Coulomb charge order, charge glass and bad metallic behavior

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Theory

S. Ciuchi (L'Aquila)
A. Ralko (Néel)
K. Driscoll (Néel)
G. D'Avino (Néel)
J. Merino (UAM)
L. Rademaker (Geneva)
V. Dobrosavljevic (FSU)

Experiments

M. Dressel (Stuttgart)
A. Pustogow (Vienna)
H. Sirringhaus (Cambridge)

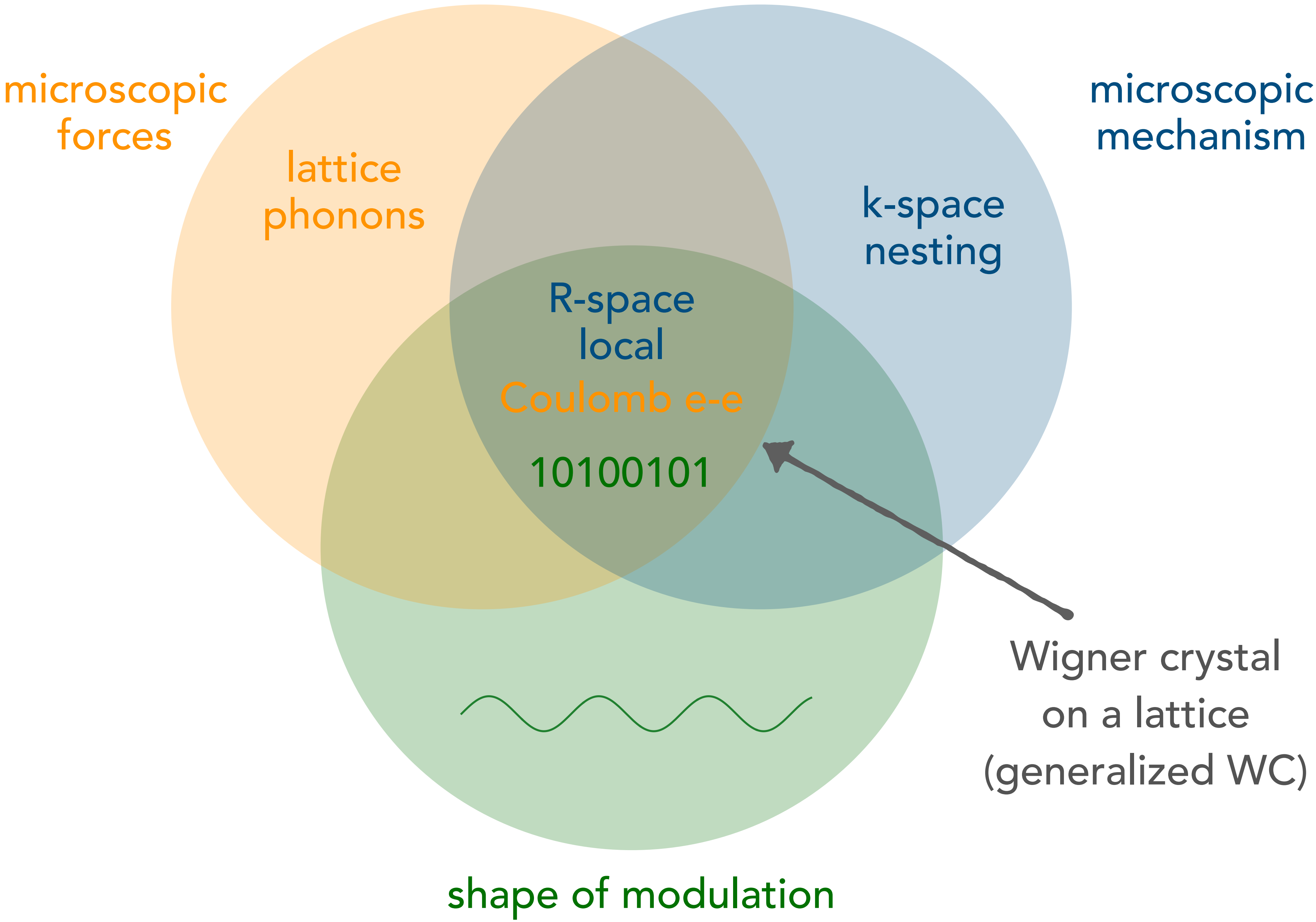
Outline

many electrons with long-range interactions

slow collective charge excitations

(self-generated disorder)

Semantics: CDW vs charge order



Wigner crystallization

DECEMBER 1, 1934 PHYSICAL REVIEW VOLUME 46

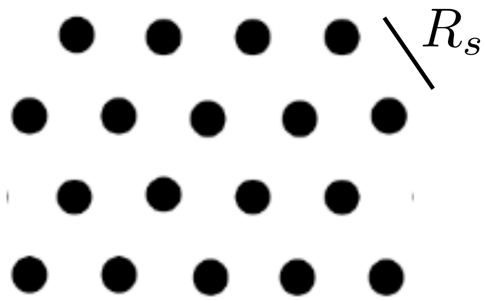
On the Interaction of Electrons in Metals

E. WIGNER, *Princeton University*

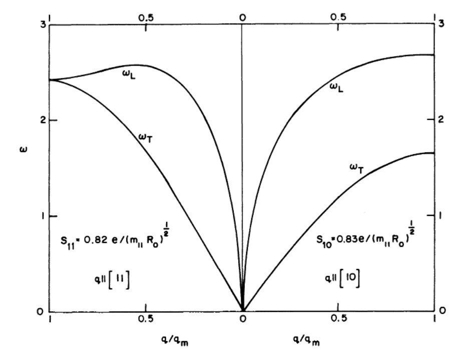
(Received October 15, 1934)

If the electrons had no kinetic energy, they would settle in configurations which correspond to the absolute minima of the potential energy. These are closed-packed lattice configurations, with energies very near to that of the body-centered lattice. Here, every electron is very

$$V(r) = \frac{e^2}{r}$$



$$\frac{e^2}{R_s} \gg \frac{\hbar^2}{2mR_s^2}$$



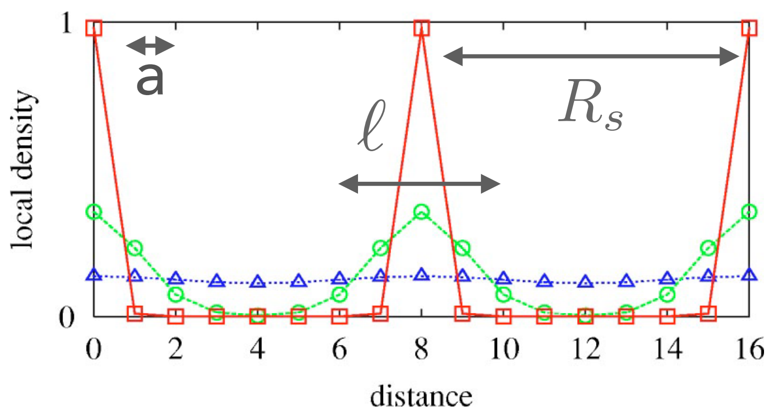
- the Wigner crystal has very low energy (shear) collective modes, they are at the origin of its fragility
- WC is notoriously difficult to observe, maybe we can suppress these modes?

Generalized Wigner crystals

- The WC is notoriously difficult to observe: are there ways to make it more stable?

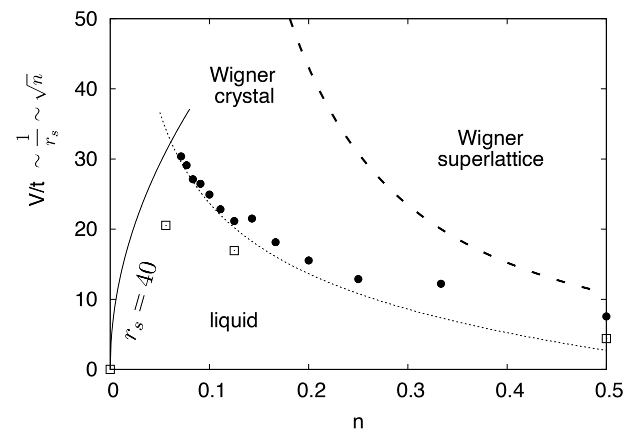
  route 1): lower the dimension r_s =**100** (3D), **40** (2D)

  route 2): get help from the periodic lattice inside materials (pin the modes)



[B. Valenzuela, SF, D. Baersiwyl, PRB 2003]

- continuum limit attained if $R_s \gg \ell \gg a$



[D. Baersiwyl, SF, ECRYS 2005]

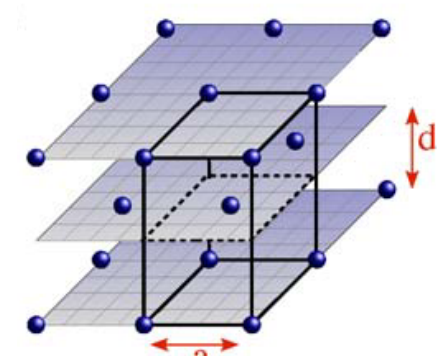
- commensurability with the underlying lattice

  -> r_s~**2** in 2D [Noda & Imada, PRL02]

- layered: 2D motion but keep 3D interactions -> r_s<**10**

  \+ naturally obtain charge order with square symmetry (cuprates?)

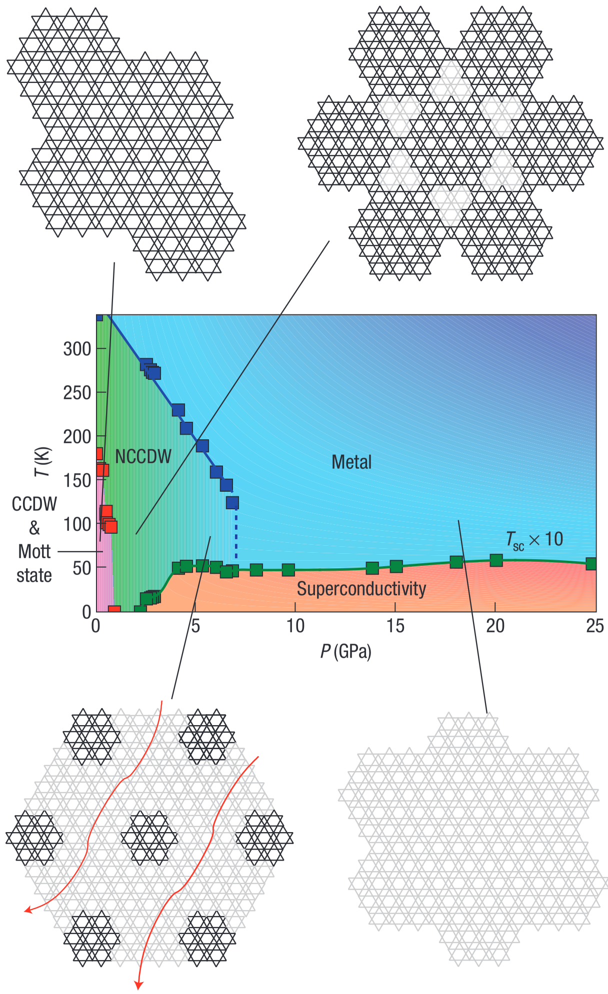
  [G. Rastelli et al EPJB04,G. Rastelli & SF PRB06]



- not surprisingly, commensurate WCs are seen in low dimensional (layered) materials

From Mott state to superconductivity in 1T-TaS_2

B. SIPOS[1]*, A. F. KUSMARTSEVA[1]*, A. AKRAP[1], H. BERGER[1], L. FORRÓ[1] AND E. TUTIŠ[2]
[1]Ecole Polytechnique Fédérale de Lausanne, IPMC, CH-1015 Lausanne, Switzerland
[2]Institute of Physics, Bijenička c. 46, Zagreb, Croatia
*e-mail: bsipos@gmail.com; anna.kusmartseva@ed.ac.uk

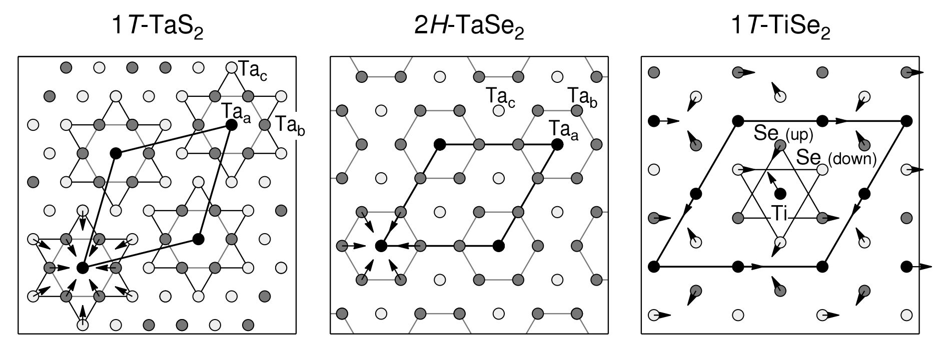


J. Phys.: Condens. Matter **23** (2011) 213001 (24pp) doi:10.1088/0953-8984/23/21/213001

TOPICAL REVIEW

On the origin of charge-density waves in select layered transition-metal dichalcogenides

