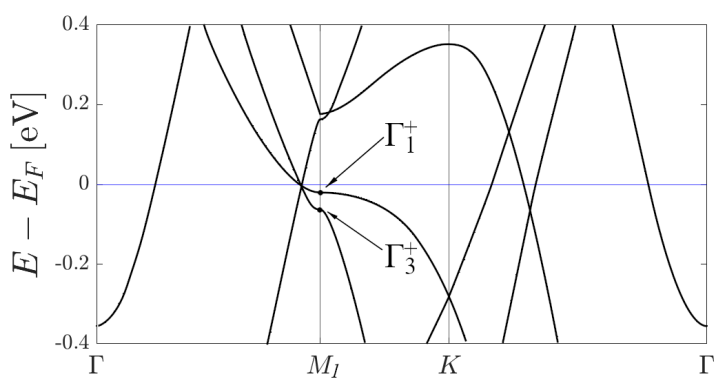


Q=M

Difference of two M points is another M point:
e.g. $M_1=M_2-M_3$ (up to RLVs)

CDW (and SC?) due to saddle point interactions?

DFT



Square lattice

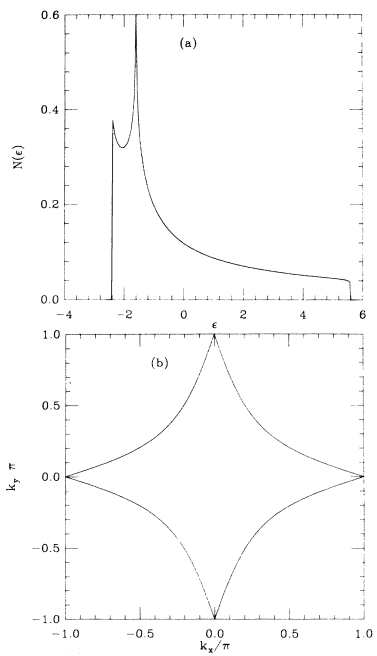
Enhanced superconductivity

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)

$$\left.\begin{aligned} G_1' &= 2G_1(G_4 - G_1)\, l_o \\ G_2' &= -2\left(G_2^2 + G_3^2\right) l \\ G_3' &= -4G_2G_3 l + 2G_3(2G_4 - G_1)\, l_o \\ G_4' &= \left(G_3^2 + G_4^2\right) l_o \end{aligned}\right\} \quad (7)$$

Square lattice

Enhanced superconductivity

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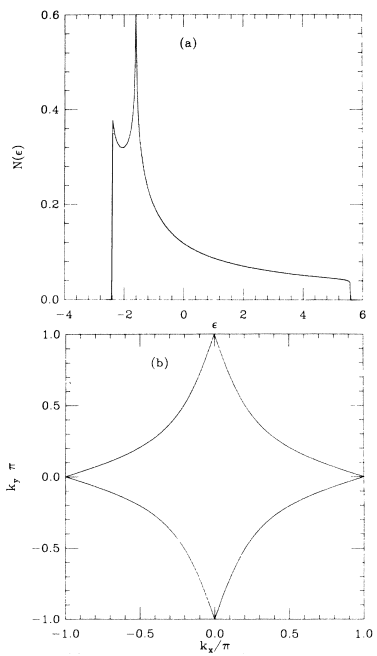


$$P_0(q) = \frac{1}{N}\sum \frac{1 - f(\epsilon_{p+q}) - f(\epsilon_p)}{\epsilon_{p+q} + \epsilon_p}.$$

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

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)

$$\dot{g}_1 = 2d_1g_1(g_2 - g_1) + 2d_2g_1g_4 - 2d_3g_1g_2, \quad (4)$$

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

$$\dot{g}_3 = -2g_3g_4 + 2d_1g_3(2g_2 - g_1), \quad (6)$$

$$\dot{g}_4 = -(g_3^2 + g_4^2) + d_2(g_1^2 + 2g_1g_2 - 2g_2^2 + g_4^2). \quad (7)$$

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

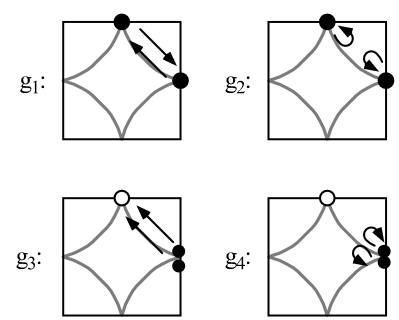


FIG. 2. The definitions of vertices for the two-patch model.

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

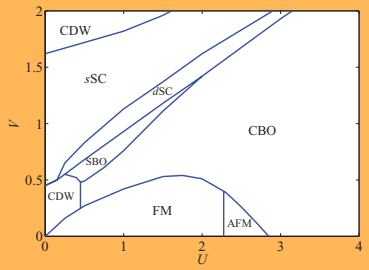
Rahul Nandkishore[1,2] and Andrey V. Chubukov[3]
[1]*Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*
[2]*Princeton Center for Theoretical Science, Princeton University, Princeton, NJ 08540, USA*
[3]*Department of Physics, University of Wisconsin-Madison, 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)

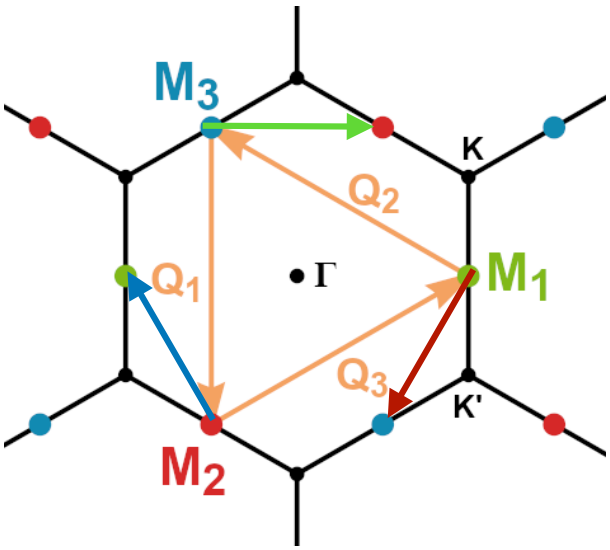
Competing electronic orders on kagome lattices at van Hove filling

