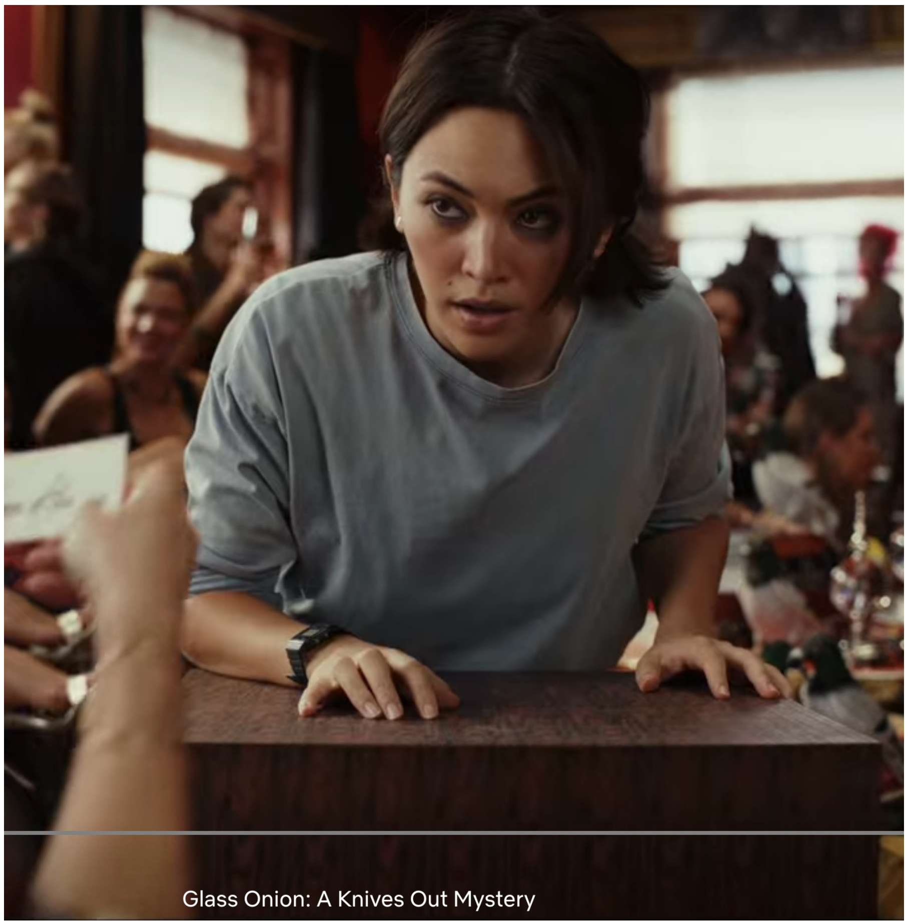
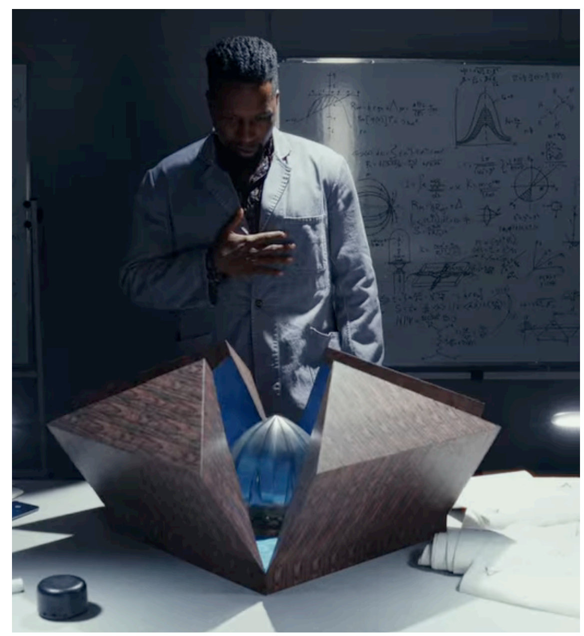
UQM and its probes: 2d materials and thermal transport

Leon Balents, UCSB

UQM meeting, Simons Foundation, January 2023

The UQM puzzle box





Outline

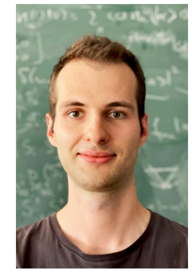
- Two on-going projects
    - **Looking for spin liquids in moiré "quantum simulators"**
    - Thermal Hall effect - towards a theoretical framework for transverse heat transport

Collaborators

TMD moiré

Zhenhao Song
UCSB

Zhu-Xi Luo
UCSB → Harvard



Urban Seifert
UCSB

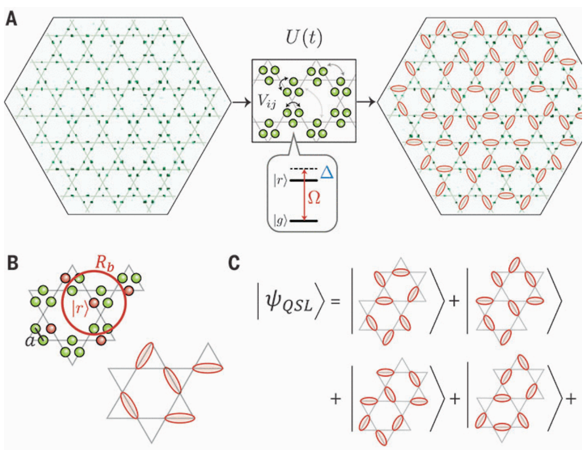
Thermal Hall

Léo Mangeolle
ENS Lyon

Lucile Savary
ENS Lyon

Scales

Quantum simulator

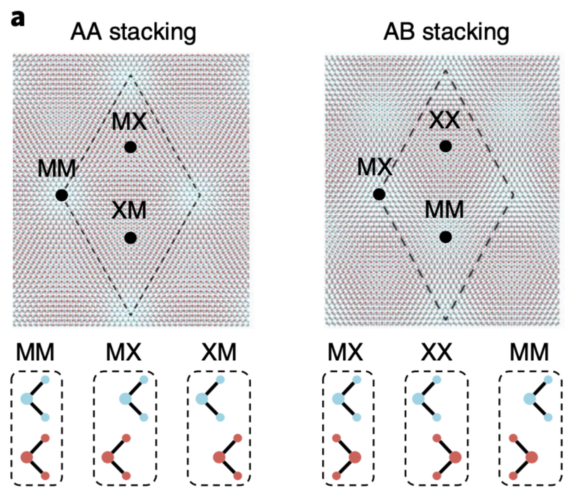


219 qubits

Very high degree of control

athermal

2d materials



10^6 qubits

Some control

meV scales

"Mesoscopic analog quantum simulator"

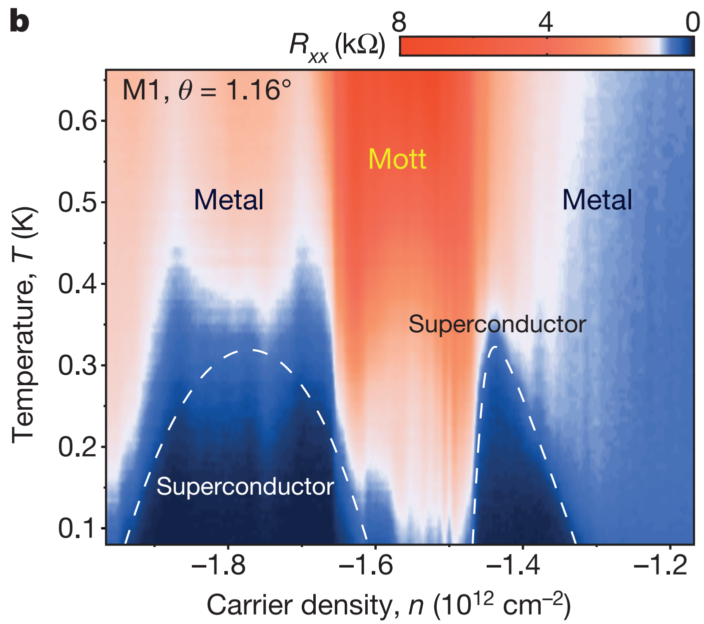
Crystals

10^{22} qubits

Caveat emptor

eV scales

Graphene



Y. Cao *et al*, 2018

PHYSICAL REVIEW X **8,** 031089 (2018)

Origin of Mott Insulating Behavior and Superconductivity in Twisted Bilayer Graphene

Hoi Chun Po,[1] Liujun Zou,[1,2] Ashvin Vishwanath,[1] and T. Senthil[2]
[1]*Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA*
[2]*Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*

PHYSICAL REVIEW LETTERS **122,** 106405 (2019)

Editors' Suggestion

Origin of Magic Angles in Twisted Bilayer Graphene

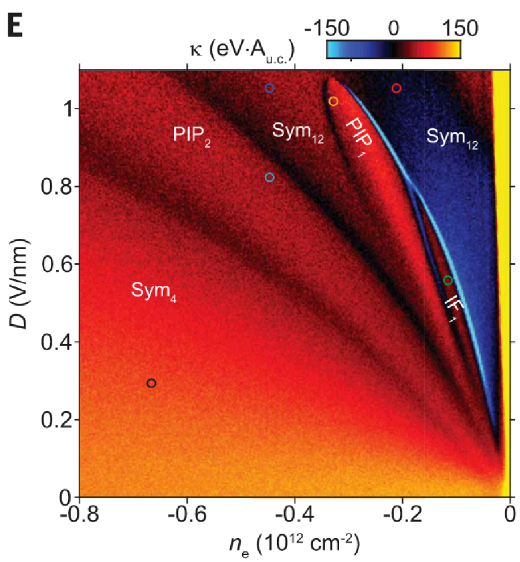
Grigory Tarnopolsky, Alex Jura Kruchkov,* and Ashvin Vishwanath
Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA

(Received 24 November 2018; published 15 March 2019; corrected 16 May 2019)

The pioneer, and the best quality

Unique features

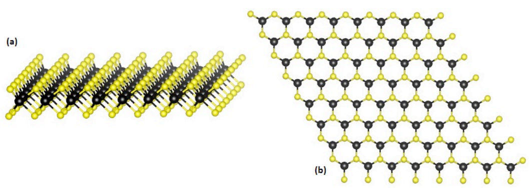
- Landau-level-like structure
- Topological obstruction to localized orbitals
- Strong tendency to form Chern bands
- Many features already present w/o moiré pattern
- Predominant generalized ferromagnetism