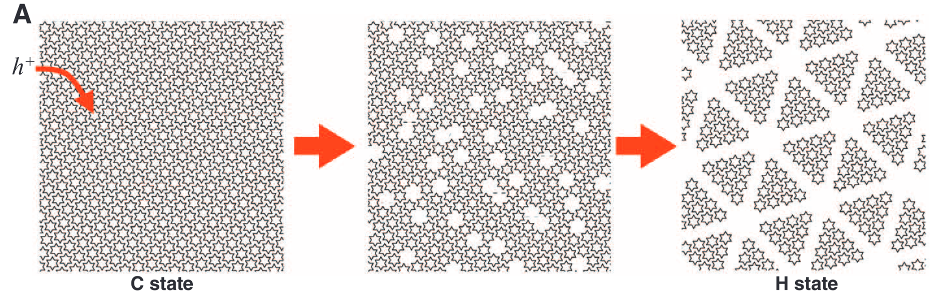
K Rossnagel



Ultrafast Switching to a Stable Hidden Quantum State in an Electronic Crystal

L. Stojchevska,[1,2] I. Vaskivskyi,[1] T. Mertelj,[1] P. Kusar,[1] D. Svetin,[1] S. Brazovskii,[3,4] D. Mihailovic[1,2,5]*

A



Article

Bilayer Wigner crystals in a transition metal dichalcogenide heterostructure

https://doi.org/10.1038/s41586-021-03560-w
Received: 4 October 2020
Accepted: 15 April 2021
Published online: 30 June 2021
Check for updates

You Zhou[1,2,9], Jiho Sung[1,2], Elise Brutschea[1], Ilya Esterlis[2], Yao Wang[2,3], Giovanni Scuri[2], Ryan J. Gelly[2], Hoseok Heo[1,2], Takashi Taniguchi[4], Kenji Watanabe[5], Gergely Zaránd[6], Mikhail D. Lukin[2], Philip Kim[2,7], Eugene Demler[2,8]✉ & Hongkun Park[1,2]✉

One of the first theoretically predicted manifestations of strong interactions in many-electron systems was the Wigner crystal[1–3], in which electrons crystallize into a

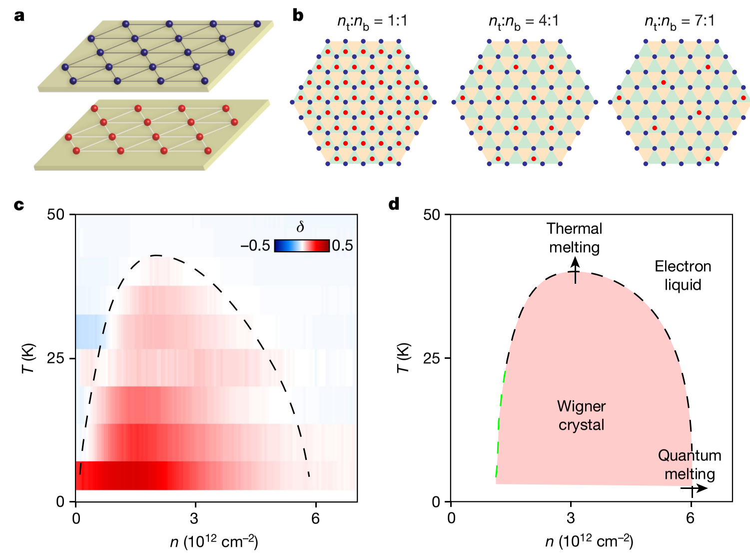
Article

Imaging two-dimensional generalized Wigner crystals

https://doi.org/10.1038/s41586-021-03874-9
Received: 3 April 2021
Accepted: 4 August 2021
Published online: 29 September 2021

Hongyuan Li[1,2,3,9], Shaowei Li[1,3,4,5,9]✉, Emma C. Regan[1,2,3], Danqing Wang[1,2], Wenyu Zhao[1], Salman Kahn[1,3], Kentaro Yumigeta[6], Mark Blei[6], Takashi Taniguchi[7], Kenji Watanabe[8], Sefaattin Tongay[6], Alex Zettl[1,3,4], Michael F. Crommie[1,3,4]✉ & Feng Wang[1,3,4]✉

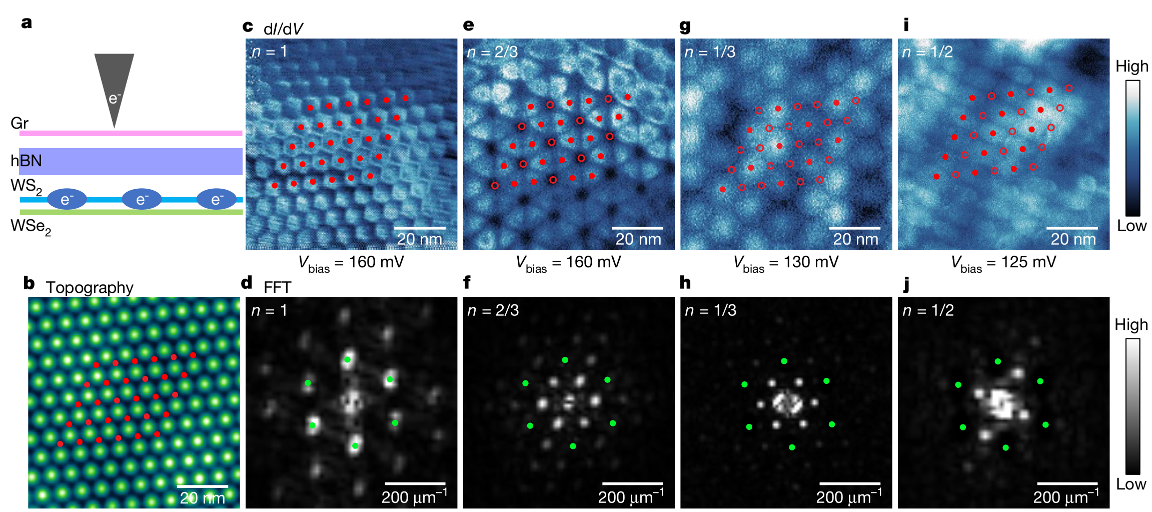
The Wigner crystal[1] has fascinated condensed matter physicists for nearly 90 years[2–14].



nature materials
LETTERS
https://doi.org/10.1038/s41563-021-00959-8
Check for updates

Stripe phases in WSe_2/WS_2 moiré superlattices

Chenhao Jin[1,7]✉, Zui Tao[1,2,7], Tingxin Li[2,7], Yang Xu[2], Yanhao Tang[2], Jiacheng Zhu[2], Song Liu[3], Kenji Watanabe[4], Takashi Taniguchi[4], James C. Hone[3], Liang Fu[5]✉, Jie Shan[1,2,6]✉ and Kin Fai Mak[1,2,6]✉



nature physics | LETTERS
PUBLISHED ONLINE: 9 JUNE 2013 | DOI: 10.1038/NPHYS2642

Charge-cluster glass in an organic conductor

F. Kagawa[1,2]*, T. Sato[1], K. Miyagawa[1], K. Kanoda[1], Y. Tokura[1,3], K. Kobayashi[4], R. Kumai[2,4] and Y. Murakami[4]

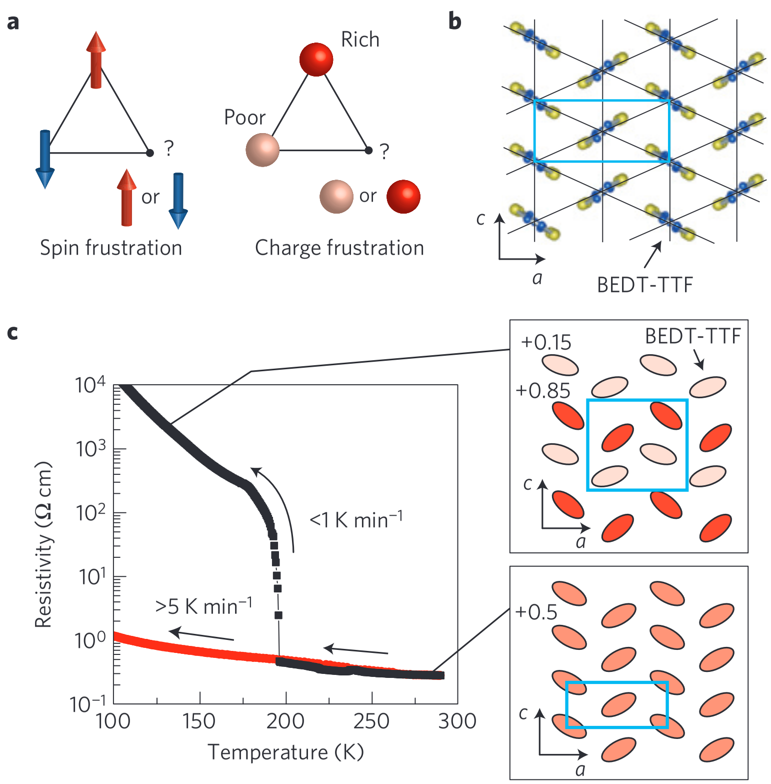
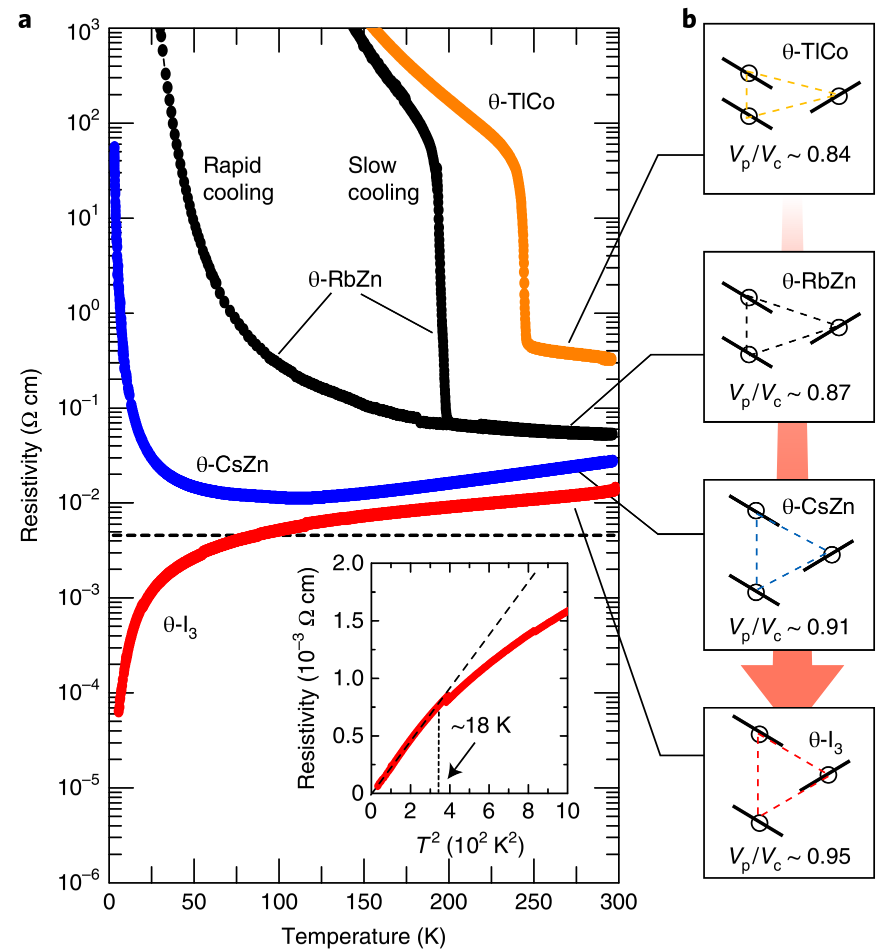