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

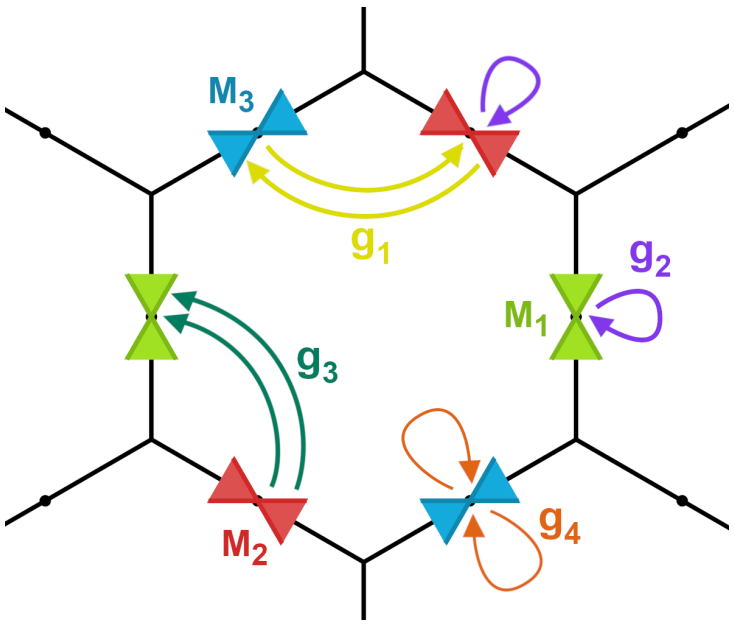
Order parameters:

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

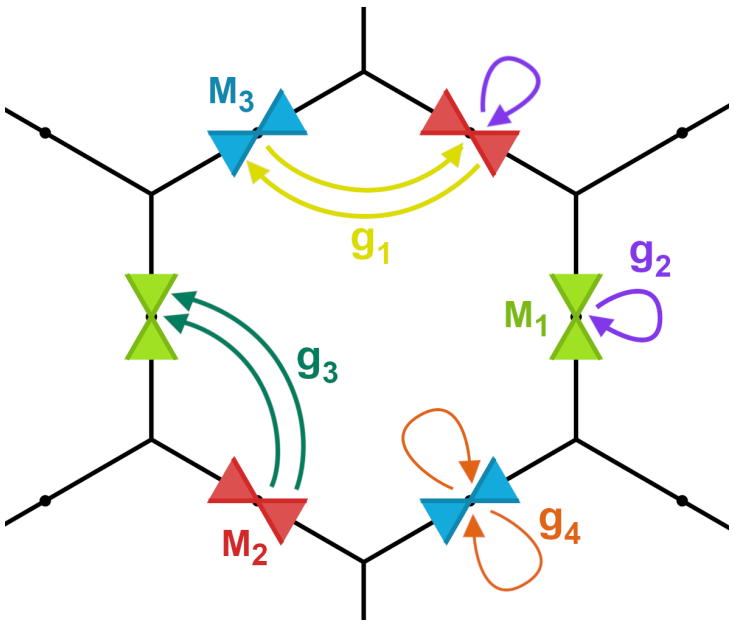
umklapp $\frac{\mathrm{d}g_3}{\mathrm{d}y} = -g_3^2 - 2g_3 g_4 + 2d_1 g_3(2g_2 - g_1),$

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 $\log^2$ is dominant even over log



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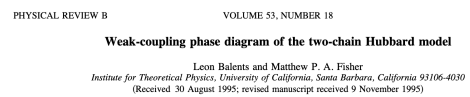
intra-valley $\frac{\mathrm{d}g_4}{\mathrm{d}y} = -2g_3^2 - g_4^2,$


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

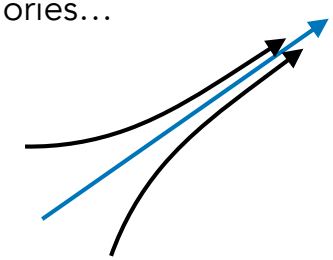
(Received 30 August 1995; revised manuscript received 9 November 1995)

memories…

Analysis:

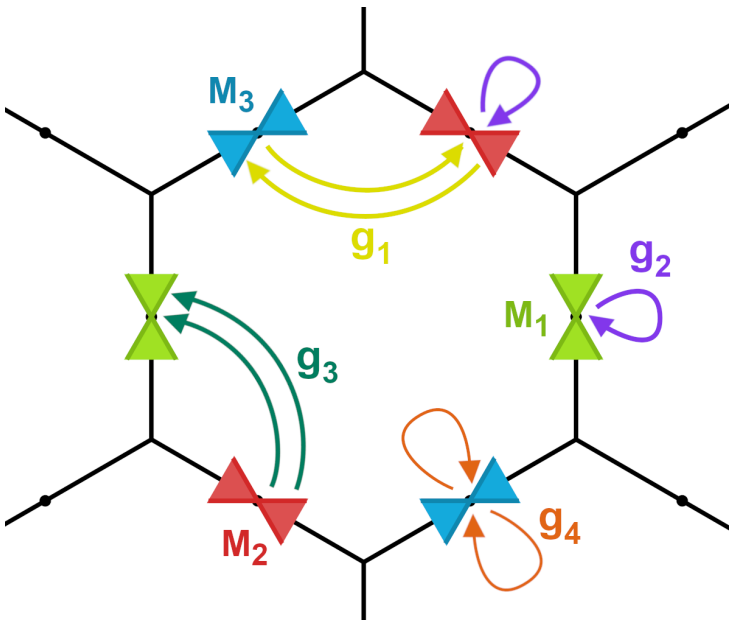
- 4 instability pathways

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

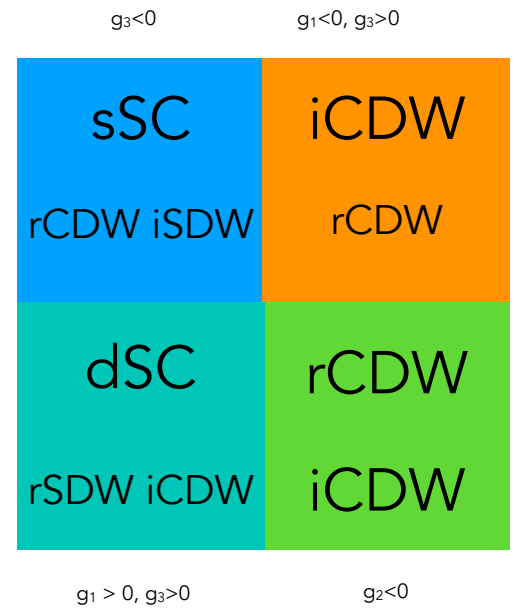


M-point RG

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



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



Analysis:

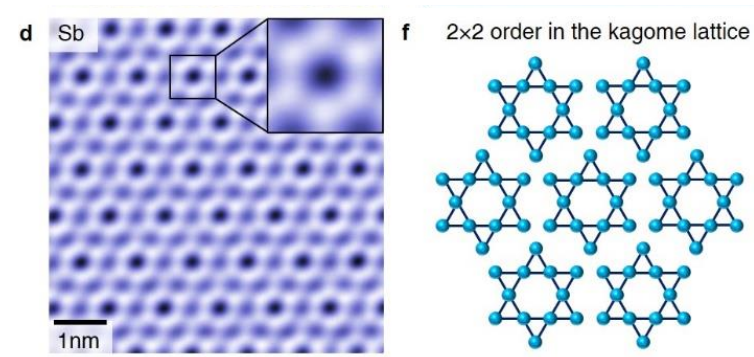
- 4 instability pathways

if bare couplings are comparable, larger order dominates

Charge density wave

Return to experiment:

sSC **rCDW** iSDW	iCDW **rCDW**
dSC rSDW iCDW	**rCDW** iCDW



rCDW order

- Occam's razor: rCDW is what is observed between 5K-90K, so it is the dominant (only?) instability

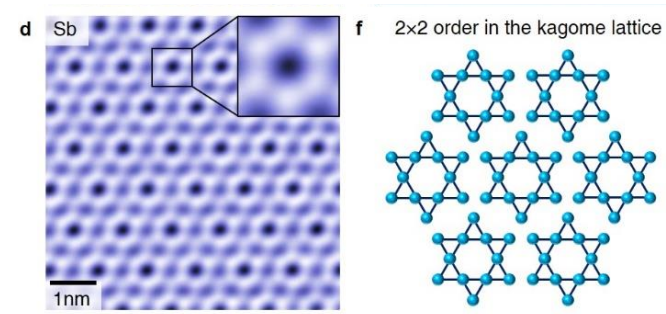
From here on we will discuss phenomenology

rCDW

Apply Landau/symmetry analysis

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

+ 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

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

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

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

$$H_2(z) = \int_0^\infty \mathrm{d}x \int_0^{x/\sqrt{3}} \mathrm{d}y \Big(\frac{F(\bar{\varepsilon}_1(x,y) - z)}{(\bar{\varepsilon}_1(x,y) - \bar{\varepsilon}_2(x,y))(\bar{\varepsilon}_1(x,y) - \bar{\varepsilon}_3(x,y))} - \frac{F(\bar{\varepsilon}_2(x,y) - z)}{(\bar{\varepsilon}_1(x,y) - \bar{\varepsilon}_2(x,y))(\bar{\varepsilon}_2(x,y) - \bar{\varepsilon}_3(x,y))} + \frac{F(\bar{\varepsilon}_3(x,y) - z)}{(\bar{\varepsilon}_1(x,y) - \bar{\varepsilon}_3(x,y))(\bar{\varepsilon}_2(x,y) - \bar{\varepsilon}_3(x,y))} \Big),$$

$$H_3(z) = \int_0^\infty \mathrm{d}x \int_0^{x/\sqrt{3}} \mathrm{d}y \Big(\frac{F'(\bar{\varepsilon}_1(x,y) - z)}{(\bar{\varepsilon}_1(x,y) - \bar{\varepsilon}_2(x,y))(\bar{\varepsilon}_1(x,y) - \bar{\varepsilon}_3(x,y))} - \frac{F'(\bar{\varepsilon}_2(x,y) - z)}{(\bar{\varepsilon}_1(x,y) - \bar{\varepsilon}_2(x,y))(\bar{\varepsilon}_2(x,y) - \bar{\varepsilon}_3(x,y))} + \frac{F'(\bar{\varepsilon}_3(x,y) - z)}{(\bar{\varepsilon}_1(x,y) - \bar{\varepsilon}_3(x,y))(\bar{\varepsilon}_2(x,y) - \bar{\varepsilon}_3(x,y))} \Big),$$

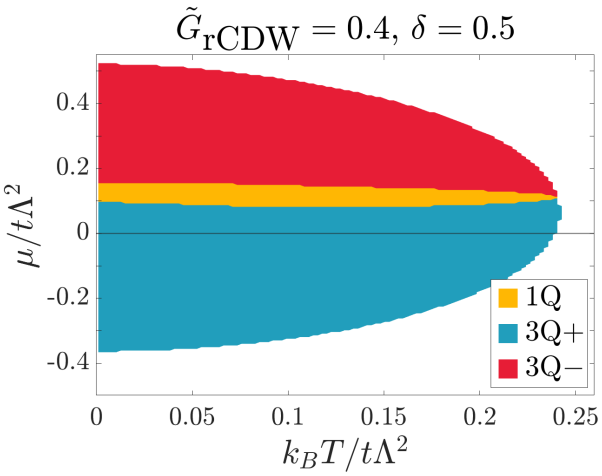
$$H_4(z) = \int_0^\infty \mathrm{d}v \left(\frac{-F(v-z) + F(-v-z)}{v^3} + \frac{F'(v-z) + F'(-v-z)}{z^2} \right).$$

sorry Taka…

Selects "star of David" or "tri-hexagonal" structure

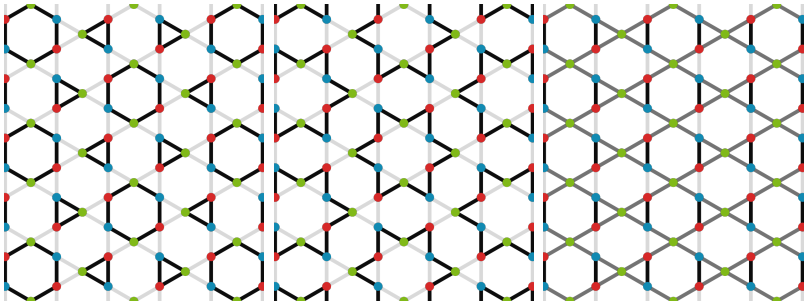
rCDW

Can also analyze via microscopic MFT w/o Landau expansion



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

1st order transition in MFT



3Q+ 3Q- 1Q

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

Comment | Published: 28 March 2022

Inverse Occam's razor

Igor Mazin

Nature Physics **18**, 367–368 (2022) | Cite this article

pluralitas non est ponenda sine necessitate

- Other orders behind the CDW?
- Unconventional superconductivity?
  - Nematicity
  - TRS breaking/Loop currents
  - Unconventional superconductivity
    - Nodes
    - Pair density wave
    - Higher charge superconductivity