H. Zhou *et al*, 2022
Untwisted bilayer

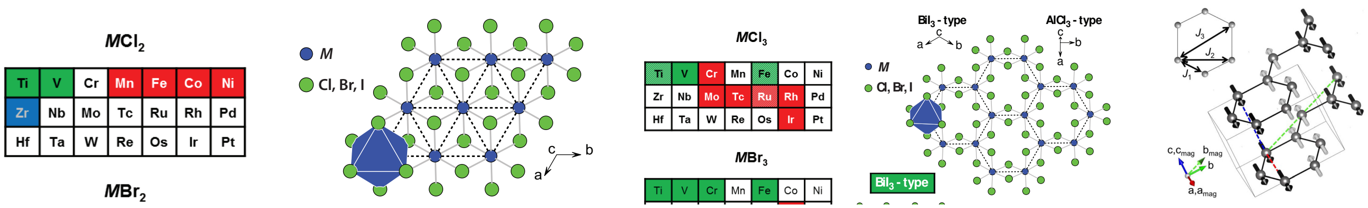
Beyond graphene: other 2d materials

- Transition metal dichalcogenide semiconductors



MX_2

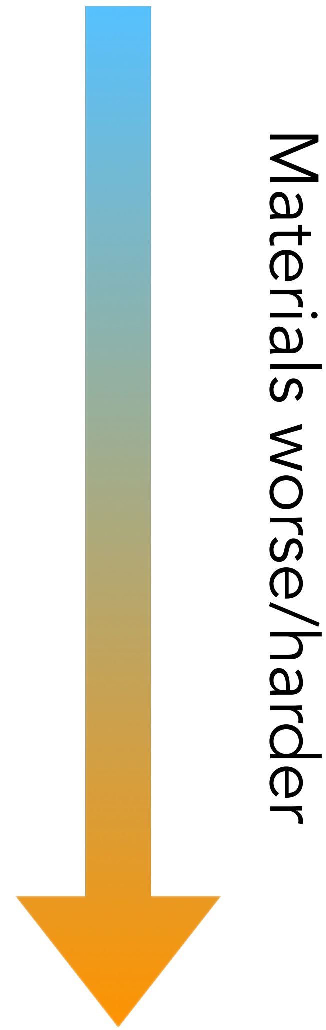
- Magnetic VdW materials



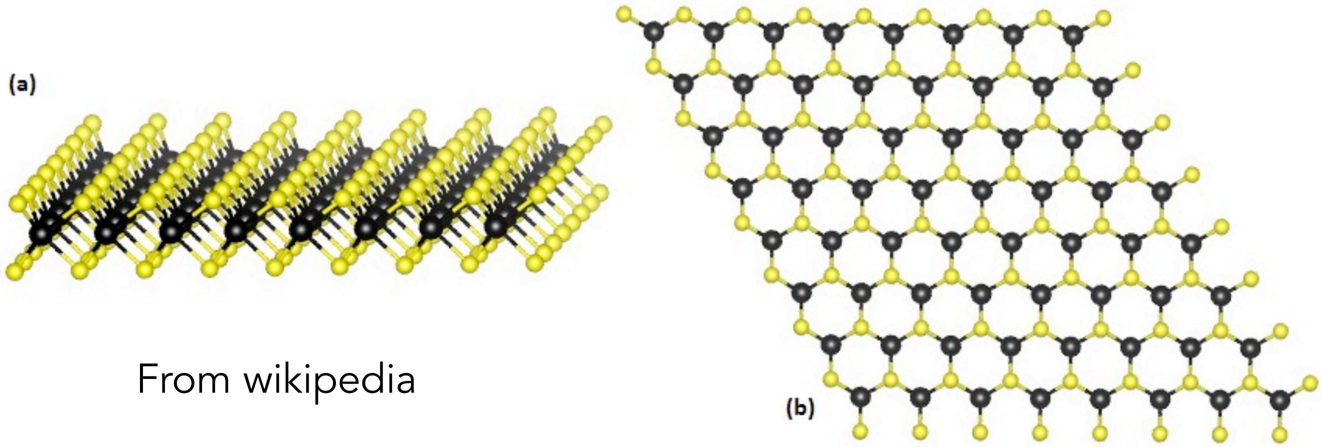
$MnPS_3$, CrI_3,…

- Intrinsically strong correlation materials

  BSCCO, $RuCl_3$, …



TMD



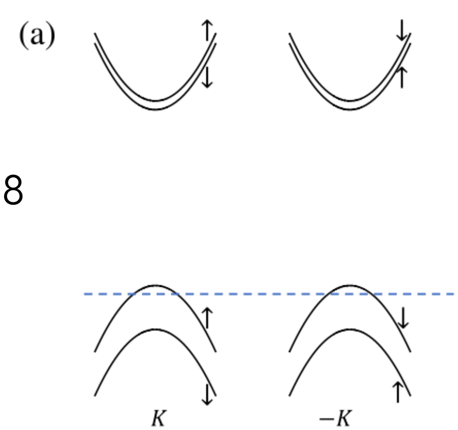
From wikipedia

MX_2

M=transition metal,
W, Mo, Nb etc.

X=chalcogenide
S,Se,Te

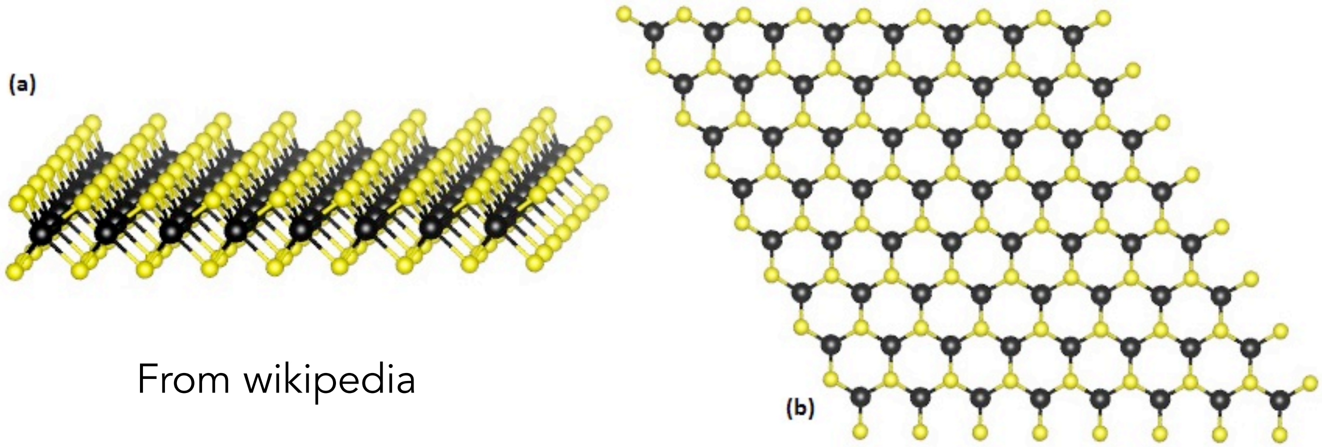
Typical band structure of TMD



F. Wu *et al*, 2018

- Quadratic dispersion: non-relativistic Schrödinger equation
- Spin-valley locking

TMD



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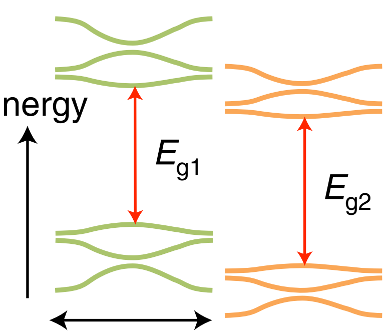


Large semiconducting gap

moiré bands localized around
band edge momenta

	graphene	TMD
Typical energy scales	$W \approx$ 10–100 meV $U \approx$ 20–40 meV	$W \approx$ 1–100 meV $U \approx$ 100–200 meV

K.-F. Mak, J. Shan, 2022

Hubbard simulator

PHYSICAL REVIEW LETTERS **121,** 026402 (2018)

Hubbard Model Physics in Transition Metal Dichalcogenide Moiré Bands

Fengcheng Wu,[1] Timothy Lovorn,[2] Emanuel Tutuc,[3] and A. H. MacDonald[2]

Article

Simulation of Hubbard model physics in WSe_2/WS_2 moiré superlattices

https://doi.org/10.1038/s41586-020-2085-3

Received: 18 August 2019

Yanhao Tang[1], Lizhong Li[1], Tingxin Li[1], Yang Xu[1], Song Liu[2], Katayun Barmak[3], Kenji Watanabe[4], Takashi Taniguchi[4], Allan H. MacDonald[5], Jie Shan[1,6,7] & Kin Fai Mak[1,6,7]

PHYSICAL REVIEW B **102**, 201104(R) (2020)

Quantum phase diagram of a Moiré-Hubbard model

Haining Pan, Fengcheng Wu, and Sankar Das Sarma

PHYSICAL REVIEW B **104**, 075150 (2021)

Editors' Suggestion

Hartree-Fock study of the moiré Hubbard model for twisted bilayer transition metal dichalcogenides

Jiawei Zang,[1] Jie Wang,[2] Jennifer Cano,[2,3] and Andrew J. Millis[1,2]

moiré (extended) Hubbard model

$$H = \sum_{s}\sum_{i,j} t_s(\boldsymbol{R}_i - \boldsymbol{R}_j) c^\dagger_{i,s} c_{j,s} + \frac{1}{2}\sum_{s,s'}\sum_{i,j} U(\boldsymbol{R}_i - \boldsymbol{R}_j) c^\dagger_{i,s} c^\dagger_{j,s'} c_{j,s'} c_{i,s},$$