Figure 1 | Charge frustration and crystal structure of θ-(BEDT-TTF)$_2$RbZn(SCN)$_4$. a, An illustration of the analogy between spin

nature materials | ARTICLES
https://doi.org/10.1038/s41563-019-0284-9

Strange metal from a frustration-driven charge order instability

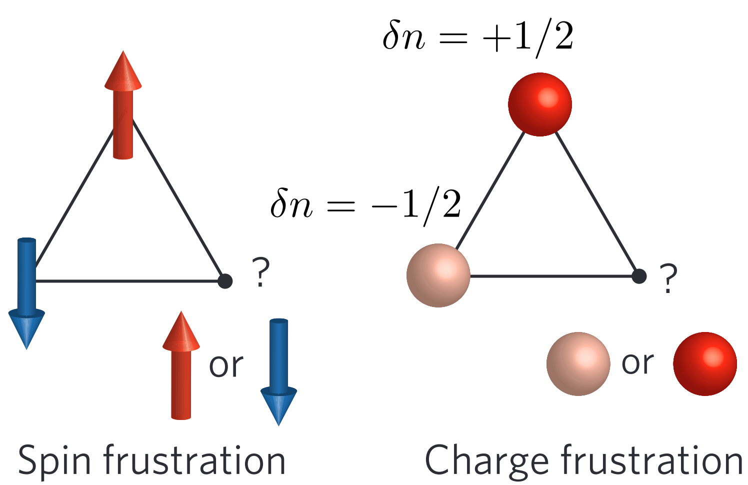
T. Sato[1,4]*, K. Kitai[1], K. Miyagawa[1], M. Tamura[2], A. Ueda[3], H. Mori[3] and K. Kanoda[1]*



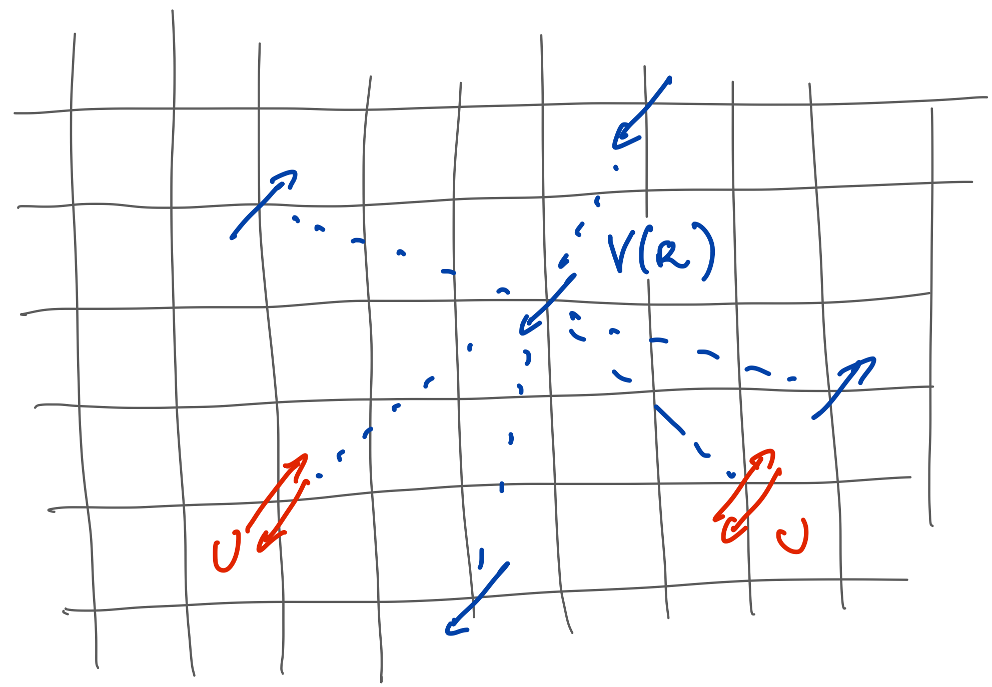
e-e interactions beyond Hubbard: 2 types of frustration

$$H = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^{+} c_{j\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow} + \frac{1}{2} \sum_{i \neq j} V(R_{ij}) n_i n_j \qquad V(R) = \frac{V}{R^\alpha}$$

- geometric: specific to triangular lattice at n=1/2 (appears already for nearest neighbor repulsion)
- long range, all electrons interact together at all distances

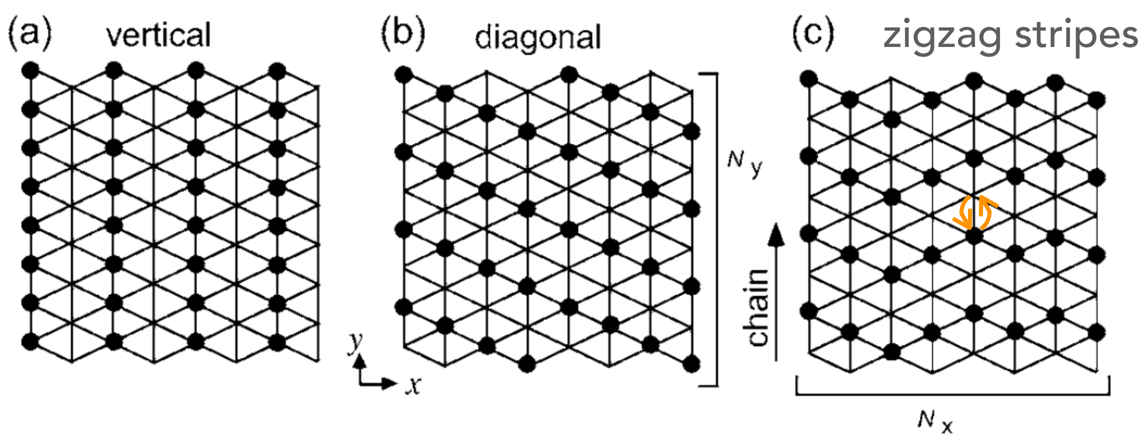


[F. Kagawa et al, NPhys 2013]

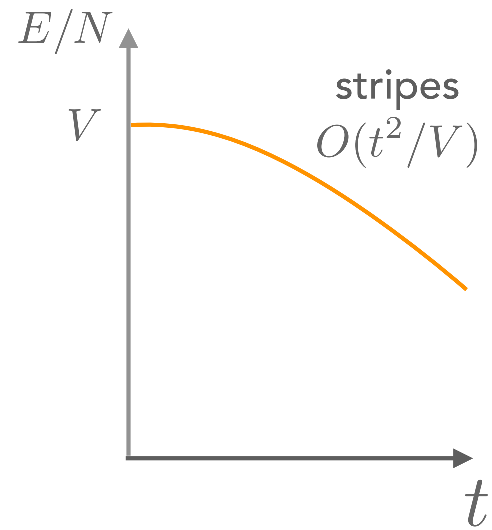


Degeneracy and lifting by quantum fluctuations

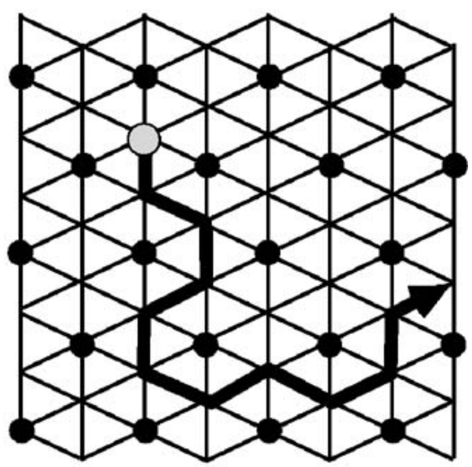
- n.n. interactions on the triangular lattice at n=1/2:
  infinitely many states with the same electrostatic energy

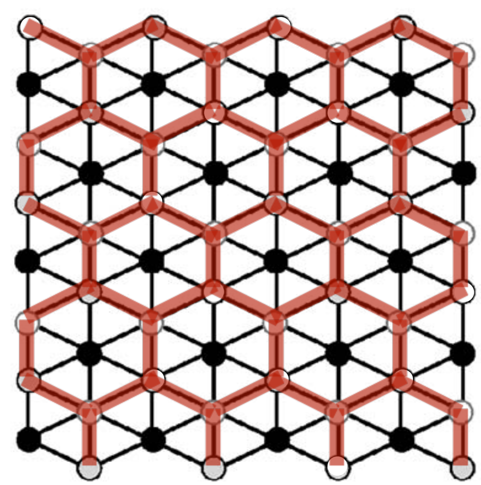


$$\frac{E}{N} = V$$



lock-in at
n=1/3





add the remaining n=1/2-1/3
on interstitials:
same $E/N = V$

quantum fluctuations:
gain Kinetic energy
O(t) (not t^2 !)

[C. Hotta, N. Furukawa, PRB 06]

Degeneracy and lifting by quantum fluctuations

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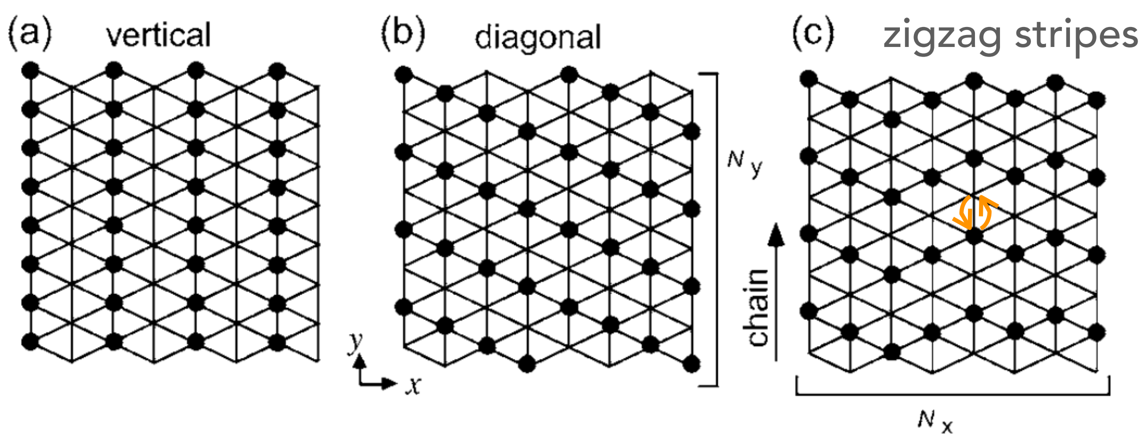

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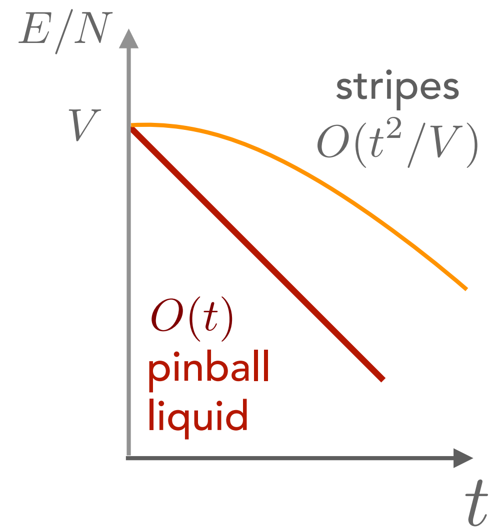
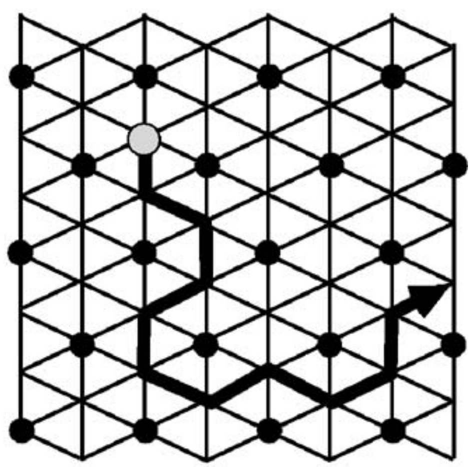
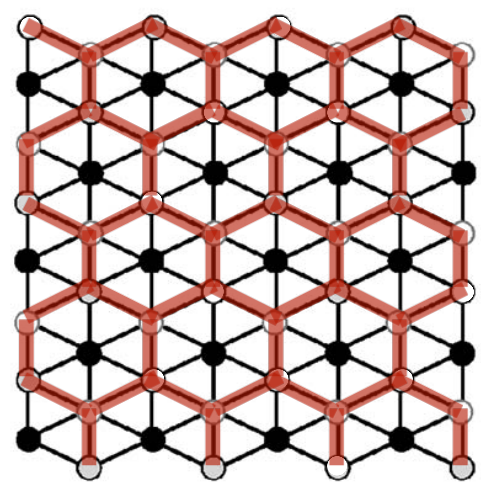


lock-in at n=1/3



[C. Hotta, N. Furukawa, PRB 06]



add the remaining n=1/2-1/3 on interstitials: same $E/N = V$

quantum fluctuations: gain Kinetic energy O(t) (not t^2 !)