Comment | Published: 28 March 2022

Inverse Occam's razor

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pluralitas non est ponenda sine necessitate

- Other orders behind the CDW?
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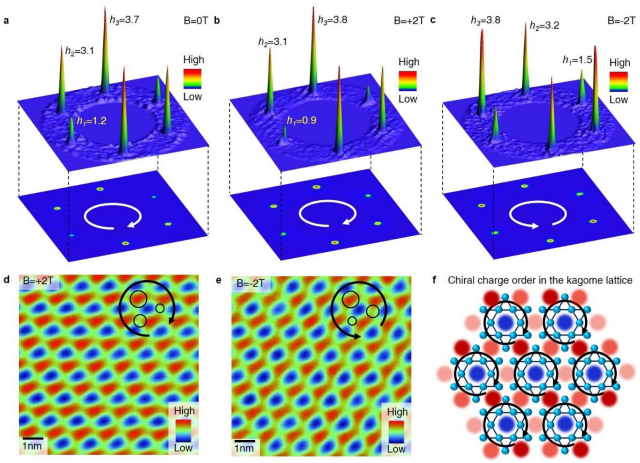
    - Nodes
    - Pair density wave
    - Higher charge superconductivity

Here we go!

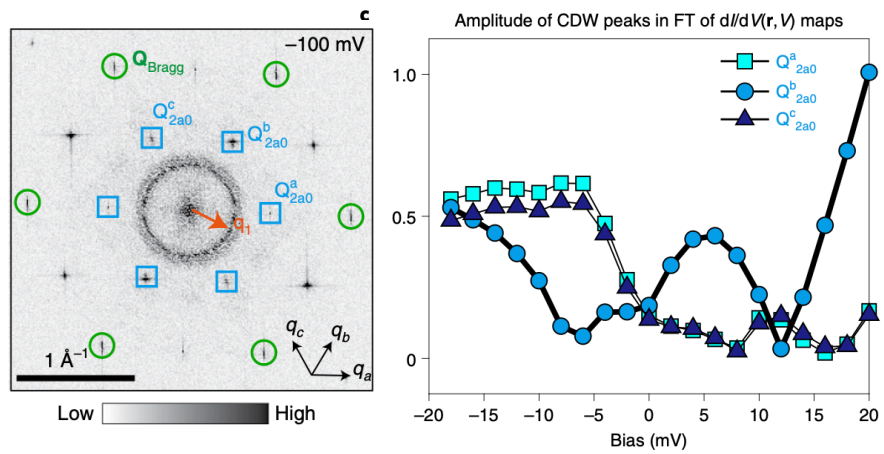
Nematicity

STM



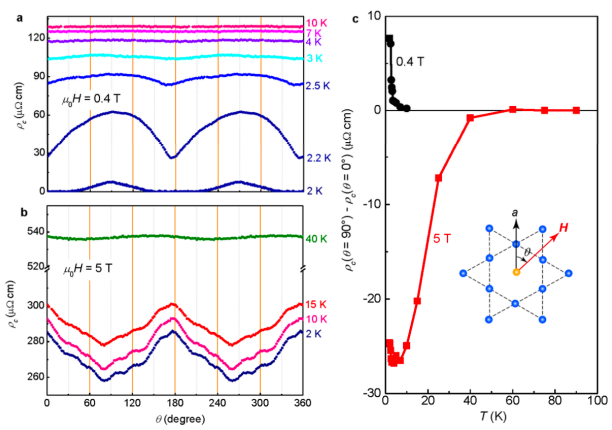
Y.-X. Jiang *et al*, 2021 (Z. Hasan)

STM



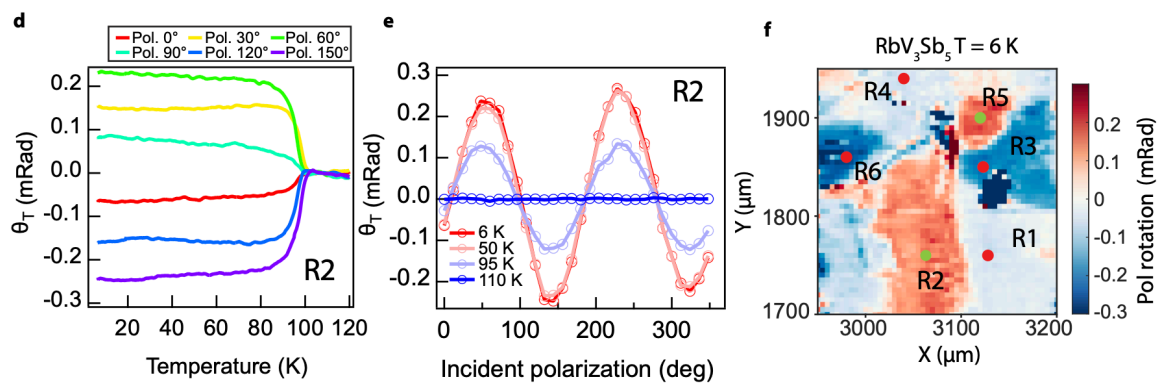
H. Li *et al*, 2022 (I. Zeljkovic)

Transport



Y. Xiang *et al*, 2021 (Hai-Hu Wen)

Birefringence



Y. Xu *et al*, 2022 - unpublished (Liang Wu)

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:

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

3d order

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

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Inter-layer free energy:

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

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

rapidly decreasing with δ

Inter-layer free energy:

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

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

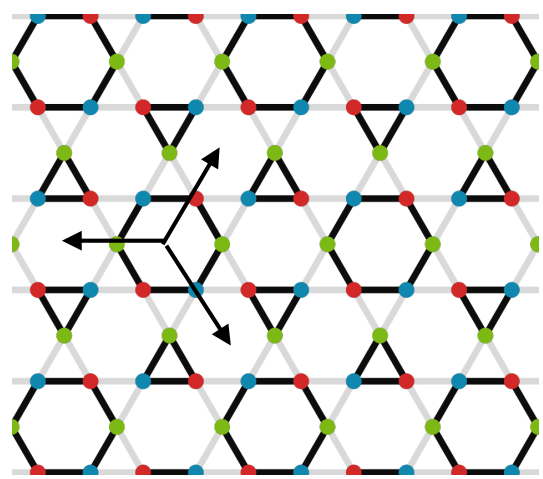
Assumption: inter-layer coupling is weak compared to intra-layer interactions, and generally decays with distance in c direction