complex hopping — Longer-range interactions

The Hubbard model is hard

D. Arovas *et al*, ARCMP, 2022

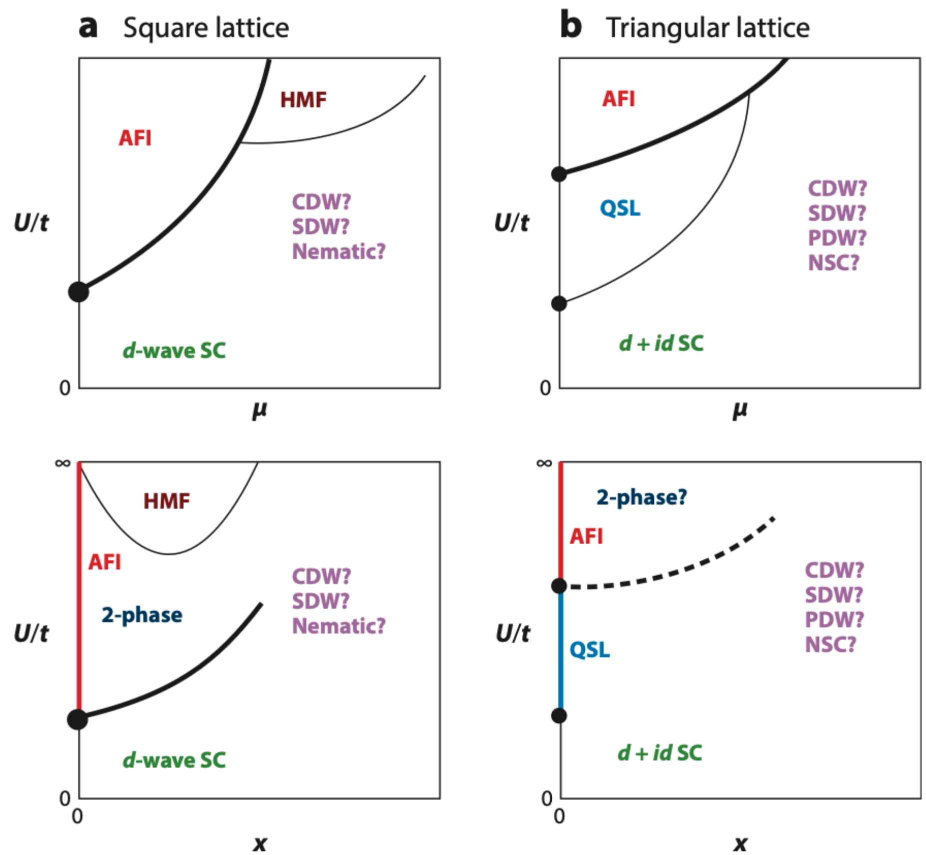


Figure 5

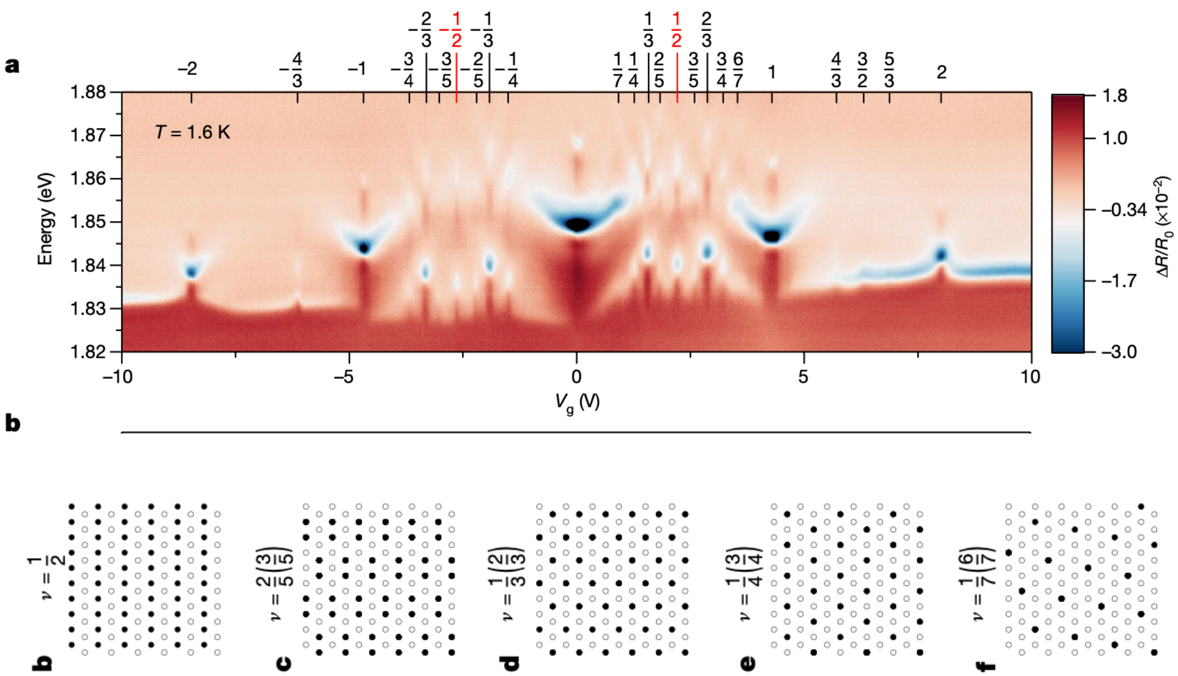
Speculative ground state phase diagrams of the Hubbard model as a function of U and chemical potential, μ

c.f.

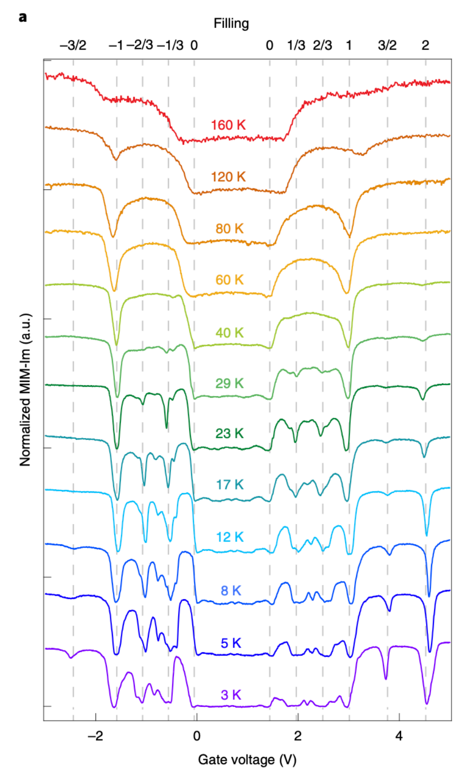
Simons Collaboration on the Many Electron Problem

Moiré Hubbard simulator

WS_2/WSe_2 bilayers



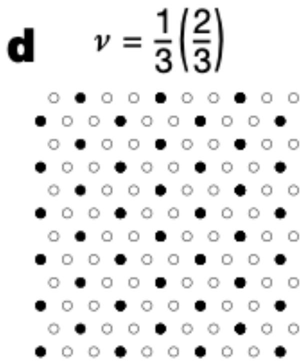
Y. Xu *et al*, 2020



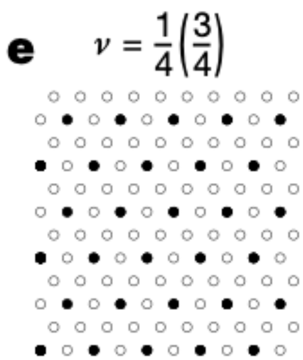
X. Huang *et al*, 2021

Fractional filling insulators: charge order

Emergent lattices



Triangular/honeycomb

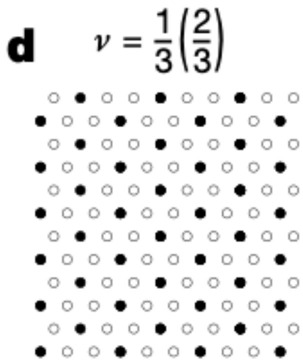


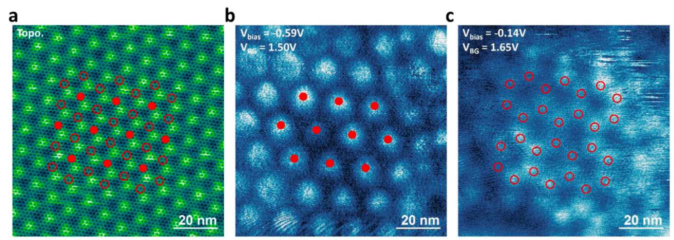
Triangular/kagomé

The Wigner crystallization is essentially classical

What are the spins doing?

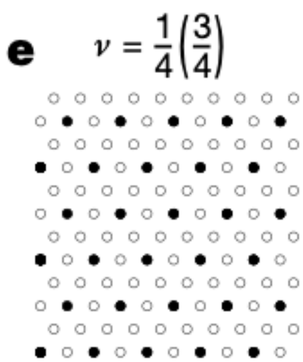
Emergent lattices





H. Li *et al*, 2022

Electron and hole excitations in twisted WS_2 imaged via graphene capping layer

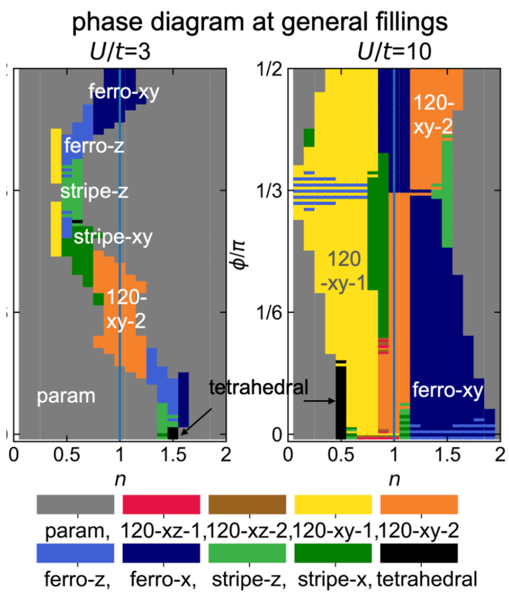


Triangular/kagomé

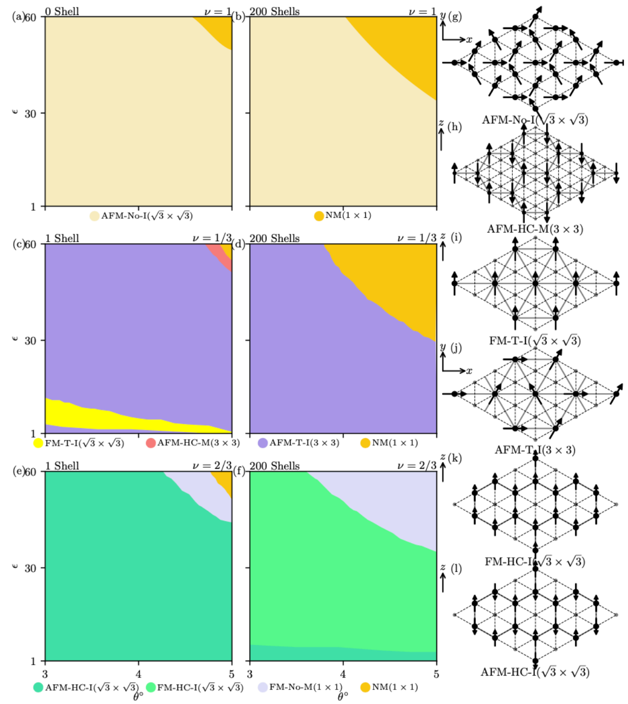
The Wigner crystallization is essentially classical

What are the spins doing?

Hartree-Fock studies



J. Zang *et al*, 2021



H. Pan + S. Das Sarma, 2022

+ many more

These studies are incapable of finding UQM

(Much fewer studies with other techniques, not global)

Slave rotor

$$c_{i\alpha} = f_{i\alpha} b_i$$

$$f_i^\dagger f_i = n_i$$ gauge constraint

$$b_i = e^{i\varphi_i}$$

$$[n_i, \varphi_j] = i\delta_{ij}$$

S. Florens + A. Georges, 2004

Slave rotor

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$$[n_i, \varphi_j] = i\delta_{ij}$$

S. Florens + A. Georges, 2004

Due to the constraint, density-density interactions can be cast entirely into the boson sector

$$H = \sum_{ij;\alpha} t_{ij,\alpha} f_{i\alpha}^\dagger f_{j\alpha} b_i^\dagger b_j + \frac{1}{2} \sum_{i,j} U_{ij} n_i n_j$$

$$\downarrow$$

$$H_{mf} = \sum_{ij;\alpha} t_{ij,\alpha}^{\text{eff}} f_i^\dagger f_j + K_{ij} b_i^\dagger b_j + \frac{1}{2} \sum_{i,j} U_{ij} n_i n_j$$

Slave rotor

$$c_{i\alpha} = f_{i\alpha} b_i \qquad f_i^\dagger f_i = n_i \quad \text{gauge constraint}$$

$$b_i = e^{i\varphi_i}$$

$$[n_i, \varphi_j] = i\delta_{ij}$$

Due to the constraint, density-density interactions can be cast entirely into the boson sector

MF conditions $\quad t^{\text{eff}}_{ij,\alpha} = t_{ij,\alpha} \langle b_i^\dagger b_j \rangle \quad K_{ij} = \sum_\alpha t_{ij,\alpha} \langle f^\dagger_{i,\alpha} f_{j,\alpha} \rangle$

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Slave rotor

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Physics:
Phases become
U(1) gauge fields

c.f. Senthil 2008

Secondary MF

MF conditions $t^{\mathrm{eff}}_{ij,\alpha} = t_{ij,\alpha}\langle b_i^\dagger b_j \rangle \quad K_{ij} = \sum_\alpha t_{ij,\alpha}\langle f_{i,\alpha}^\dagger f_{j,\alpha} \rangle$