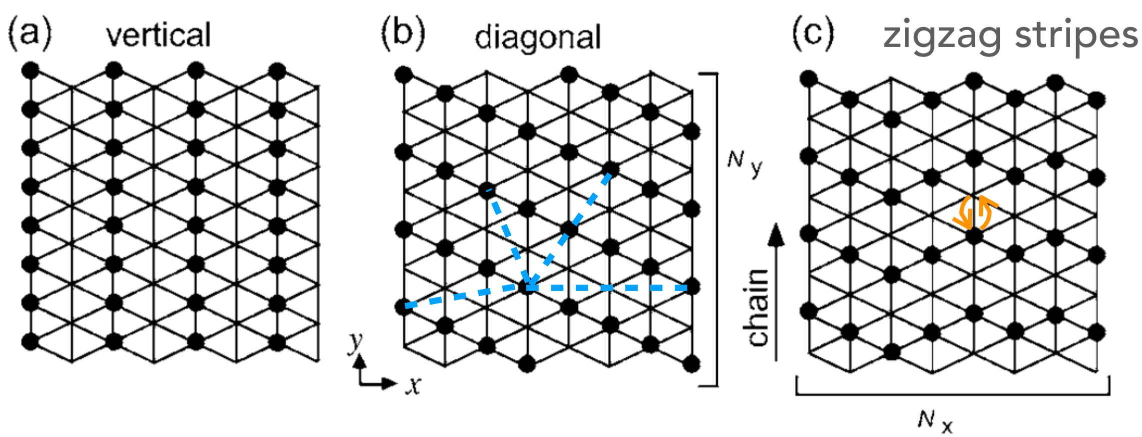
pinball liquid (unique ground state)

observed experimentally in $AgNiO_2$

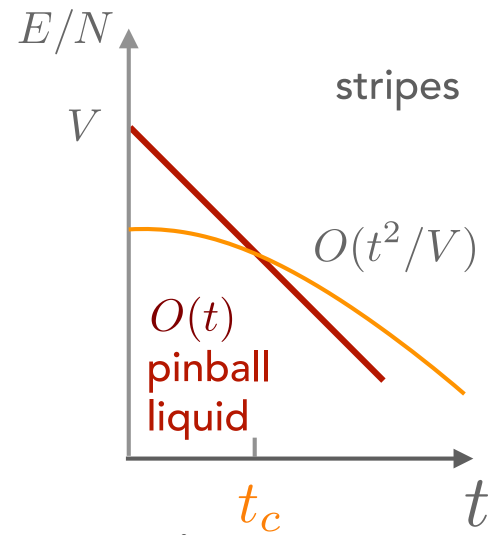
[R. Coldea et al PRL 2007, PRL 2011; A. Ralko, J. Merino, SF, PRB 15]

Degeneracy, lifting by long range interactions

- n.n. interactions on the triangular lattice at n=1/2:
  infinitely many states with the same electrostatic energy



$$\frac{E}{N} = V$$



- add long range interactions: stripes now have the lowest electrostatic energy, all other states become metastable
- stripe to pinball transition occurs at a critical t/V

Degeneracy, lifting by long range interactions

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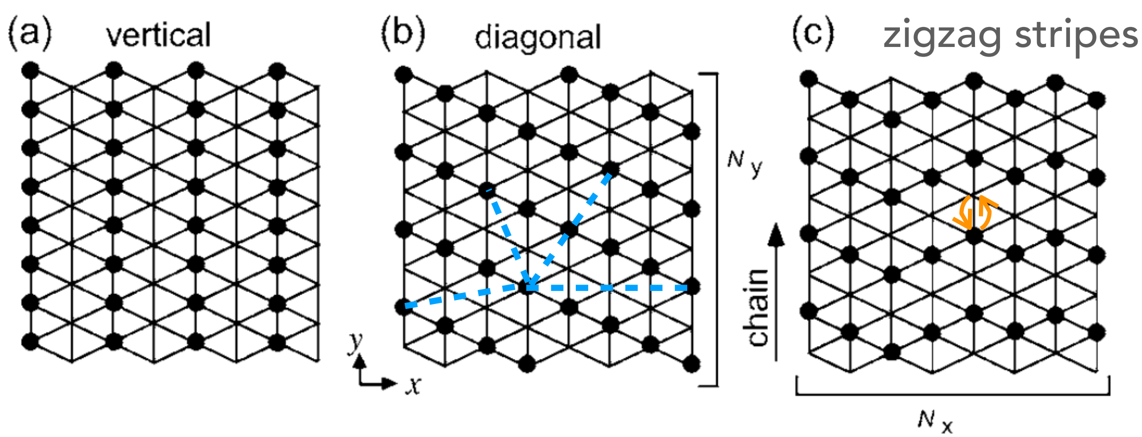
  infinitely many states with the same electrostatic energy



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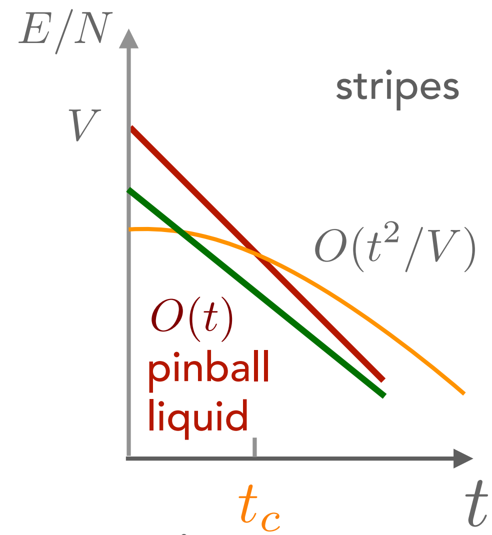
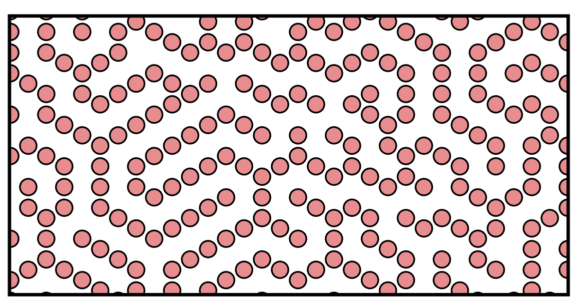


- add long range interactions: stripes now have the lowest electrostatic energy, all other states become metastable
- stripe to pinball transition occurs at a critical t/V
- can we find a state that combines the electrostatic gain ~V of the stripes and the quantum gain ~t of the pinball, and is therefore more stable than both?



(spoiler: "hidden state" or charge glass)

Long Range Coulomb on triangular lattice

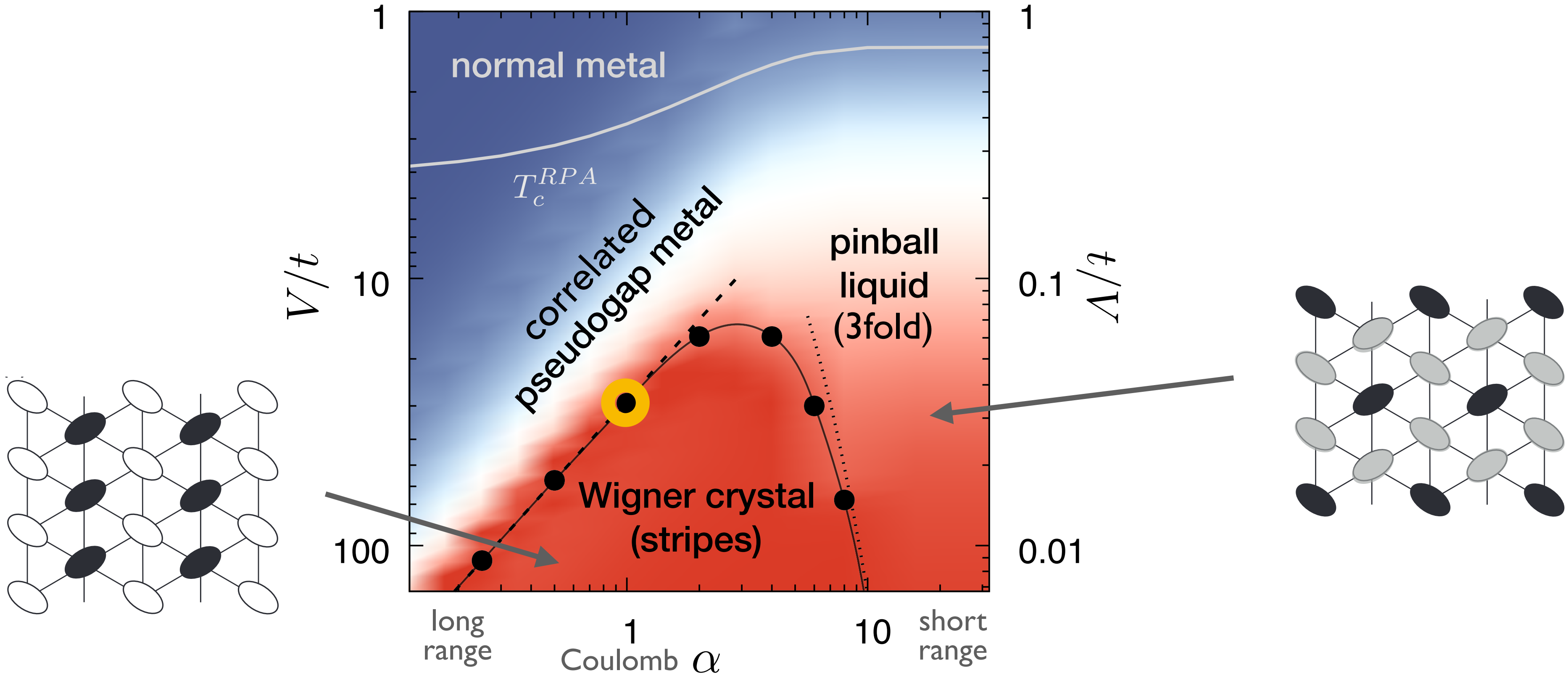
$$H = -t \sum_{\langle ij \rangle \sigma} (c^{+}_{i\sigma} c_{j\sigma} + h.c.) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + \frac{1}{2} \sum_{i \neq j} V(R_{ij}) n_i n_j \qquad V(R) = \frac{V}{R^{\alpha}}$$

- quantum ED T=0: spinful/spinless, n=0.5, use Ewald and TBC averaging
  [SF, J. Merino, PRB 2009; K. Driscoll, A. Ralko and SF, PRB(L) 2021]
- classical MC T>0: spinless, n=0.5 [Mahmoudian et al., PRL 2015]
- mixed quantum/classical T>0: classical MC + quantum calculation of conductivity, all n
  [SF, K. Driscoll, S. Ciuchi, A. Ralko, arXiv 2208.06260 this week]
- fully quantum T>0: FTLM solution in progress, KPM solution in progress

focus on the metal near the Wigner crystal melting where LR interactions matter

Long Range Coulomb on triangular lattice

$$H = -t\sum_{\langle ij\rangle\sigma}(c^+_{i\sigma}c_{j\sigma}+h.c.) + U\sum_i n_{i\uparrow}n_{i\downarrow} + \frac{1}{2}\sum_{i\neq j}V(R_{ij})n_in_j \qquad V(R)=\frac{V}{R^\alpha}$$

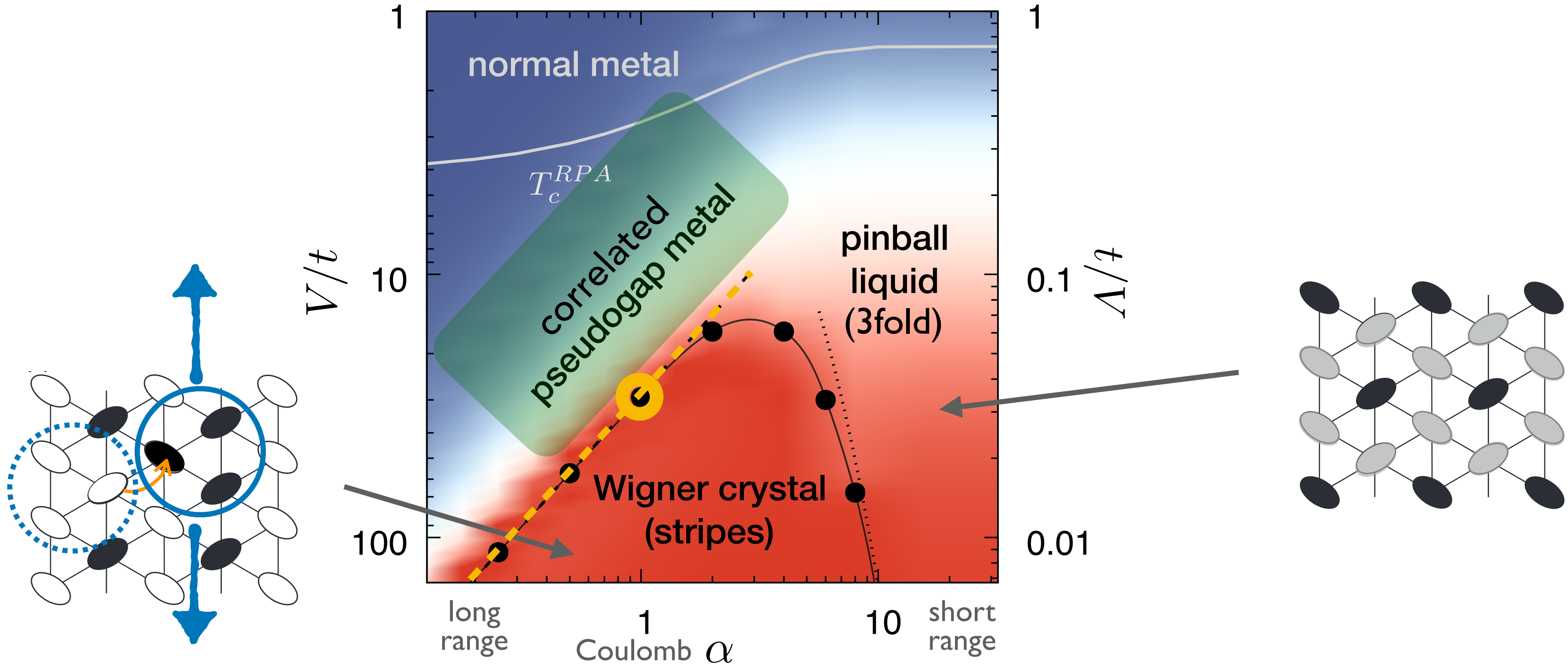


- $r_s = 7.2$ due to commensurability with underlying lattice

[K. Driscoll, A. Ralko and SF, PRB(L) 2021]