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

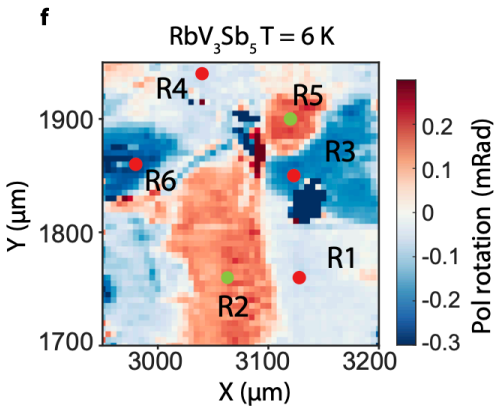
Upshot: iCDW and rSDW should have k_z=0 rCDW order

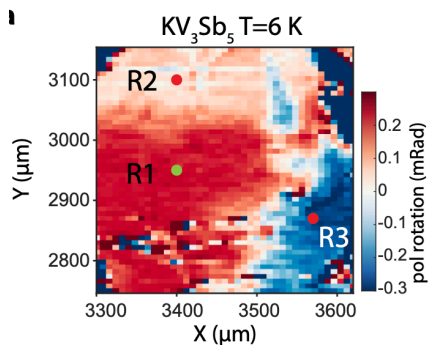
Experiments (x-rays):

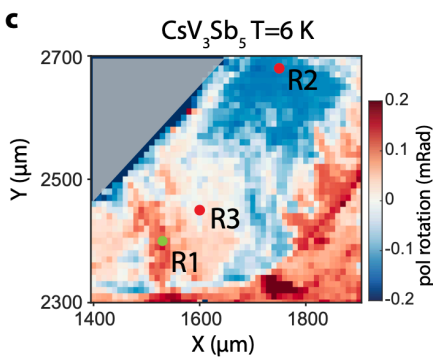
A	k_z
Cs	¼
K	½
Rb	½

consistent with primary rCDW

Nematicity

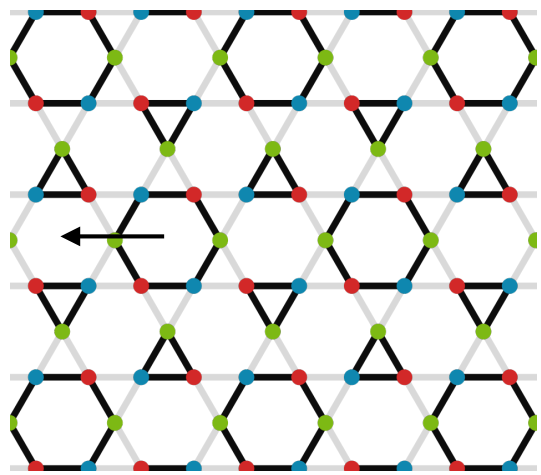


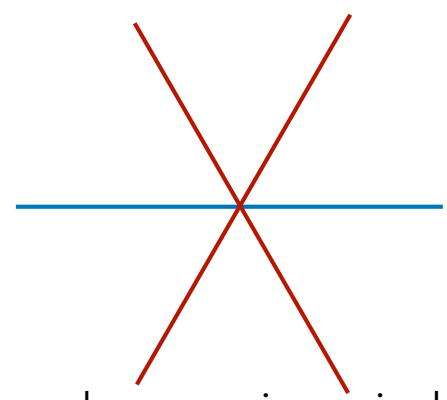




Period 2 and period 4 layerings necessarily break C_3 symmetry and form 3 rotational domains

Pattern of 2+1 charge peaks expected





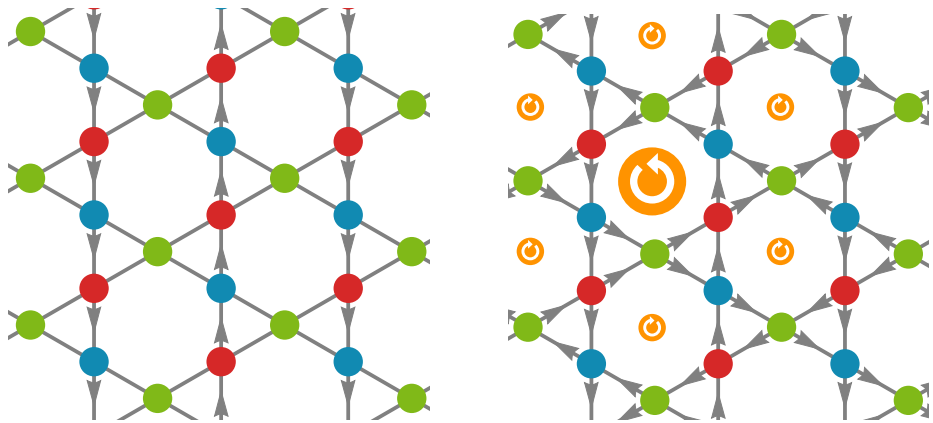
axes become inequivalent

Observed in all 3 compounds

Y. Xu *et al*, 2022 - unpublished (Liang Wu)

TRS breaking

Numerous experiments *suggestive* of weak orbital? magnetism



3Q state *macroscopically* breaks TR

$$\Phi = \phi_1 \phi_2 \phi_3$$

transforms like M_z

Loop currents?

"iCDW" is almost degenerate with rCDW - only distinguished by umklapp g_3 coupling

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

Anomalous Hall effect

PHYSICS Sci. Adv. 2020

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

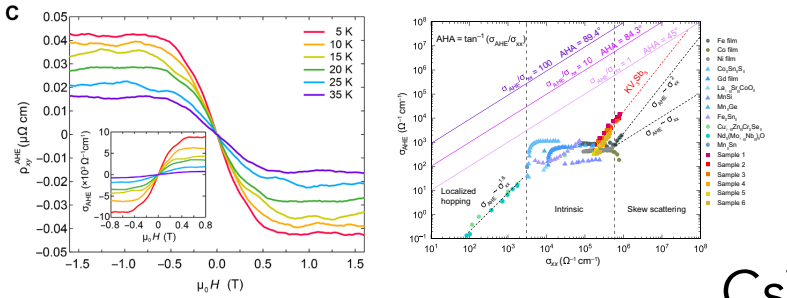
Shuo-Ying Yang[1]*, Yaojia Wang[1]*, Brenden R. Ortiz[2], Defa Liu[1], Jacob Gayles[3,4], Elena Derunova[1], Rafael Gonzalez-Hernandez[5,6], Libor Šmejkal[6,7,8], Yulin Chen[9], Stuart S. P. Parkin[1], Stephen D. Wilson[2], Eric S. Toberer[10], Tyrel McQueen[11], Mazhar N. Ali[1†]