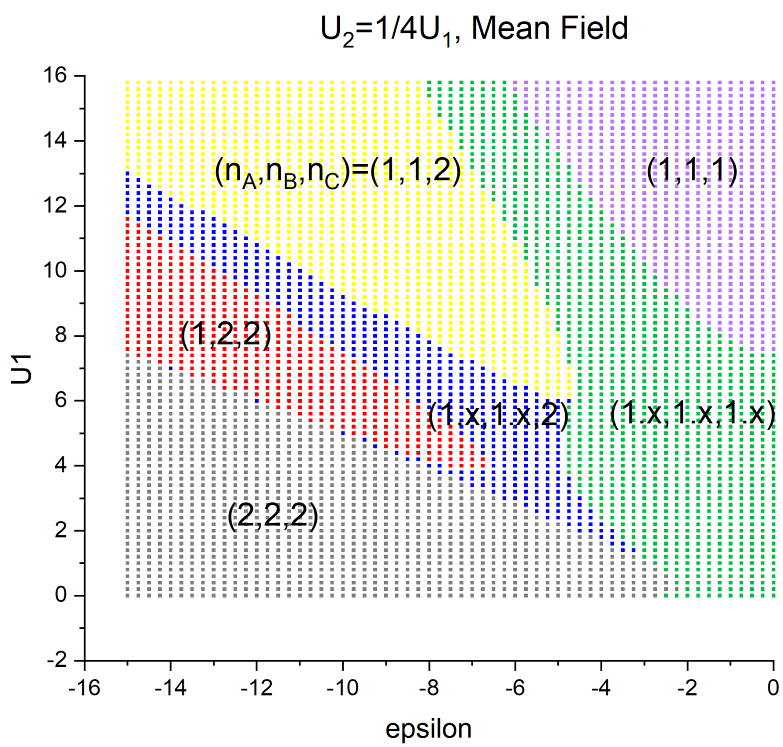
$$H_{mf} = \sum_{ij;\alpha} t^{\mathrm{eff}}_{ij,\alpha} f_i^\dagger f_j + K_{ij} b_i^\dagger b_j + \frac{1}{2}\sum_{i,j} U_{ij} n_i n_j$$

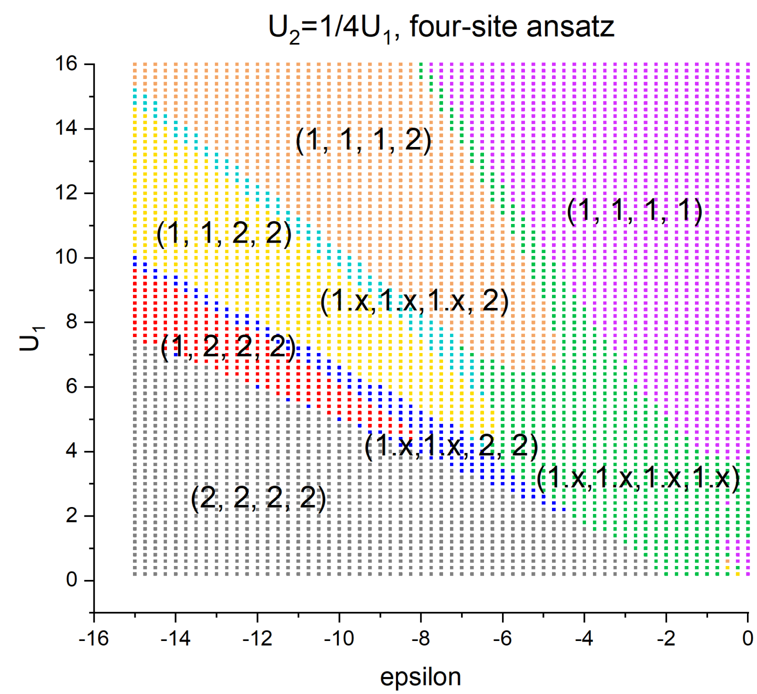
Boson rotor model still non-trivial: a canonical model for Bose Mott and Bose crystal transitions

For a tractable calculation we carry out a secondary MF for the boson problem, and work to quadratic order in the fluctuations around it. This is sufficient to obtain all necessary expectation values, and becomes exact in the large U limit.

MF Results

Phase diagrams allowing 3 or 4 site unit cells





MF Results

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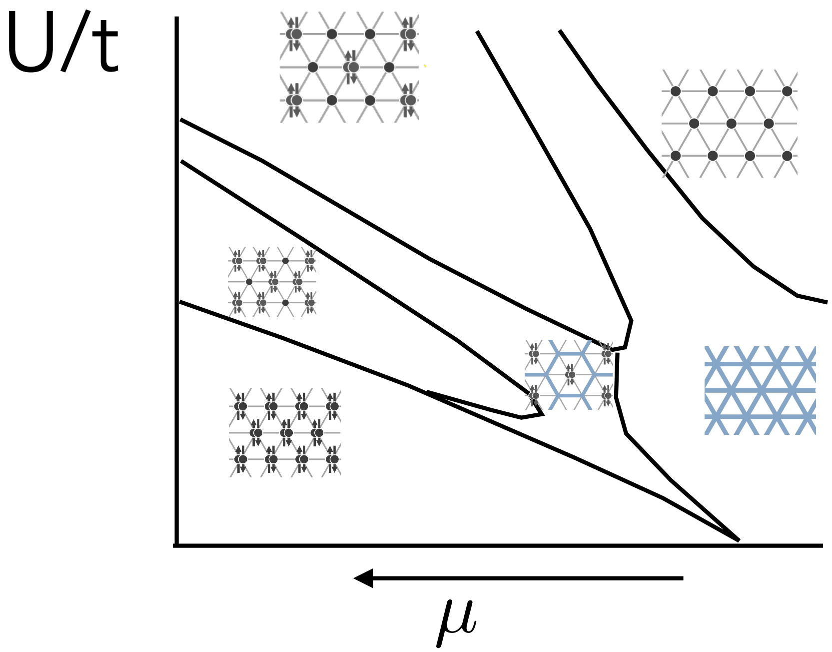
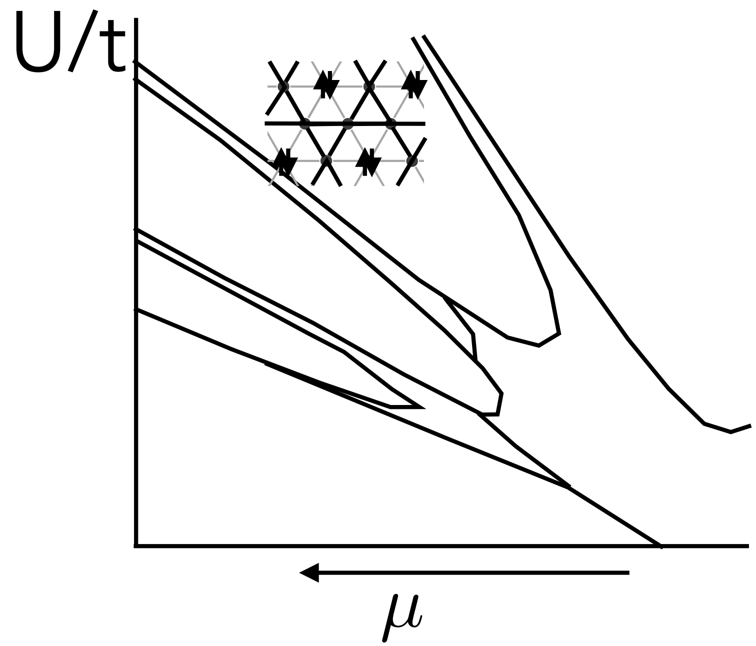
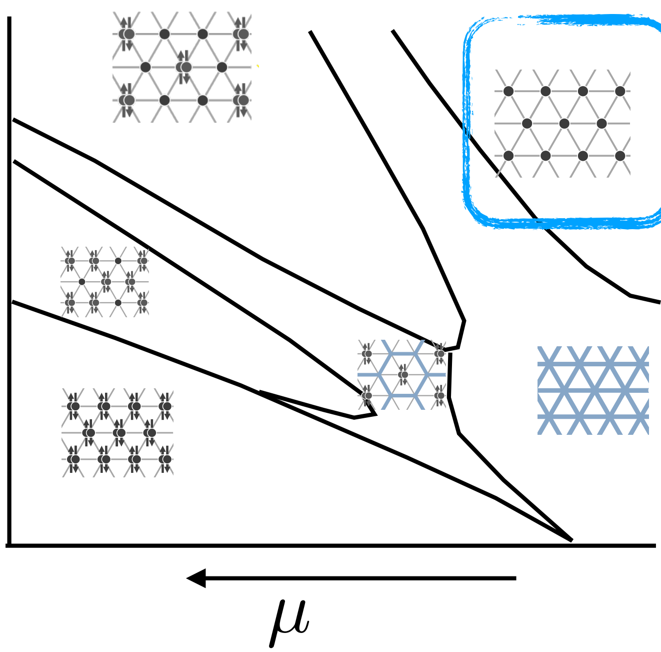


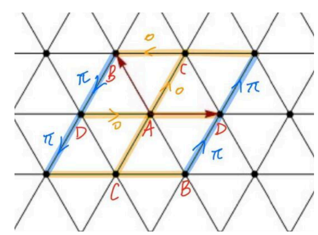


Uniform Mott state



U(1) Fermi surface state?

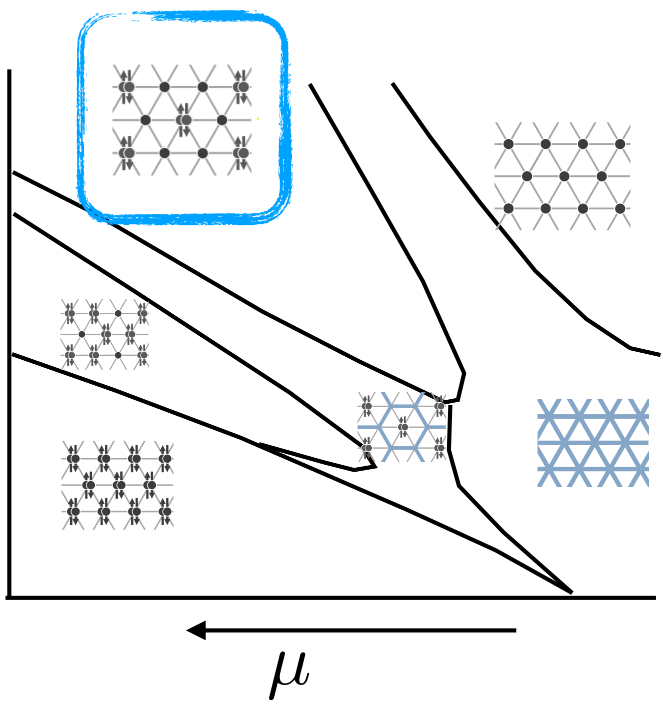
Slightly lower energy:

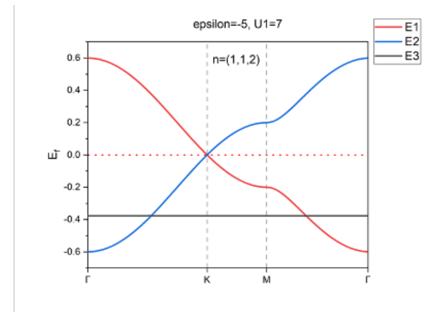


Broken C_3 symmetry

Emergent pi-flux Dirac state

Honeycomb Wigner Crystal



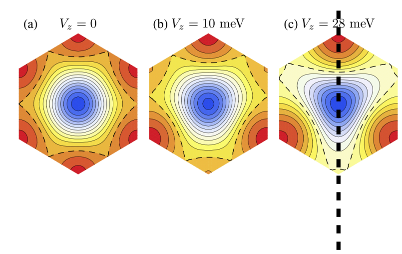


U(1) Dirac spin liquid?