Long Range Coulomb on triangular lattice

$$H = -t\sum_{\langle ij\rangle\sigma}(c^+_{i\sigma}c_{j\sigma} + h.c.) + U\sum_i n_{i\uparrow}n_{i\downarrow} + \frac{1}{2}\sum_{i\neq j}V(R_{ij})n_in_j \qquad V(R) = \frac{V}{R^\alpha}$$

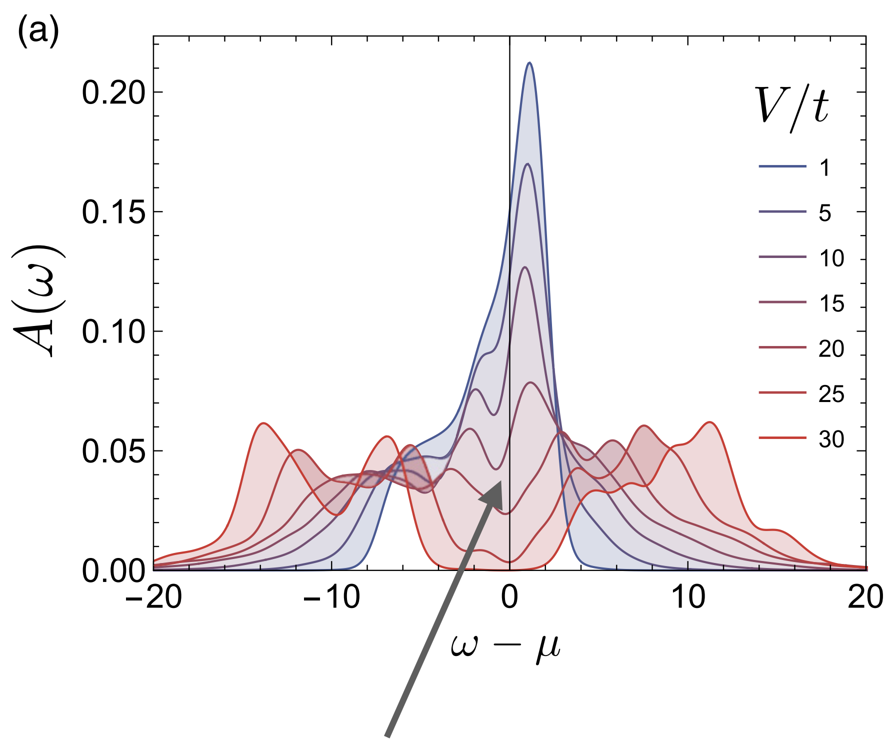


- $r_s = 7.2$ due to commensurability with underlying lattice
- increasing Vc/t with range of interactions indicates key role of charge defects for melting of long range order (lattice equivalent of soft collective excitations)
- short range order persists in the metal up to the mean field transition (V/t~1)

[K. Driscoll, A. Ralko and SF, PRB(L) 2021]

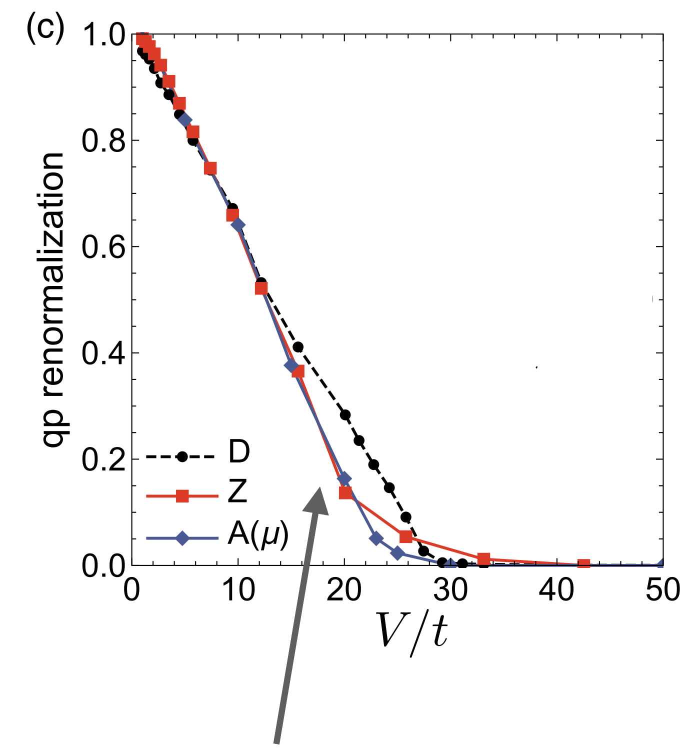
Correlated pseudogap metal

spectral function



pseudogap emerges in the interacting liquid

Drude and q.p. weight

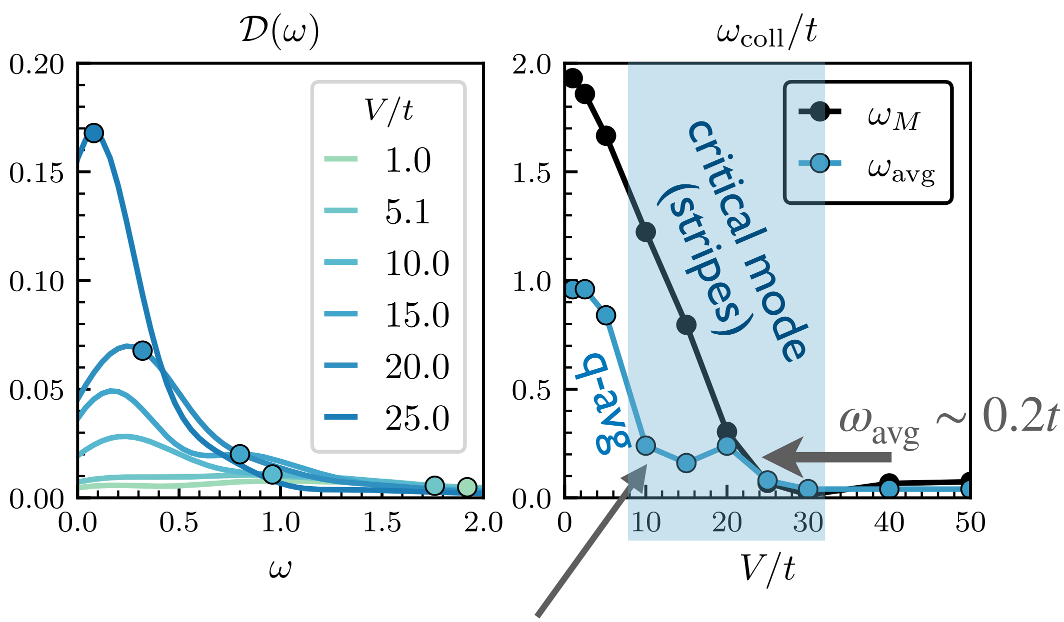


pseudogap regime is strongly correlated, (no local U, no magnetic moments!)

[K. Driscoll, A. Ralko and SF, PRB(L) 2021]

Self-generated disorder

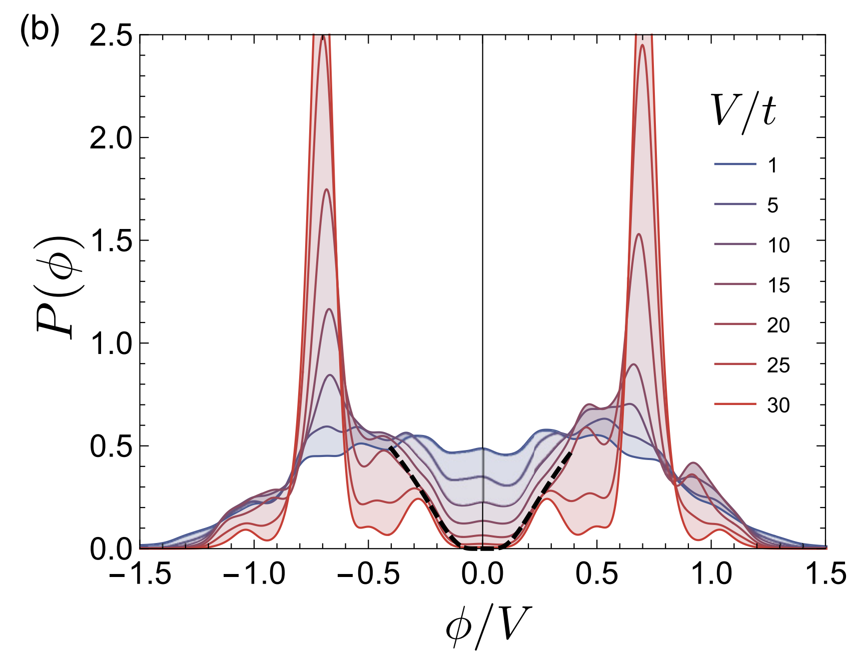
spectrum of collective charge excitations



the overall timescale of collective motions is slow within the entire pseudogap phase

$\phi_i = \sum_j V_{ij} n_j$

distribution of instantaneous site potentials



separation of timescales

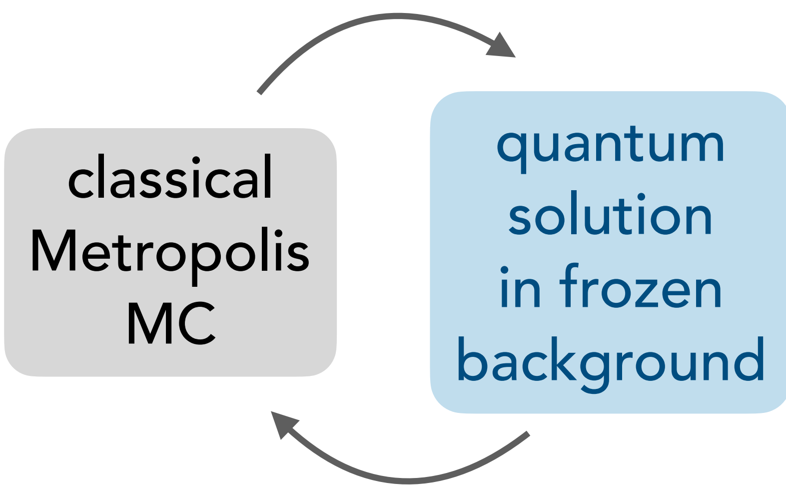
$\omega_0 \simeq 0.2t$ << bandwidth

the collective motions are much slower than the indvidual motions: the electrons move in a self-generated disordered background
cf. Andreev and Kosevic (1979) and Efros (1992)