arXiv:2102.10987

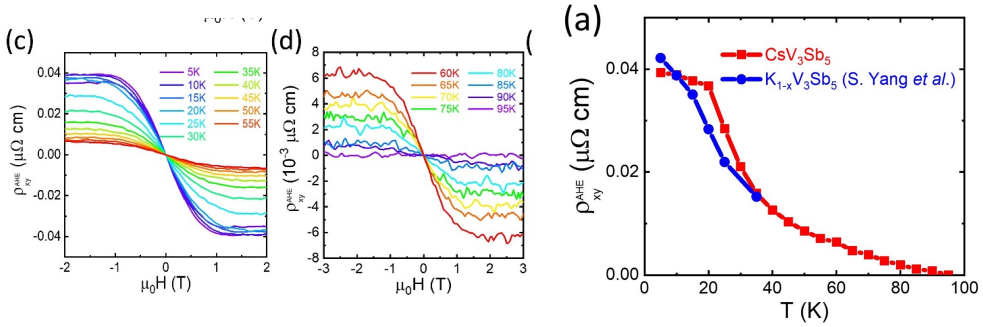
Concurrence of anomalous Hall effect and charge density wave in a superconducting topological kagome metal

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†]

KV_3Sb_5



CsV_3Sb_5



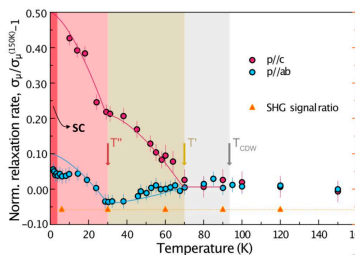
Not directly indicative of TRSB but suggestive

muSR

arXiv:2107.10714

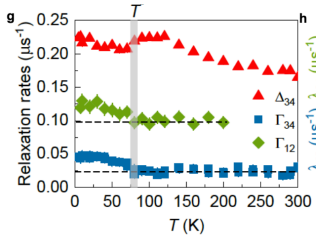
Evidence of a hidden flux phase in the topological kagome metal CsV_3Sb_5

Li Yu[1,6,9†*], Chennan Wang[2†], Yuhang Zhang[1,6†], Mathias Sander[3,4], Shunli Ni[1,6], Zouyouwei Lu[1,6], Sheng Ma[1,6], Zhengguo Wang[10], Zhen Zhao[1,6], Hui Chen[1,6,7,9], Kun Jiang[1], Yan Zhang[10], Haitao Yang[1,6,7,9*], Fang Zhou[1,6,9], Xiaoli Dong[1,6,9], Steven L. Johnson[3,4], Michael J. Graf [5*], Jiangping Hu[1,8], Hong-Jun Gao[1,6,7,9], Zhongxian Zhao[1,6,9]



Time-reversal symmetry-breaking charge order in a correlated kagome superconductor

C. Mielke III,[1,2,*] D. Das,[1,*] J.-X. Yin,[3,*] H. Liu,[4,5,*] R. Gupta,[1] C.N. Wang,[1] Y.-X. Jiang,[3] M. Medarde,[6] X. Wu,[7] H.C. Lei,[8] J.J. Chang,[2] P. Dai,[9] Q. Si,[9] H. Miao,[10] R. Thomale,[11,12] T. Neupert,[2] Y. Shi,[4,5,13] R. Khasanov,[1] M.Z. Hasan,[3,14,15,16,†] H. Luetkens,[1] and Z. Guguchia[1,‡]



arXiv:2203.0577

Muon-spin relaxation study of the layered kagome superconductor CsV_3Sb_5

Zhaoyang Shan,[1,2] Pabitra K. Biswas,[3,*] Sudeep K. Ghosh,[4,†] T. Tula,[4] Adrian D. Hillier,[3] Devashibhai Adroja,[3,5] Stephen Cottrell,[3] Guang-Han Cao,[1,2,6] Yi Liu,[7] Xiaofeng Xu,[7] Yu Song,[1,2] Huiqiu Yuan,[1,2,6] and Michael Smidman[1,2,‡]

and superconductivity in this material. From zero-field μSR, we find that spontaneous magnetic fields appear below 50 K which is well below the charge-density wave transition ($T^* \sim 93$ K). We show that these spontaneous fields are dynamic in nature making it difficult to associate them with a hidden static order. The superconducting state of CsV_3Sb_5 is found to preserve time-reversal symmetry and the transverse-field μSR results are consistent with a superconducting state that has two fully open gaps.

arXiv:2203.12317

Charge order breaks time-reversal symmetry in CsV_3Sb_5

Rustem Khasanov,[1,*] Debarchan Das,[1] Ritu Gupta,[1] Charles Mielke III,[1] Matthias Elender,[1] Qiangwei Yin,[2] Zhijun Tu,[2] Chunsheng Gong,[2] Hechang Lei,[2,†] Ethan Ritz,[3] Rafael M. Fernandes,[4] Turan Birol,[3] Zurab Guguchia,[1,‡] and Hubertus Luetkens[1,§]

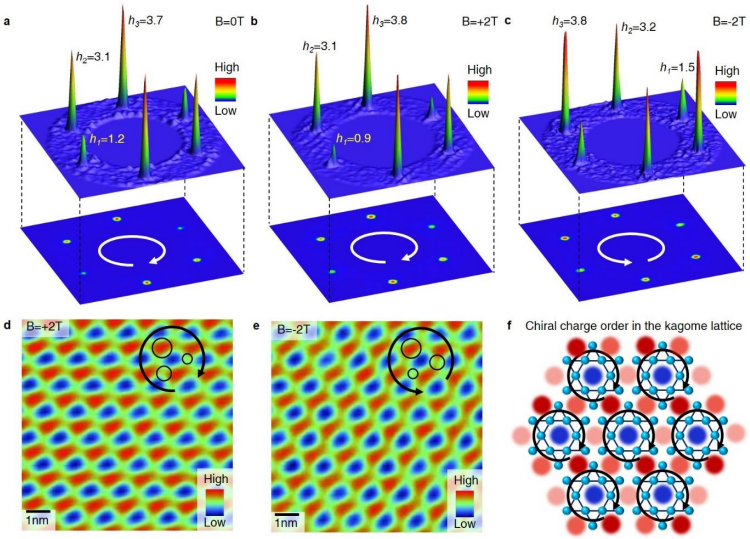
muSR seems to be somewhat controversial

STM

Nat. Mat. 2021

Unconventional chiral charge order in kagome superconductor KV_3Sb_5

Yu-Xiao Jiang[1,13], Jia-Xin Yin[1,13], M. Michael Denner[2,13], Nana Shumiya[1,13], Brenden R. Ortiz[3,13], Gang Xu[4,13], Zurab Guguchia[5], Junyi He[4], Md Shafayat Hossain[1], Xiaoxiong Liu[2], Jacob Ruff[6], Linus Kautzsch[6], Songtian S. Zhang[1], Guoqing Chang[7], Ilya Belopolski[1], Qi Zhang[1], Tyler A. Cochran[1], Daniel Multer[1], Maksim Litskevich[1], Zi-Jia Cheng[1], Xian P. Yang[1], Ziqiang Wang[8], Ronny Thomale[9], Titus Neupert[2], Stephen D. Wilson[3] and M. Zahid Hasan[1,10,11,12]