Symmetry of moiré TMD

α atom in the bottom layer is vertically aligned with the β atom in the top layer. The twisted bilayer has D_3 point-group symmetry generated by a threefold rotation C_{3z} around the $\hat{z}$ axis and a twofold rotation C_{2y} around the in-plane $\hat{y}$ axis that swaps the two layers. The D_3 point group is reduced to C_3 when an external out-of-plane displacement field is applied to the system.

H. Pan *et al*, 2020



(Homobilayer: heterobilayer is even lower)

Accidental reflection symmetry

Kagome Wigner crystal

Likely also U(1) Dirac ?

Or chiral SL?

(Analysis in progress)

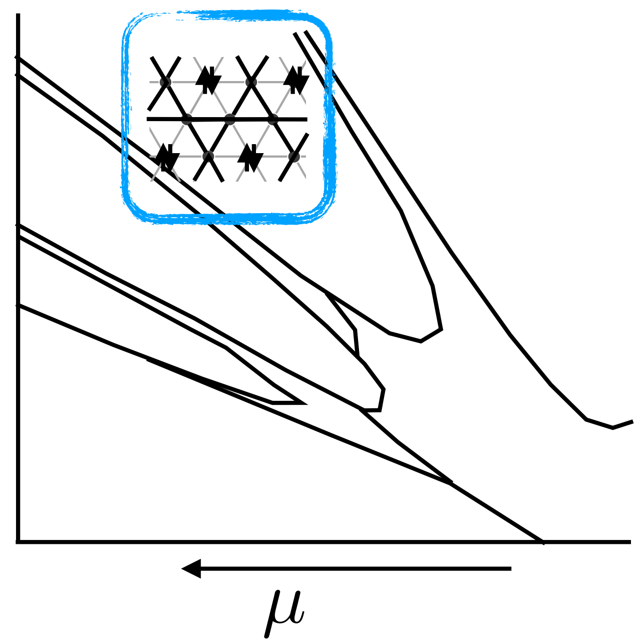
Kagome Chiral Spin Liquid in Transition Metal Dichalcogenide Moiré Bilayers

Johannes Motruk,[1,*] Dario Rossi,[1] Dmitry A. Abanin,[1,2] and Louk Rademaker[1]

[1] *Department of Theoretical Physics, University of Geneva, Quai Ernest-Ansermet 24, 1205 Geneva, Switzerland*

[2] *Google Research, Mountain View, CA, USA*

(Dated: November 30, 2022)



Next steps

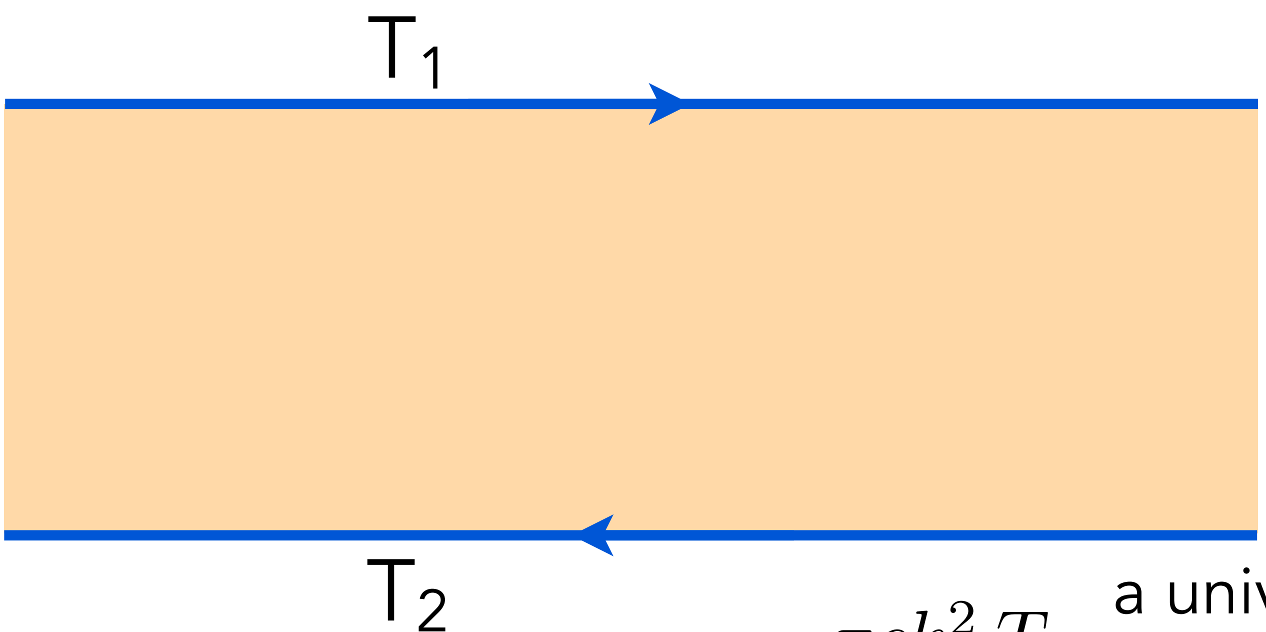
- Mapping to wave functions, corrected energies.
- Competition with magnetic order
- Maximizing energy scale for entanglement: some O(1) fraction of bandwidth t??
- What are the observables for spin liquids in TMDs?

Outline

- Two on-going projects
  - Looking for spin liquids in moiré “quantum simulators”
  - **Thermal Hall effect - towards a theoretical framework for transverse heat transport**

Thermal Hall effect

- Motivation: a probe of exotic phases. In insulators, "must" come from electrons

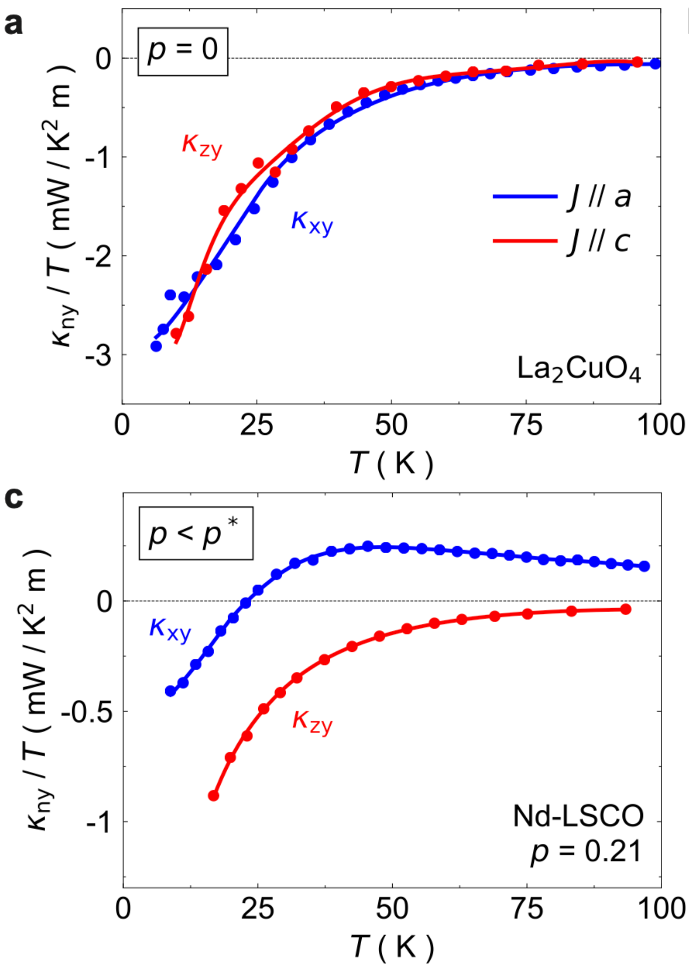


$$I_x = \kappa_H \Delta T_y$$

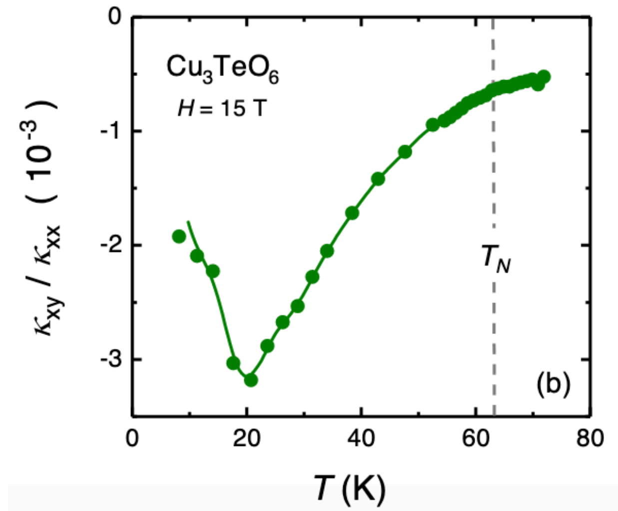
$$\kappa_H = \frac{\pi c k_B^2 T}{6\hbar}$$

a universal prediction for chiral "Ising anyon" phase: *agnostic to microscopic spin interactions*

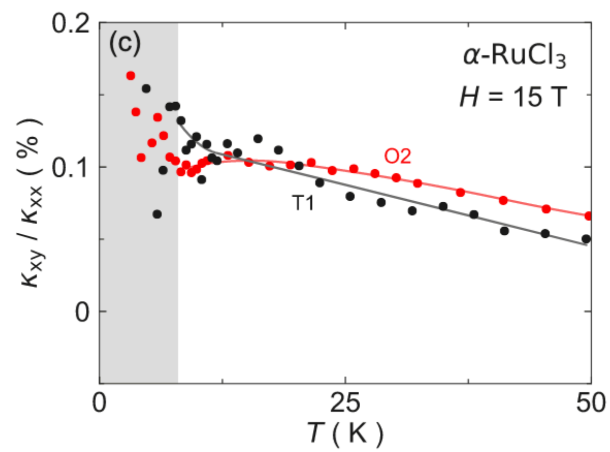
Phonons



Grissonanche *et al*, 2020



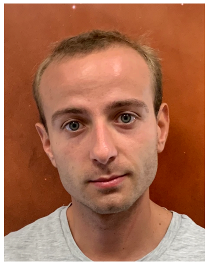
L. Chen *et al*, 2021



Evidence of a Phonon Hall Effect in the Kitaev Spin Liquid Candidate α-$RuCl_3$

É. Lefrançois,[1] G. Grissonnanche,[1] J. Baglo,[1] P. Lampen-Kelley,[2,3] J. Yan,[2] C. Balz,[4,*]
D. Mandrus,[2,3] S. E. Nagler,[4] S. Kim,[5] Young-June Kim,[5] N. Doiron-Leyraud,[1] and L. Taillefer[1,6]

Two types of effects



Phonon Boltzmann equation

- Phonons are good quasiparticles

Convective derivative. Dynamics.