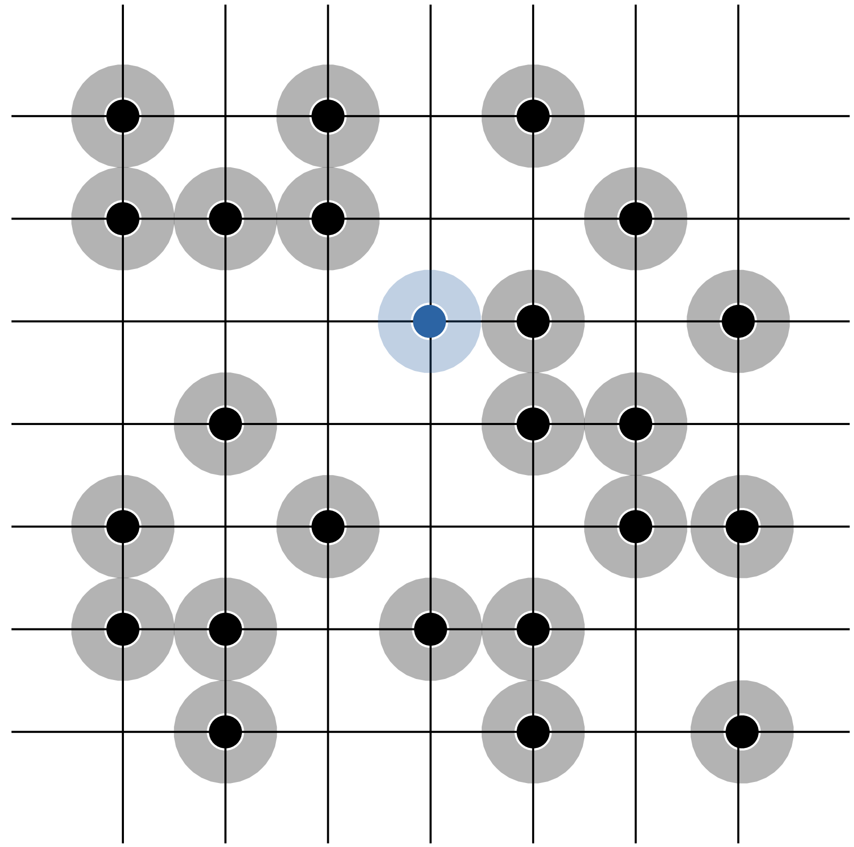
[K. Driscoll, A. Ralko and SF, PRB(L) 2021]

Mixed quantum/classical treatment

individual motions, fast:
quantum electrons in
the collective landscape



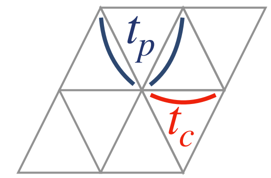
collective motions, slow: classical MC

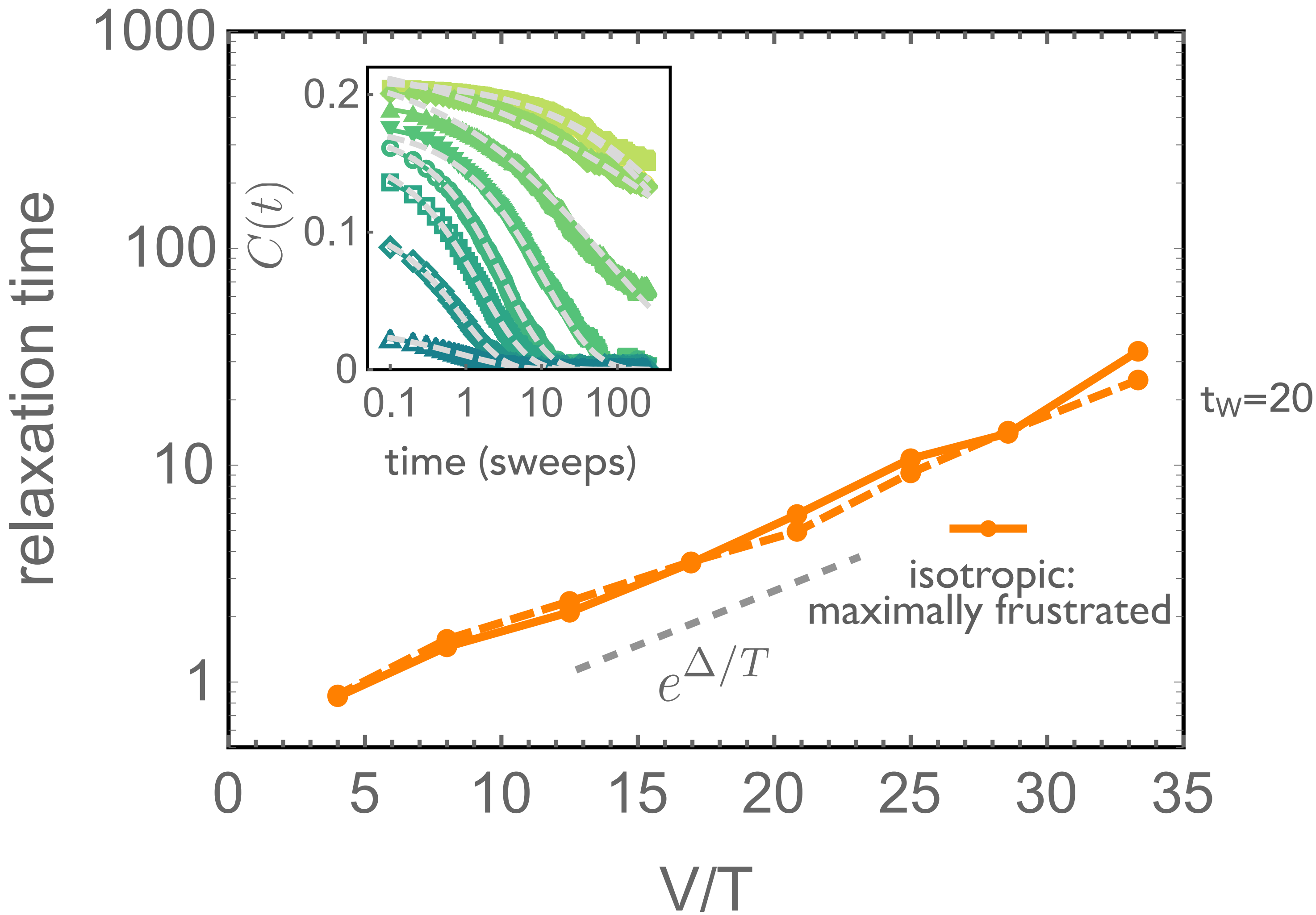


- metastable states
- crystallization dynamics and aging
- impact on electron transport
- P(n), C(q), sigma(w), rho(T), A(k,w), Cv/T…

Exponential slowing down vs frustration

$$C(t, t_W) = \sum_i \langle n_i(t + t_W) n_i(t_W) \rangle$$

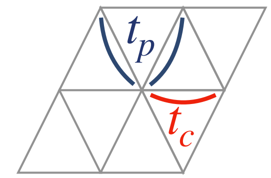


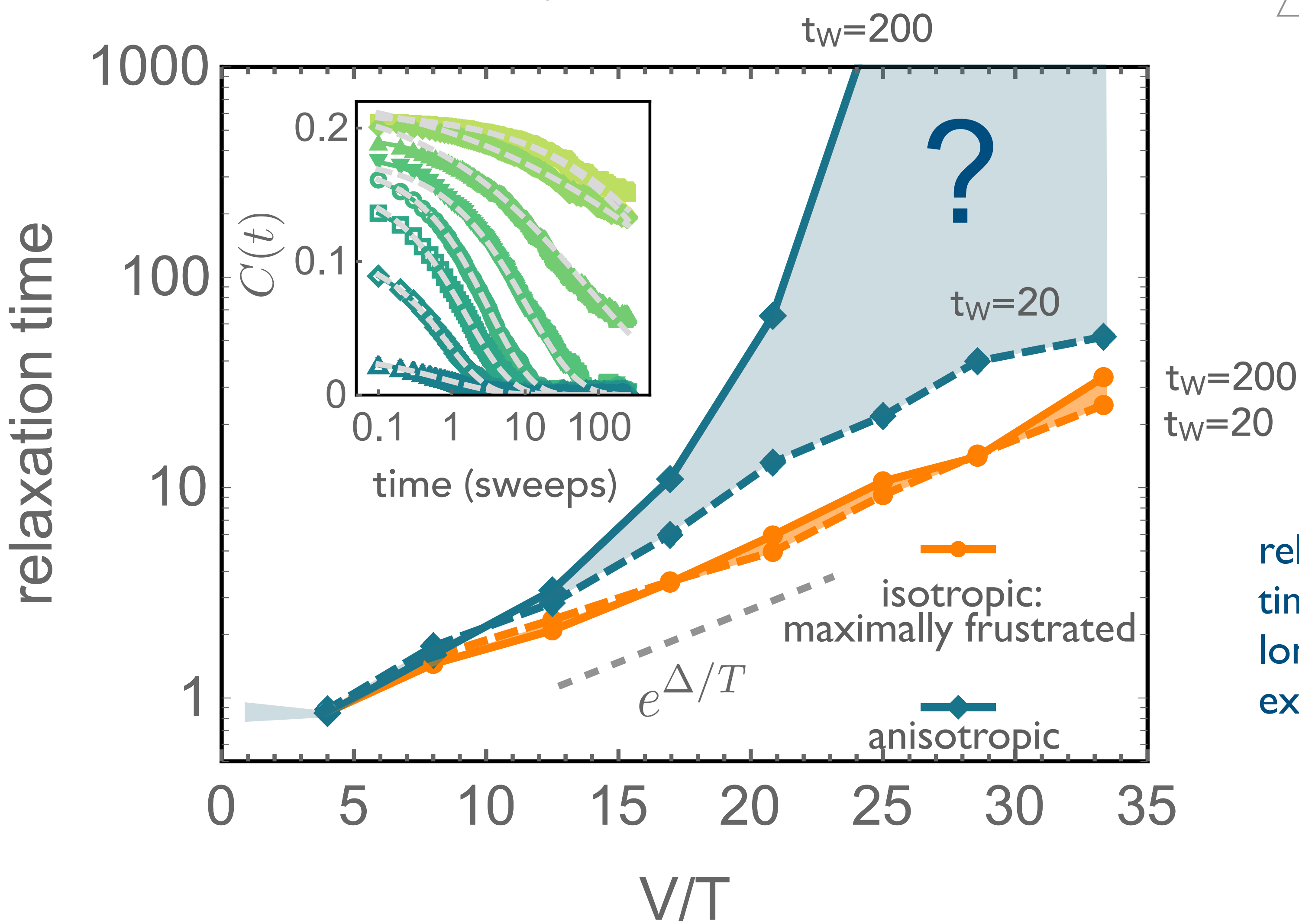


[SF, K. Driscoll, S. Ciuchi, A. Ralko, arXiv 2208.06260 this week]

Exponential slowing down vs frustration

$$C(t,t_W) = \sum_i \langle n_i(t+t_W) n_i(t_W) \rangle$$

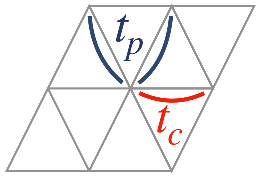




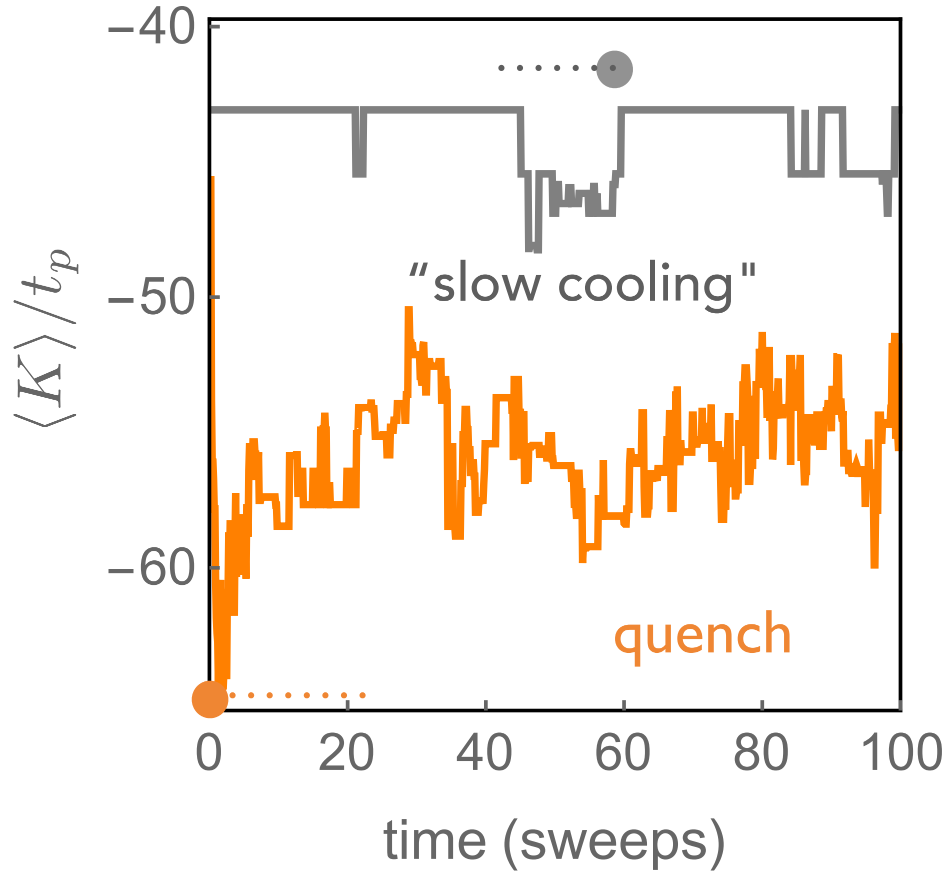
relaxation time grows longer than exponential