Claim: "chiral charge order":

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

Nat. Phys. 2022

Rotation symmetry breaking in the normal state of a kagome superconductor KV_3Sb_5

Hong Li[1,7], He Zhao[1,7], Brenden R. Ortiz[2,3], Takamori Park[4], Mengxing Ye[5], Leon Balents[5,6], Ziqiang Wang[1], Stephen D. Wilson[2,3] and Ilija Zeljkovic[1]

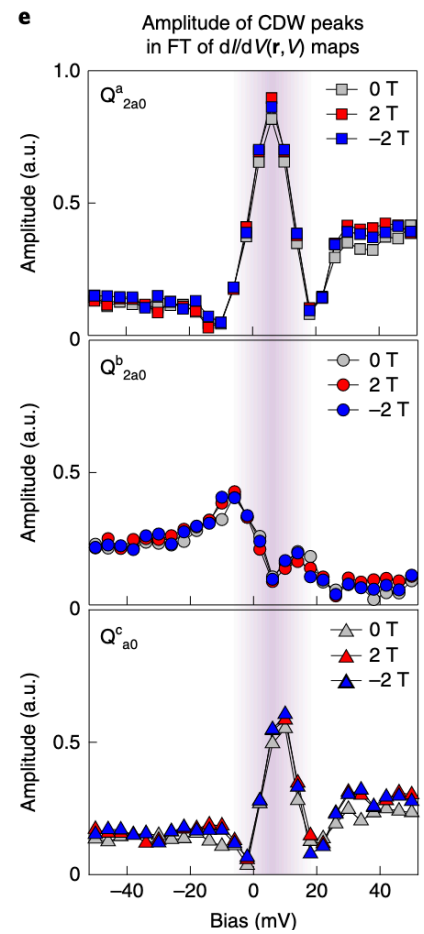
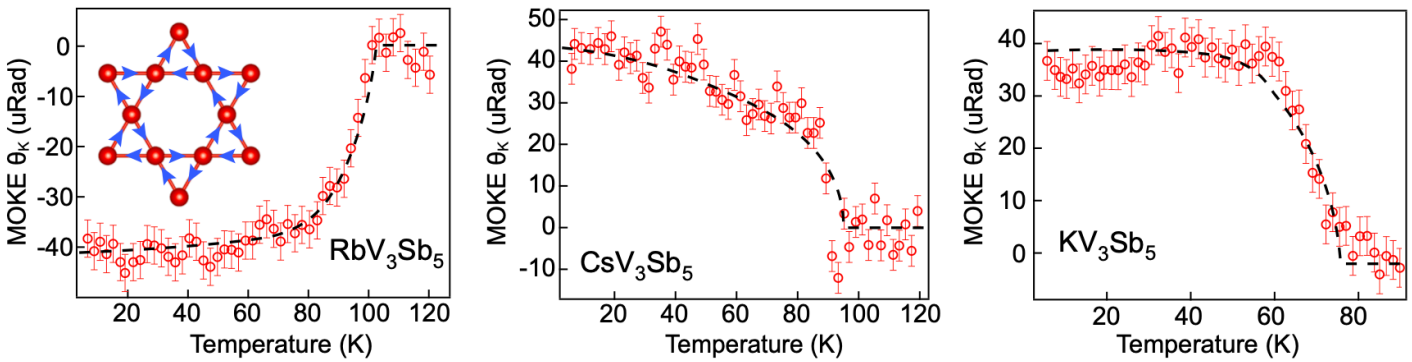


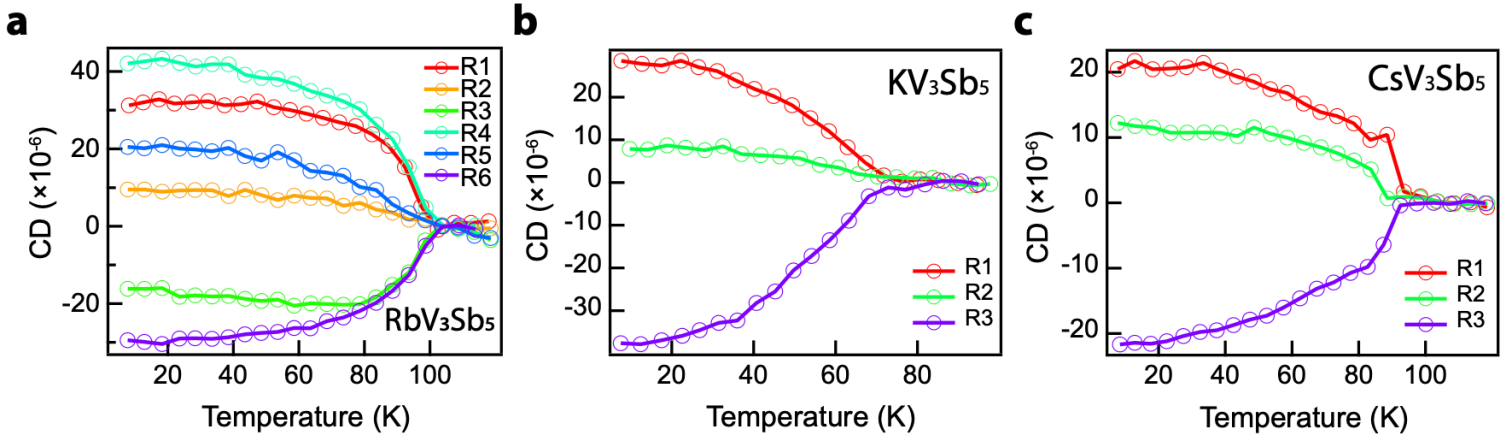
Fig. 4 | Insensitivity of CDW to external magnetic-field direction. a–c, S