- Non-dissipative effects: modifications of intrinsic dynamics of individual quasiparticles, e.g. Berry phase effects, etc.

$$D_t p = \Gamma[p]$$

- Dissipative effects: modifications of scattering of quasiparticles

Collision term

Goals: use phonons as a *probe* of UQM, and understand THE well enough to extract true UQM physics, eventually formulate quantum kinetics for perhaps more interesting fluids

Two types of effects

- Phonons are good quasiparticles

Phonon Boltzmann equation

Convective derivative. Dynamics.

- Non-dissipative effects: modifications of intrinsic dynamics of individual quasiparticles, e.g. Berry phase effects, etc.

$$D_t p = \Gamma[p]$$

- Dissipative effects: modifications of scattering of quasiparticles

Collision term

Talk about 2nd, and work in progress combining with the first

Dissipative effects

- Basically, this is "skew scattering" of phonons
- We ask how this arises through coupling to electronic degrees of freedom
- Transition matrix in *full many-body space of phonons+electrons:*

$$T_{\mathtt{i}\to\mathtt{f}} = T_{\mathtt{fi}} = \langle \mathtt{f}|H'|\mathtt{i}\rangle + \sum_{\mathtt{n}} \frac{\langle \mathtt{f}|H'|\mathtt{n}\rangle\langle \mathtt{n}|H'|\mathtt{i}\rangle}{E_{\mathtt{i}} - E_{\mathtt{n}} + i\eta} + \cdots$$

Important point: 1st order term is Hermitian, so 1st order T-matrix is effectively time-reversal invariant

- No Hall effect at leading order.

From T-matrix to collision term

- Coupling Hamiltonian

$$H' = \sum_{n\boldsymbol{k}} \left(a^\dagger_{n\boldsymbol{k}} Q^\dagger_{n\boldsymbol{k}} + a_{n\boldsymbol{k}} Q_{n\boldsymbol{k}} \right)$$

"Spin"

Can be anything non-phononic, e.g. electronic

- Full transition rate

$$\Gamma_{\mathbf{i}\to\mathbf{f}} = \frac{2\pi}{\hbar} |T_{\mathbf{i}\to\mathbf{f}}|^2 \delta(E_{\mathbf{i}} - E_{\mathbf{f}}). \qquad p_{i_s} = \frac{1}{Z_s} e^{-\beta E_{i_s}}$$

- Phonon transition rate

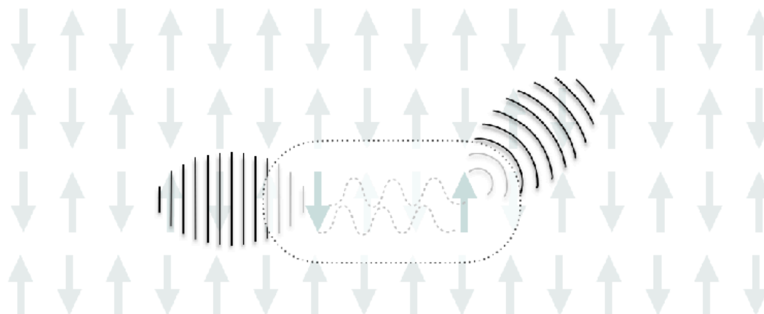
$$\tilde{\Gamma}_{i_p\to f_p} = \sum_{i_s f_s} \Gamma_{\mathbf{i}\to\mathbf{f}}\, p_{i_s},$$

- Master equation

$$\mathcal{C}_{n\mathbf{k}} = \sum_{i_p, f_p} \tilde{\Gamma}_{i_p\to f_p} \left(N_{n\mathbf{k}}(f_p) - N_{n\mathbf{k}}(i_p) \right) p_{i_p}$$

In this way we can construct C_{nk} for any "spin" subsystem

Scattering rates



O(Q²)

$$D_{n\mathbf{k}} = -\frac{1}{\hbar^2}\int dt\, e^{-i\omega_{n\mathbf{k}}t}\left\langle [Q_{n\mathbf{k}}(t), Q^{\dagger}_{n\mathbf{k}}(0)]\right\rangle_{\beta} + \breve{D}_{n\mathbf{k}}$$

O(Q⁴)

$$\mathfrak{W}^{\ominus,qq'}_{n\mathbf{k}n'\mathbf{k}'} = \frac{2N_{\mathrm{uc}}}{\hbar^4}\mathfrak{Re}\int_{t,t_1,t_2} e^{i[\Sigma^{q,q'}_{n\mathbf{k}n'\mathbf{k}'}t+\Delta^{q,q'}_{n\mathbf{k}n'\mathbf{k}'}(t_1+t_2)]}\mathrm{sign}(t_2)\left\langle\left[Q^{-q}_{n\mathbf{k}}(-t-t_2), Q^{-q'}_{n'\mathbf{k}'}(-t+t_2)\right]\left\{Q^{q'}_{n'\mathbf{k}'}(-t_1), Q^{q}_{n\mathbf{k}}(t_1)\right\}\right\rangle$$

commutator anti-commutator

Anti-detailed balance

$$\mathfrak{W}^{\ominus,qq'}_{n\mathbf{k}n'\mathbf{k}'} = -\, e^{-\beta(q\omega_{n\mathbf{k}}+q'\omega_{n'\mathbf{k}'})}\, \mathfrak{W}^{\ominus,-q-q'}_{n\mathbf{k}n'\mathbf{k}'}$$

Thermal Hall effect

Anti-symmetric part

$$\kappa_H^{\mu\nu} = \frac{\hbar^2}{k_B T^2} \frac{1}{V} \sum_{n\mathbf{k}n'\mathbf{k}'} J_{n\mathbf{k}}^{\mu} \frac{e^{\beta\hbar\omega_{n\mathbf{k}}/2}}{2D_{n\mathbf{k}}} \left(\frac{1}{N_{\mathrm{uc}}} \sum_{q=\pm} \frac{\left(e^{\beta\hbar\omega_{n\mathbf{k}}} - e^{q\beta\hbar\omega_{n'\mathbf{k}'}}\right) \mathfrak{W}_{n\mathbf{k},n'\mathbf{k}'}^{\ominus,+,q}}{\sinh(\beta\hbar\omega_{n\mathbf{k}}/2)\sinh(\beta\hbar\omega_{n'\mathbf{k}'}/2)} \right) \frac{e^{\beta\hbar\omega_{n'\mathbf{k}'}/2}}{2D_{n'\mathbf{k}'}} J_{n'\mathbf{k}'}^{\nu}$$

$$J_{n\mathbf{k}}^{\mu} = N_{n\mathbf{k}}^{\mathrm{eq}}\, \omega_{n\mathbf{k}} v_{n\mathbf{k}}^{\mu}$$

Thermal Hall effect

Anti-symmetric part

$$\kappa_H^{\mu\nu} = \frac{\hbar^2}{k_B T^2} \frac{1}{V} \sum_{n\mathbf{k}n'\mathbf{k}'} J^{\mu}_{n\mathbf{k}} \frac{e^{\beta\hbar\omega_{n\mathbf{k}}/2}}{2D_{n\mathbf{k}}} \left(\frac{1}{N_{\mathrm{uc}}} \sum_{q=\pm} \frac{\left(e^{\beta\hbar\omega_{n\mathbf{k}}} - e^{q\beta\hbar\omega_{n'\mathbf{k}'}}\right) \mathfrak{W}^{\ominus,+,q}_{n\mathbf{k},n'\mathbf{k}'}}{\sinh(\beta\hbar\omega_{n\mathbf{k}}/2)\sinh(\beta\hbar\omega_{n'\mathbf{k}'}/2)} \right) \frac{e^{\beta\hbar\omega_{n'\mathbf{k}'}/2}}{2D_{n'\mathbf{k}'}} J^{\nu}_{n'\mathbf{k}'}$$

$$J^{\mu}_{n\mathbf{k}} = N^{\mathrm{eq}}_{n\mathbf{k}}\,\omega_{n\mathbf{k}} v^{\mu}_{n\mathbf{k}}$$

Basic idea

$$\#\nabla T = -\frac{1}{\tau}\delta n - \frac{1}{\tau_{\mathrm{skew}}}\delta n$$

$$\delta n = -\tau\#\nabla T - \frac{\tau}{\tau_{\mathrm{skew}}}\delta n$$

$$\approx -\tau\#\nabla T - \frac{\tau^2}{\tau_{\mathrm{skew}}}\#\nabla T$$

Thermal Hall effect

Conductivity versus resistivity

$$\kappa_H \sim \frac{\tau^2}{\tau_{\text{skew}}}$$

Sensitive to all ordinary scattering mechanisms. Very non-universal

$$\varrho_H \sim -\frac{\kappa_H}{\kappa^2} \sim \frac{1}{\tau_{\text{skew}}}$$

Only sensitive to skew scattering. A better quantity to study.

$$\varrho_H \sim \mathfrak{W}^{\ominus,\text{eff}}$$

Indeed follows from our formulae

Many-body skew scattering

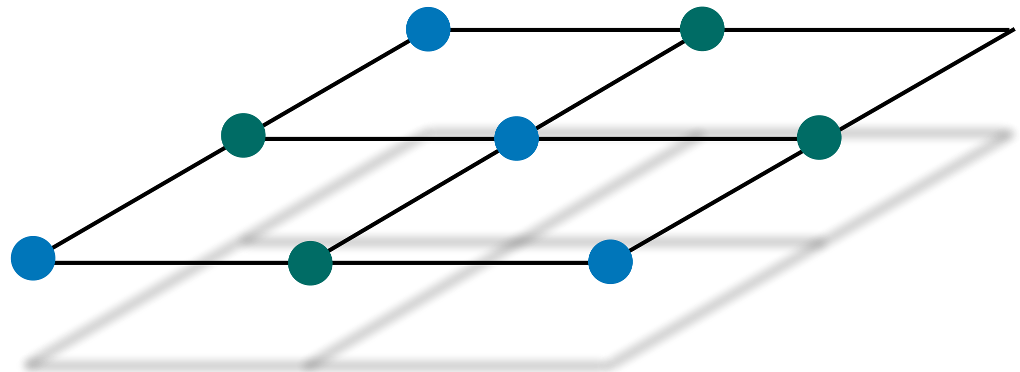
$$\mathfrak{W}^{\ominus,qq'}_{n\mathbf{k}n'\mathbf{k}'} = \frac{2N_{\mathrm{uc}}}{\hbar^4}\mathfrak{Re}\int_{t,t_1,t_2} e^{i[\Sigma^{q,q'}_{n\mathbf{k}n'\mathbf{k}'}t+\Delta^{q,q'}_{n\mathbf{k}n'\mathbf{k}'}(t_1+t_2)]}\mathrm{sign}(t_2)\left\langle\left[Q^{-q}_{n\mathbf{k}}(-t-t_2), Q^{-q'}_{n'\mathbf{k}'}(-t+t_2)\right]\left\{Q^{q'}_{n'\mathbf{k}'}(-t_1), Q^{q}_{n\mathbf{k}}(t_1)\right\}\right\rangle$$

What good is it?

- In principle, this can be applied for any Q, could be e.g. quantum critical field etc.
- Can be used to analyze symmetries, *ala* Onsager
- That said, it is very hard to calculate such real-time correlation functions…maybe with a quantum simulator?