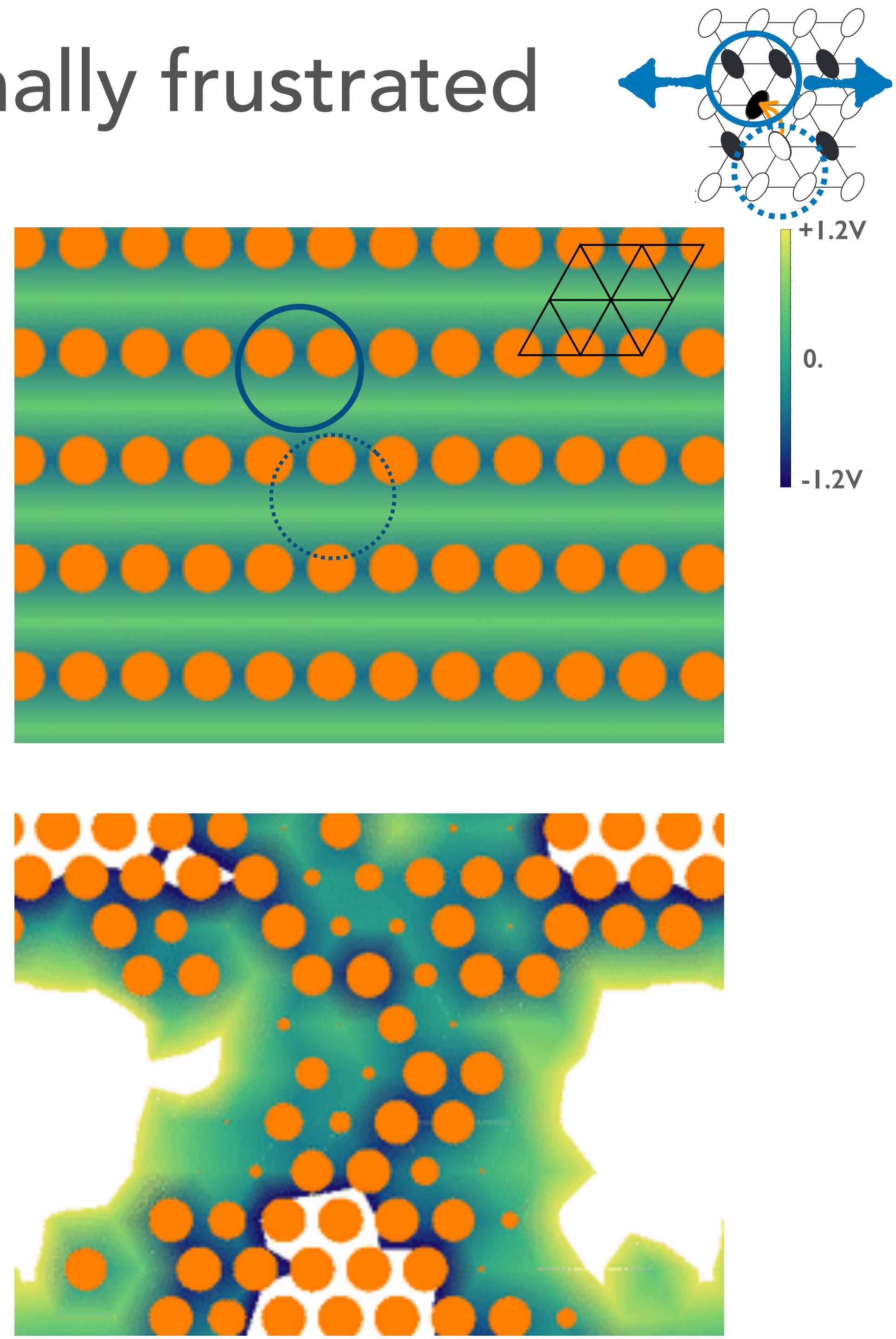
[SF, K. Driscoll, S. Ciuchi, A. Ralko, arXiv 2208.06260 this week]

Phase dynamics: maximally frustrated



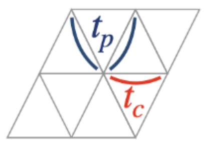
$t_p = t_c = 0.090V$
$T = 0.025V$



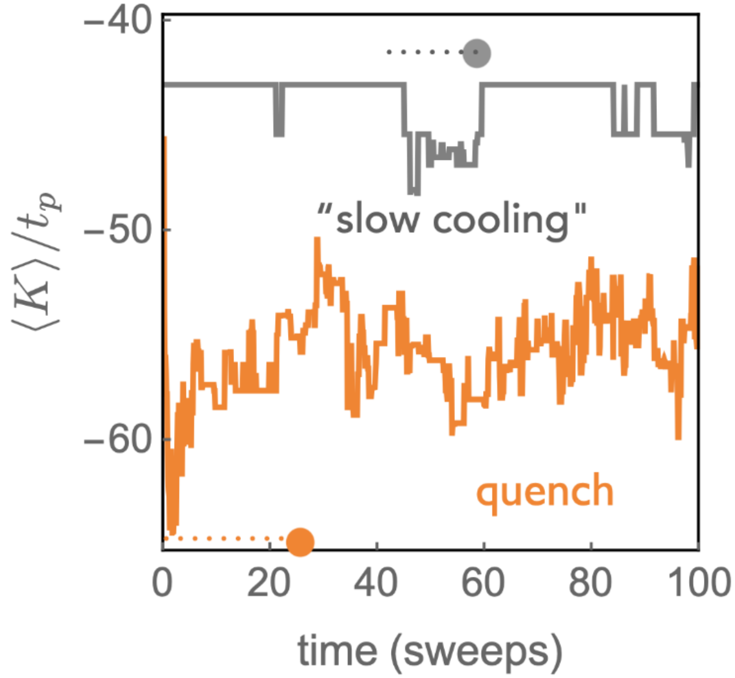


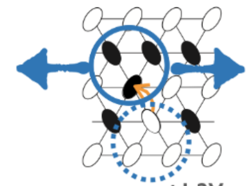
[SF, K. Driscoll, S. Ciuchi, A. Ralko, arXiv 2208.06260 this week]

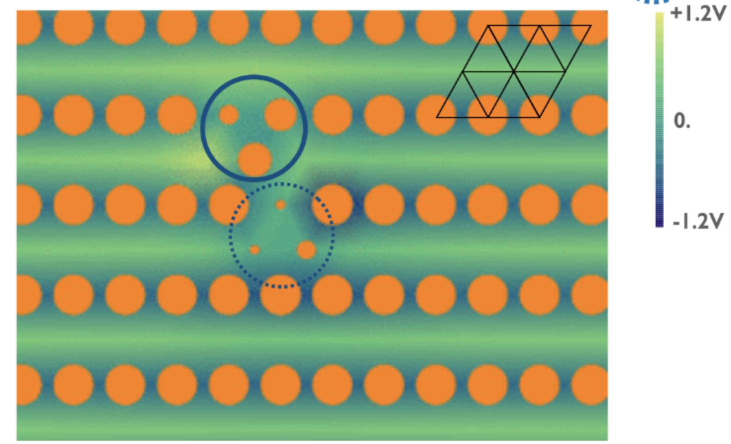
Phase dynamics: maximally frustrated

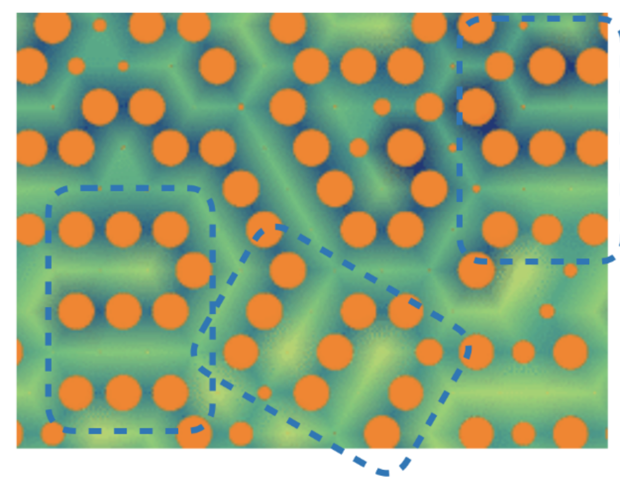


$t_p = t_c = 0.090V$
$T = 0.025V$





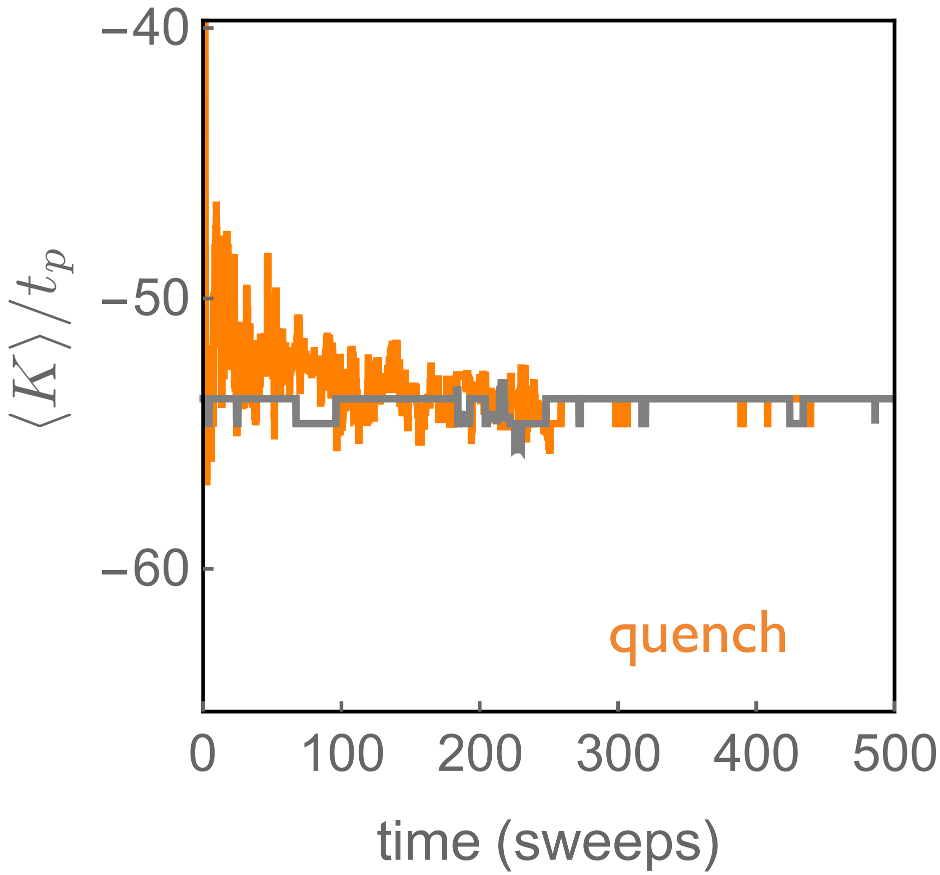


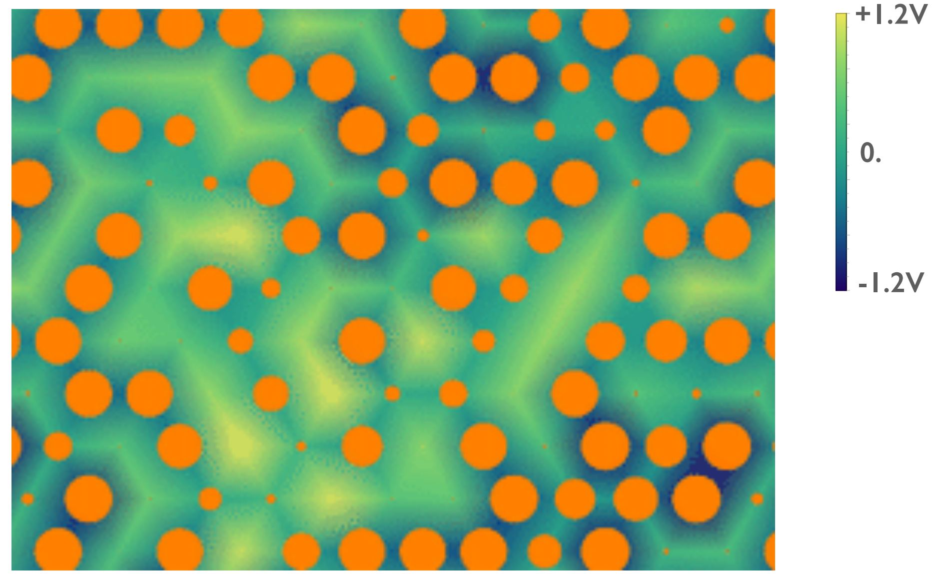


[SF, K. Driscoll, S. Ciuchi, A. Ralko, arXiv 2208.06260 this week]