Optics

Magneto-optical Kerr rotation



Circular dichroism



Probably the strongest evidence so far

Y. Xu *et al*, 2022 - unpublished (Liang Wu)

Unconventional superconductivity

Thermal conductivity

Nodal superconductivity and superconducting domes in the topological Kagome metal CsV_3Sb_5

C. C. Zhao[1,6], L. S. Wang[1,6], W. Xia[2,3,6], Q. W. Yin[4,6], J. M. Ni[1], Y. Y. Huang[1], C. P. Tu[1], Z. C. Tao[2], Z. J. Tu[4], C. S. Gong[4], H. C. Lei[4,+], Y. F. Guo[2,†], X. F. Yang[1,#], and S. Y. Li[1,5*]

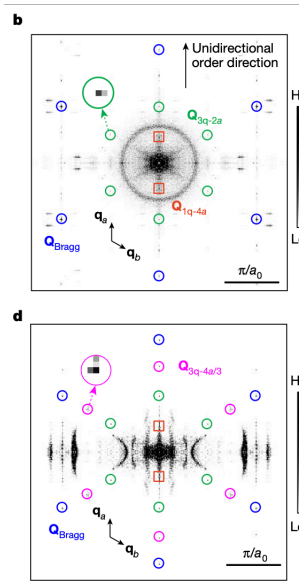
Penetration depth

Nodeless superconductivity in the kagome metal CsV_3Sb_5

Weiyin Duan[1,2], Zhiyong Nie[1,2], Shuaishuai Luo[1,2], Fanghang Yu[3], Brenden R. Ortiz[4], Lichang Yin[1,2], Hang Su[1,2], Feng Du[1,2], An Wang[1,2], Ye Chen[1,2], Xin Lu[1,2], Jianjun Ying[3], Stephen D. Wilson[4], Xianhui Chen[3,5,6], Yu Song[1,2*], and Huiqiu Yuan[1,2,6,7*]

SC-STM

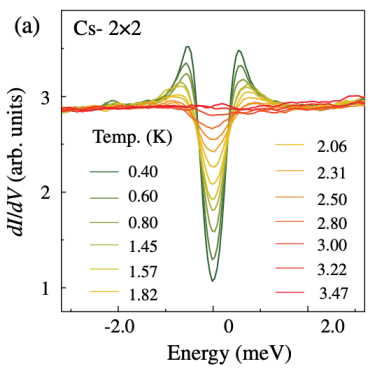
H. Chen *et al*, 2021



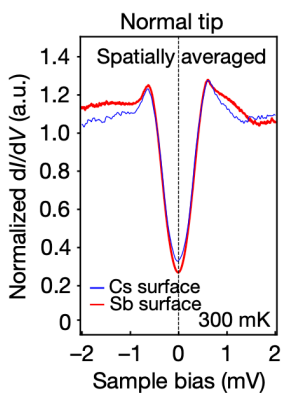
c, **d**, dI/dV(**r**, −5 mV) map (**c**) and the magnitude of the drift-corrected, two-fold symmetrized Fourier transform (**d**), revealing new 3Q PDW modulations at $\mathbf{Q}_{3q\text{-}4a/3}$ ($V_s = -5$ mV, $I_t = 1$ nA, $V_{mod} = 0.2$ mV). **e**, **f**, dI/dV(**r**, −0.25 mV) (**e**) and

STM

Z. Liang *et al*, 2021



H. Chen *et al*, 2021

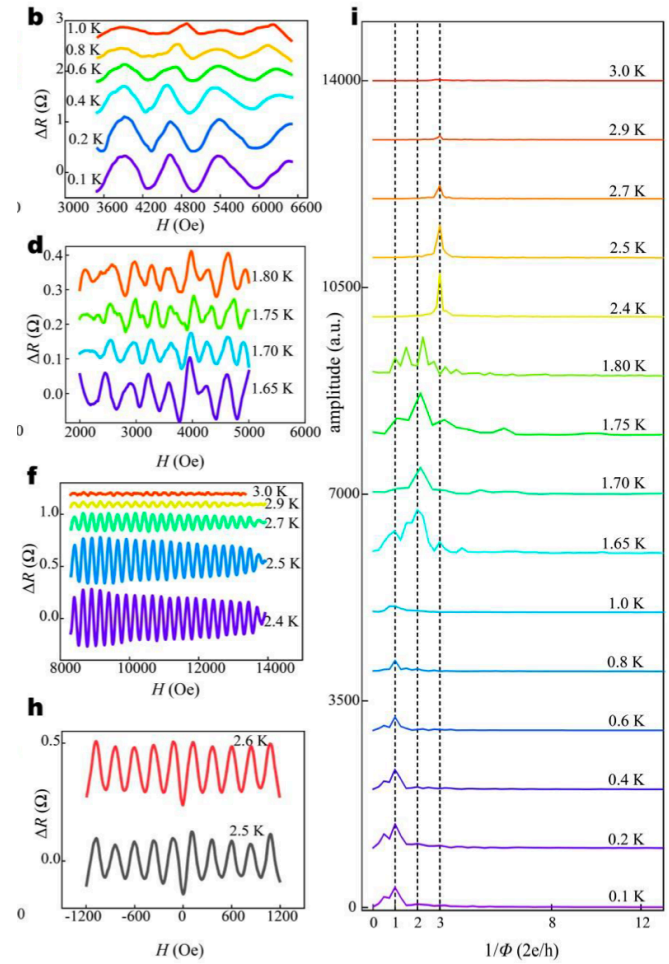


Unconventional superconductivity

Discovery of charge-4*e* and charge-6*e* superconductivity in kagome superconductor CsV_3Sb_5

Jun Ge[1#], Pinyuan Wang[1#], Ying Xing[1,2], Qiangwei Yin[3], Hechang Lei[3], Ziqiang Wang[4] & Jian Wang[1,5,6*]

Authors suggest this is related to "vestigial" order of PDW



Summary

- AV_3Sb_5 kagomé metals may realize van Hove scenario of electronic instabilities
  - Gap at M points (ARPES, ~10-20meV) consistent with BCS relation $2\Delta/kT_c \sim 3.5$.
  - Still pretty weak evidence
- Observed 3Q real CDW order, with staggered layered structure, inducing nematicity.
- Hints of exotic physics: time-reversal symmetry breaking, pair density wave, higher charge superconductivity
  - Occam's razor or the inverse?
- Needed: clarify minimal models/bands, apply many body computations
- Superconducting order parameter. Much more to be done.

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