Application to an antiferromagnet

For concreteness,
2d, layered



Spin waves

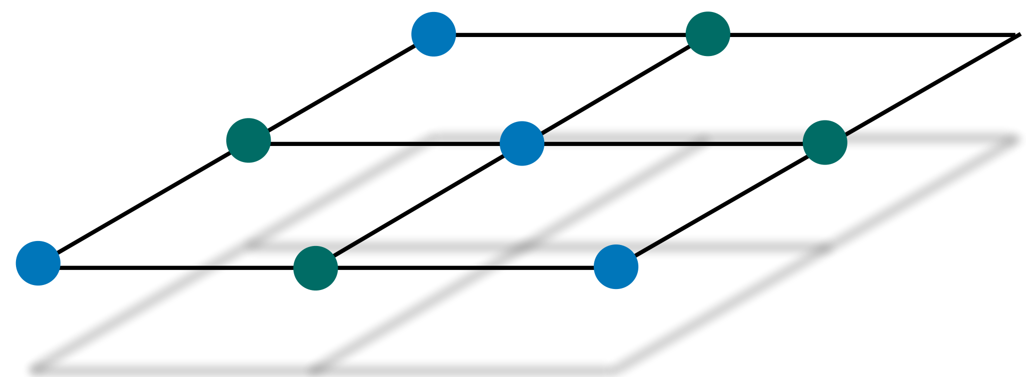
$$H_{\mathrm{NLS}} + H_{\mathrm{field}} = \sum_{\ell} \sum_{\mathbf{k}} \Omega_{\mathbf{k},\ell} b^{\dagger}_{\mathbf{k},\ell} b_{\mathbf{k},\ell}$$

Collective field

$$Q^{q}_{n\mathbf{k}} = \sum_{\ell,q_1,z} \mathcal{A}^{n,\ell|q_1 q}_{\mathbf{k}} \, e^{ik_z z} b^{q_1}_{\ell,\mathbf{k},z} \; + \frac{1}{\sqrt{N_{\mathrm{uc}}}} \sum_{\substack{\mathbf{p},\ell,\ell' \\ q_1,q_2,z}} \mathcal{B}^{n,\ell_1,\ell_2|q_1 q_2 q}_{\mathbf{k};\mathbf{p}} \; e^{ik_z z} b^{q_1}_{\ell_1,\mathbf{p}+\frac{q}{2}\mathbf{k},z} b^{q_2}_{\ell_2,-\mathbf{p}+\frac{q}{2}\mathbf{k},z}$$

Application to an antiferromagnet

For concreteness, 2d, layered



Spin waves

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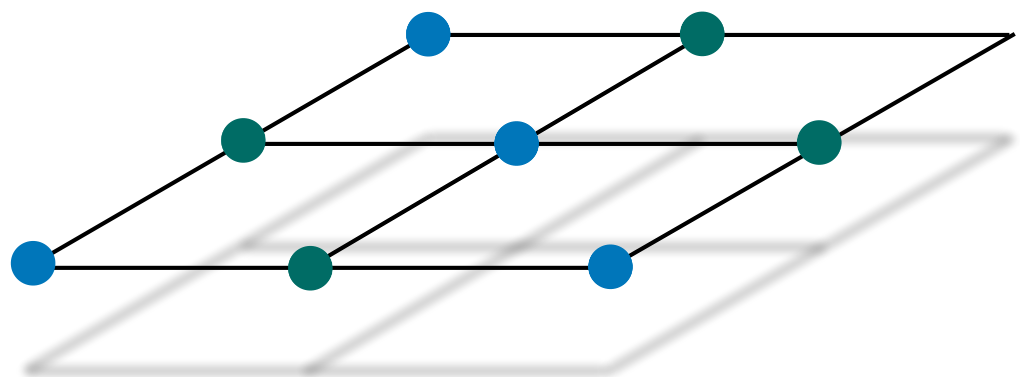
Collective field

$$Q^{q}_{n\mathbf{k}} = \sum_{\ell,q_1,z} \mathcal{A}^{n,\ell|q_1 q}_{\mathbf{k}} e^{ik_z z} b^{q_1}_{\ell,\mathbf{k},z} + \frac{1}{\sqrt{N_{\rm uc}}} \sum_{\substack{\mathbf{p},\ell,\ell' \\ q_1,q_2,z}} \mathcal{B}^{n,\ell_1,\ell_2|q_1 q_2 q}_{\mathbf{k};\mathbf{p}} \; e^{ik_z z} b^{q_1}_{\ell_1,\mathbf{p}+\frac{q}{2}\mathbf{k},z} b^{q_2}_{\ell_2,-\mathbf{p}+\frac{q}{2}\mathbf{k},z}$$

Negligible phase space

Application to an antiferromagnet

For concreteness,
2d, layered



Spin waves

$$H_{\text{NLS}} + H_{\text{field}} = \sum_{\ell} \sum_{\mathbf{k}} \Omega_{\mathbf{k},\ell} b^{\dagger}_{\mathbf{k},\ell} b_{\mathbf{k},\ell}$$

Collective field

$$Q^{q}_{n\mathbf{k}} = \sum_{\ell,q_1,z} \mathcal{A}^{n,\ell|q_1 q}_{\mathbf{k}} e^{ik_z z} b^{q_1}_{\ell,\mathbf{k},z} + \frac{1}{\sqrt{N_{\text{uc}}}} \sum_{\substack{\mathbf{p},\ell,\ell' \\ q_1,q_2,z}} \mathcal{B}^{n,\ell_1,\ell_2|q_1 q_2 q}_{\mathbf{k};\mathbf{p}} e^{ik_z z} b^{q_1}_{\ell_1,\mathbf{p}+\frac{q}{2}\mathbf{k},z} b^{q_2}_{\ell_2,-\mathbf{p}+\frac{q}{2}\mathbf{k},z}$$

Negligible phase space

Structure hidden here

General result

- Diagonal scattering rate:

$$D^{(s)}_{n\mathbf{k}} = \frac{(3-s)\pi}{\hbar^2 N^{\mathrm{2d}}_{\mathrm{uc}}} \sum_{\mathbf{p}} \sum_{\ell,\ell'} \frac{\sinh(\frac{\beta}{2}\hbar\omega_{n\mathbf{k}})}{\sinh(\frac{\beta}{2}\hbar\Omega_{\ell,\mathbf{p}})\sinh(\frac{\beta}{2}\hbar\Omega_{\ell',\mathbf{p}-\mathbf{k}})} \quad \delta(\omega_{n\mathbf{k}} - \Omega_{\ell,\mathbf{p}} - s\Omega_{\ell',\mathbf{p}-\mathbf{k}}) \left|\mathcal{B}^{n,\ell,\ell'|+s-}_{\mathbf{k};-\mathbf{p}+\frac{\mathbf{k}}{2}}\right|^2$$

- Skew scattering rate:

$$\mathfrak{W}^{\ominus,qq'}_{n\mathbf{k},n'\mathbf{k}'} = \frac{64\pi^2}{\hbar^4}\frac{1}{N^{2d}_{\mathrm{uc}}}\sum_{\mathbf{p}}\sum_{\{\ell_i,q_i\}} \mathfrak{D}^{nn'|q_1q_2q_3,\ell_1\ell_2\ell_3}_{q\mathbf{k}q'\mathbf{k}',\mathbf{p}} \; \mathfrak{F}^{q_1q_2q_4,\ell_1\ell_2\ell_3}_{q\mathbf{k}q'\mathbf{k}',\mathbf{p}} \; \mathfrak{Im}\Big\{ \mathcal{B}^{n\ell_2\ell_3|q_2q_3q}_{\mathbf{k},\mathbf{p}+\frac{1}{2}q\mathbf{k}+q'\mathbf{k}'} \mathcal{B}^{n'\ell_3\ell_1|-q_3q_1q'}_{\mathbf{k}',\mathbf{p}+\frac{1}{2}q'\mathbf{k}'}$$

$$\times\,\mathrm{PP}\Bigg[\frac{\mathcal{B}^{n\ell_1\ell_4|-q_1q_4-q}_{\mathbf{k},\mathbf{p}+\frac{1}{2}q\mathbf{k}}\mathcal{B}^{n'\ell_4\ell_2|-q_4-q_2-q'}_{\mathbf{k}',\mathbf{p}+q\mathbf{k}+\frac{1}{2}q'\mathbf{k}'}}{\Delta^{qq'}_{n\mathbf{k}n'\mathbf{k}'} + q_1\Omega_{\ell_1,\mathbf{p}} - q_2\Omega_{\ell_2,\mathbf{p}+q\mathbf{k}+q'\mathbf{k}'} - 2q_4\Omega_{\ell_4,\mathbf{p}+q\mathbf{k}}} + \frac{\mathcal{B}^{n'\ell_1\ell_4|-q_1-q_4-q'}_{\mathbf{k}',\mathbf{p}+\frac{1}{2}q'\mathbf{k}'}\mathcal{B}^{n\ell_4\ell_2|q_4-q_2-q}_{\mathbf{k},\mathbf{p}+\frac{1}{2}q\mathbf{k}+q'\mathbf{k}'}}{\Delta^{qq'}_{n\mathbf{k}n'\mathbf{k}'} - q_1\Omega_{\ell_1,\mathbf{p}} + q_2\Omega_{\ell_2,\mathbf{p}+q\mathbf{k}+q'\mathbf{k}'} - 2q_4\Omega_{\ell_4,\mathbf{p}+q'\mathbf{k}'}}\Bigg]\Big\}$$

$$\mathfrak{D}^{nn'|q_1q_2q_3,\ell_1\ell_2\ell_3}_{q\mathbf{k}q'\mathbf{k}',\mathbf{p}} = \delta\left(\Sigma^{qq'}_{n\mathbf{k}n'\mathbf{k}'} + q_1\Omega_{\ell_1,\mathbf{p}} + q_2\Omega_{\ell_2,\mathbf{p}+q\mathbf{k}+q'\mathbf{k}'}\right)\delta\left(\Delta^{qq'}_{n\mathbf{k}n'\mathbf{k}'} + 2q_3\Omega_{\ell_3,\mathbf{p}+q'\mathbf{k}'} - q_1\Omega_{\ell_1,\mathbf{p}} + q_2\Omega_{\ell_2,\mathbf{p}+q\mathbf{k}+q'\mathbf{k}'}\right),$$

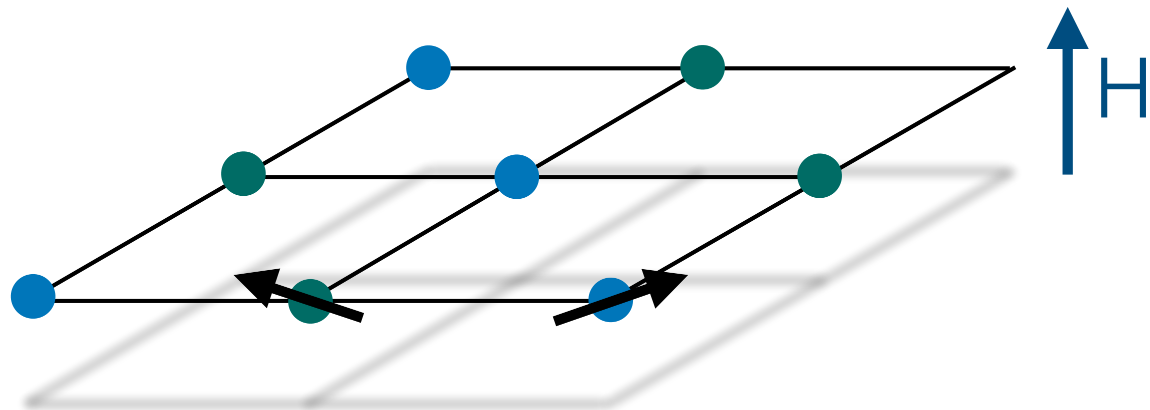
$$\mathfrak{F}^{q_1q_2q_4,\ell_1\ell_2\ell_3}_{q\mathbf{k}q'\mathbf{k}',\mathbf{p}} = q_4\left(2n_{\mathrm{B}}(\Omega_{\ell_3,\mathbf{p}+q'\mathbf{k}'})+1\right)\left(2n_{\mathrm{B}}(\Omega_{\ell_1,\mathbf{p}})+q_1+1\right)\left(2n_{\mathrm{B}}(\Omega_{\ell_2,\mathbf{p}+q\mathbf{k}+q'\mathbf{k}'})+q_2+1\right).$$