Phase dynamics: strained (anisotropic)

$t_c/t_p = 0.1$
$t_p = 0.12V$
$T = 0.03V$





- outcome depends on history
- outcome depends on anisotropy of quantum electrons

[SF, K. Driscoll, S. Ciuchi, A. Ralko, arXiv 2208.06260 this week]

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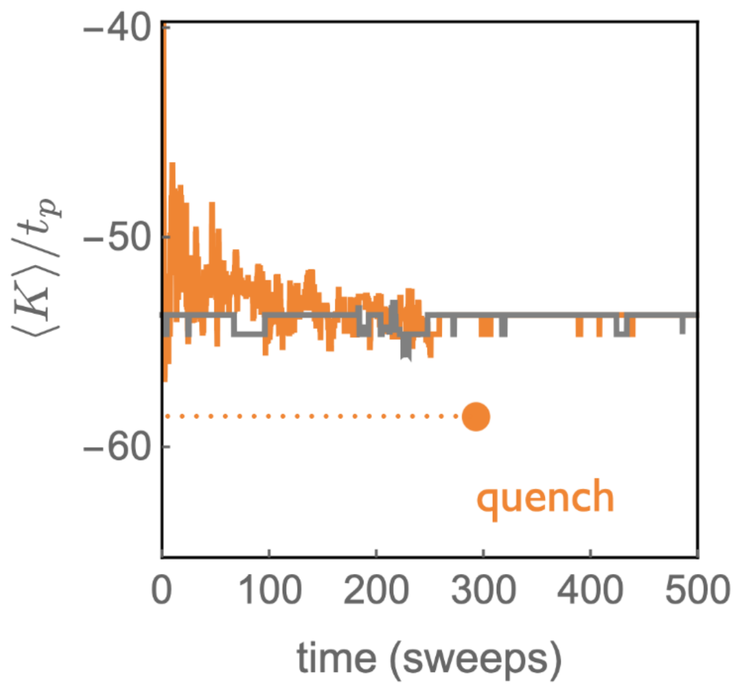
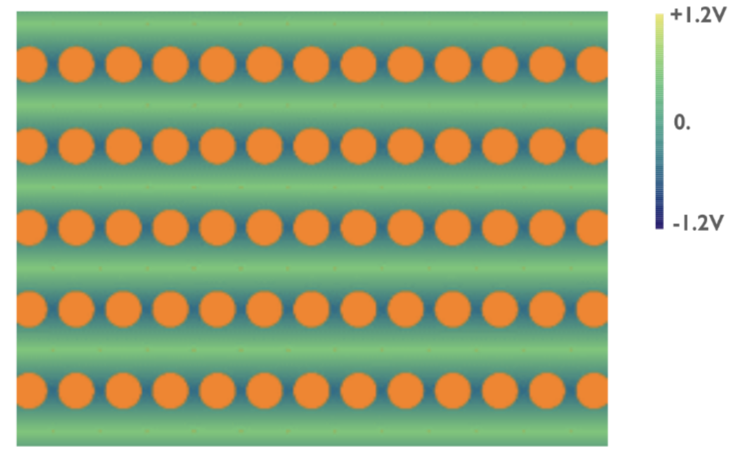


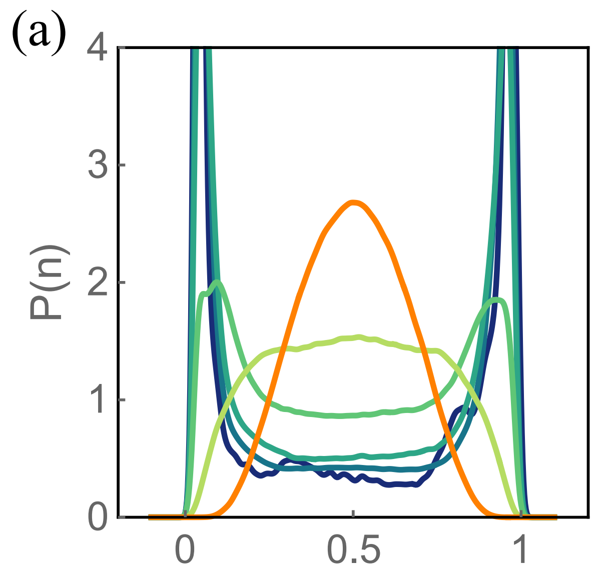


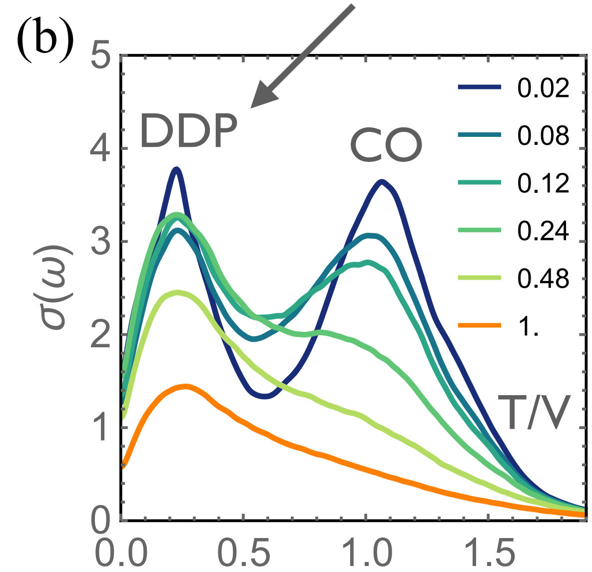
- outcome depends on history
- outcome depends on anisotropy of quantum electrons

[SF, K. Driscoll, S. Ciuchi, A. Ralko, arXiv 2208.06260 this week]

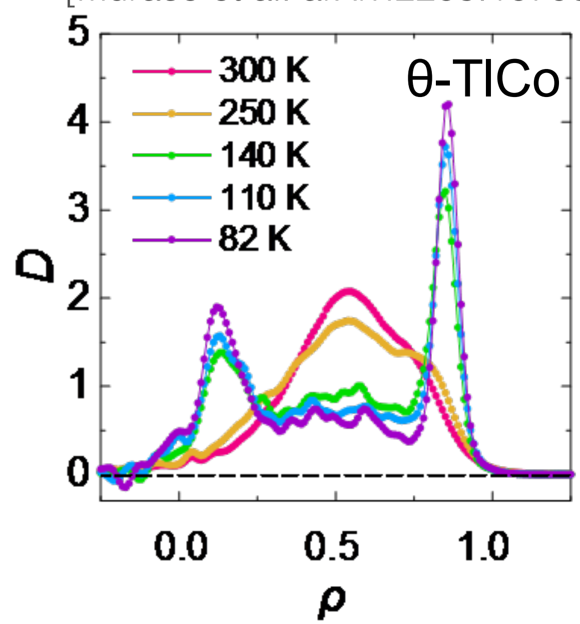
Characterization of charge glass

(localization in self generated disorder)

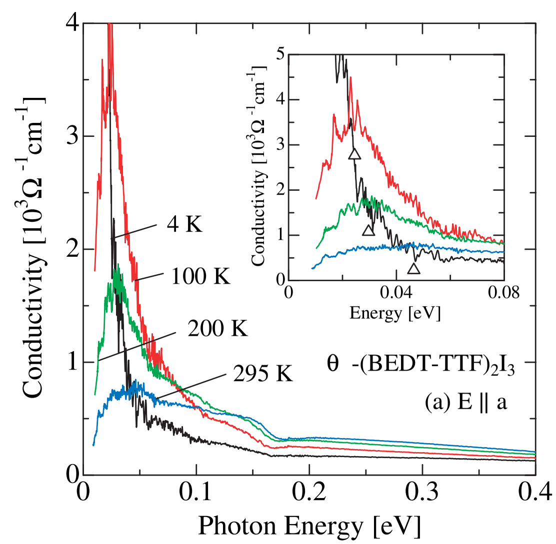




[Murase et al. arXiv:2205.10795]

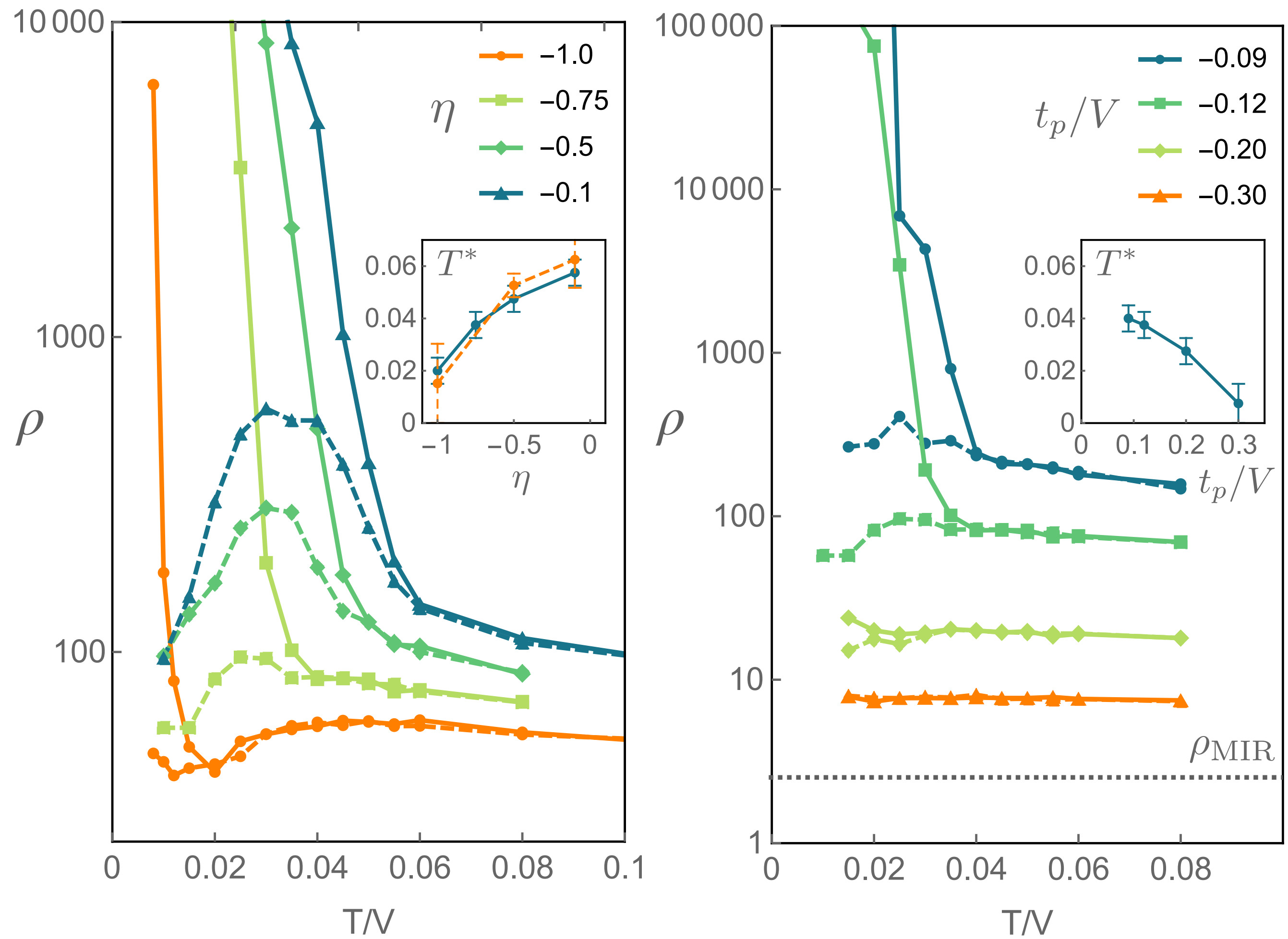


[Takenaka et al, PRL (2005)]



[SF, K. Driscoll, S. Ciuchi, A. Ralko, arXiv 2208.06260 this week]

Self-generated disorder (MC,classical)



[SF, K. Driscoll, S. Ciuchi, A. Ralko, arXiv 2208.06260 this week]

Concluding remarks

- Long range interacting electrons on lattices display charge frustration, at the origin of a variety of original physical phenomena.
- One of the most interesting is the emergence of self-generated disorder due to charge frustration (very **slow collective charge dynamics**), which is at the origin go the observed glass phase.
- This is also one plausible mechanism for bad metal behavior: it increases the resistivity above the semiclassical value, and Coulomb interactions are ubiquitous after all. It can also lead to strange T-linear behavior.