Could be applied to any magnet

Continuum magnons

Hamiltonian

$$\mathcal{H}_{\rm NLS} = \frac{\rho}{2}\left(|\underline{\boldsymbol{\nabla}} n_y|^2 + |\underline{\boldsymbol{\nabla}} n_z|^2\right) + \frac{1}{2\chi}(m_y^2 + m_z^2) + \sum_{a,b=y,z} \frac{\Gamma_{ab}}{2} n_a n_b$$



Spin-lattice coupling

$$\mathcal{H}_{\rm s-l} = \sum_{\substack{\alpha,\beta \\ a,b=x,y,z}} \mathcal{E}_{\mathbf{r}}^{\alpha\beta} \left(\Lambda_{ab}^{(\rm n),\alpha\beta} {\rm n}_a {\rm n}_b + \frac{\Lambda_{ab}^{(\rm m),\alpha\beta}}{n_0^2} {\rm m}_a {\rm m}_b \right)\Bigg|_{\mathbf{x},z}$$

$$|\mathbf{n}|^2 + \frac{\mathfrak{a}^4}{\mu_0^2}|\mathbf{m}|^2 = 1, \qquad \mathbf{m}\cdot\mathbf{n} = 0.$$

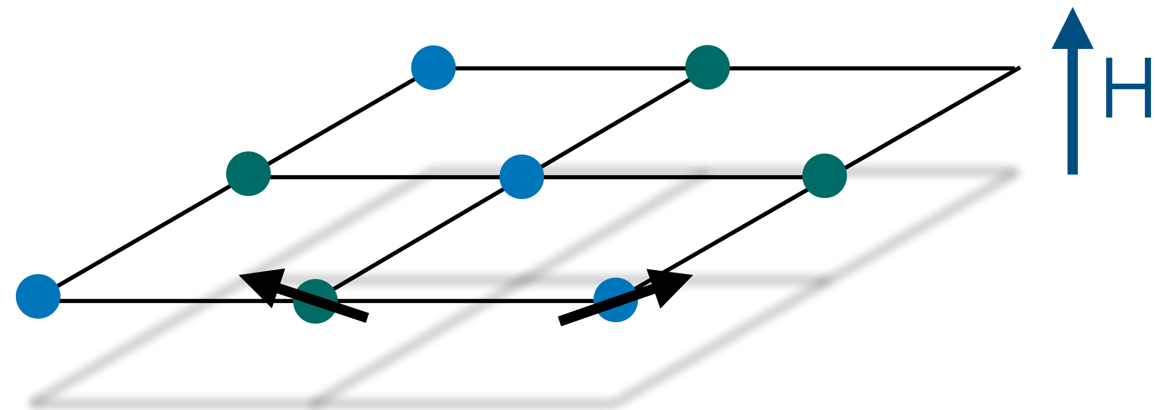
Solve NLSM constraints, expand around canted state

$$\mathcal{H}_{\rm s-l} \approx \sum_{\alpha\beta} \mathcal{E}_{\mathbf{r}}^{\alpha\beta} \sum_{a,b=y,z} \sum_{\xi,\xi'=m,n} \lambda^{\alpha\beta}_{\xi_a,\xi'_b} n_0^{-\xi-\xi'} \xi_{a\mathbf{r}} \xi'_{b\mathbf{r}}$$

Continuum magnons

Hamiltonian

$$\mathcal{H}_{\mathrm{NLS}} = \frac{\rho}{2}\left(|\nabla n_y|^2 + |\nabla n_z|^2\right) + \frac{1}{2\chi}(m_y^2 + m_z^2) + \sum_{a,b=y,z}\frac{\Gamma_{ab}}{2} n_a n_b$$



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$$\mathcal{H}_{\mathrm{s-l}} = \sum_{\substack{\alpha,\beta \\ a,b=x,y,z}} \mathcal{E}_{\mathbf{r}}^{\alpha\beta}\left(\Lambda_{ab}^{(\mathrm{n}),\alpha\beta}\mathrm{n}_a\mathrm{n}_b + \frac{\Lambda_{ab}^{(\mathrm{m}),\alpha\beta}}{n_0^2}\mathrm{m}_a\mathrm{m}_b\right)\Bigg|_{\mathbf{x},z}$$

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n.b.

m m

n n

m n

Effective TRS breaking

Scaling

- B coefficients: $\Omega \sim \omega \sim v_{\mathrm{ph}} k \sim k_B T$

$$\mathcal{B} \sim \left(\frac{k_B T}{M v_{\mathrm{ph}}^2}\right)^{\frac{1}{2}} n_0^{-1} \left(\lambda_{mm} \frac{\chi k_B T}{n_0} + \lambda_{mn} + \lambda_{nn} \frac{n_0}{\chi k_B T}\right) \quad \sim T^{1/2+x}$$

smallness: ions are heavy.

Antiferromagnet: order-parameter (n) has strongest correlations

- Diagonal scattering rate: $D^{(s)}_{n\mathbf{k}} = \frac{(3-s)\pi}{\hbar^2 N_{\mathrm{uc}}^{2\mathrm{d}}} \sum_{\mathbf{p}} \sum_{\ell,\ell'} \frac{\sinh(\frac{\beta}{2}\hbar\omega_{n\mathbf{k}})}{\sinh(\frac{\beta}{2}\hbar\Omega_{\ell,\mathbf{p}}) \sinh(\frac{\beta}{2}\hbar\Omega_{\ell',\mathbf{p}-\mathbf{k}})} \quad \delta(\omega_{n\mathbf{k}} - \Omega_{\ell,\mathbf{p}} - s\Omega_{\ell',\mathbf{p}-\mathbf{k}}) \left|\mathcal{B}^{n,\ell,\ell'|+s-}_{\mathbf{k};-\mathbf{p}+\frac{\mathbf{k}}{2}}\right|^2$

$$\frac{1}{\tau} \sim T^{d-1} |\mathcal{B}|^2 \sim T^{d+2x}$$

$\sim T^{d+2}, T^{d}, T^{d-2}$?

Scaling

- B coefficients: $\Omega \sim \omega \sim v_{\mathrm{ph}} k \sim k_B T$

$$\mathcal{B} \sim \left(\frac{k_B T}{M v_{\mathrm{ph}}^2}\right)^{\frac{1}{2}} n_0^{-1} \left(\lambda_{mm} \frac{\chi k_B T}{n_0} + \lambda_{mn} + \lambda_{nn} \frac{n_0}{\chi k_B T}\right) \sim T^{1/2+x}$$

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Antiferromagnet: order-parameter (n) has strongest correlations

- Diagonal scattering rate:

$$D_{n\mathbf{k}}^{(s)} = \frac{(3-s)\pi}{\hbar^2 N_{\mathrm{uc}}^{2\mathrm{d}}} \sum_{\mathbf{p}} \sum_{\ell,\ell'} \frac{\sinh(\frac{\beta}{2}\hbar\omega_{n\mathbf{k}})}{\sinh(\frac{\beta}{2}\hbar\Omega_{\ell,\mathbf{p}})\sinh(\frac{\beta}{2}\hbar\Omega_{\ell',\mathbf{p}-\mathbf{k}})} \delta(\omega_{n\mathbf{k}} - \Omega_{\ell,\mathbf{p}} - s\Omega_{\ell',\mathbf{p}-\mathbf{k}}) \left|\mathcal{B}_{\mathbf{k};-\mathbf{p}+\frac{\mathbf{k}}{2}}^{n,\ell,\ell'|+s-}\right|^2$$

$$\frac{1}{\tau} \sim T^{d-1}|\mathcal{B}|^2 \sim T^{d+2x}$$

$\sim T^{d+2}$, T^{d}, T^{d-2}

Spin–phonon interactions in a Heisenberg antiferromagnet: II. The phonon spectrum and spin–lattice relaxation rate

M G Cottam
Department of Physics, University of Essex, Colchester CO4 3SQ, England

Received 11 March 1974

$$\frac{1}{\tau_{\mathrm{SL}}} \simeq \frac{b_1 S^2(r^2-1)}{D^{10}}\left(\frac{5T_{\mathrm{D}}^3}{12\pi^4} + \frac{\pi^2 D^3}{24V}\right) Q_0^2 T^5$$

Scaling: Hall

From the formula:

$$\mathfrak{W}^{\ominus} \sim T^{d-3}\mathcal{B}^4$$

Effective TRS breaking: one factor of m-n coupling:

$$\sim T^{d-1}\lambda_{mn}\left(\lambda_{mm}T + \lambda_{nn}T^{-1}\right)^3 \sim T^{d-1+3x},$$

This gives Hall resistivity:

$$\varrho_H \sim \mathfrak{W}^{\ominus,\mathrm{eff}} \sim T^{d-1+3x}$$

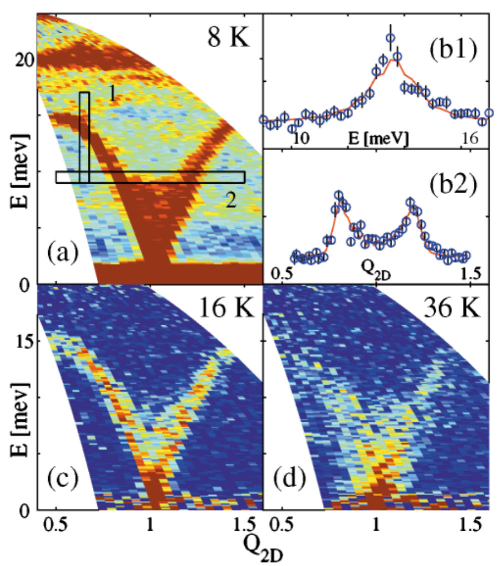
Check: numerical calculation

Many parameters: loosely inspired by Copper Deuteroformate Tetradeuterate (CFTD)

VOLUME 87, NUMBER 3 PHYSICAL REVIEW LETTERS 16 JULY 2001

Spin Dynamics of the 2D Spin $\frac{1}{2}$ Quantum Antiferromagnet Copper Deuteroformate Tetradeuterate (CFTD)

H. M. Rønnow,[1,2] D. F. McMorrow,[1] R. Coldea,[3,4] A. Harrison,[5] I. D. Youngson,[5] T. G. Perring,[4] G. Aeppli,[6] O. Syljuåsen,[7] K. Lefmann,[1] and C. Rischel[8]



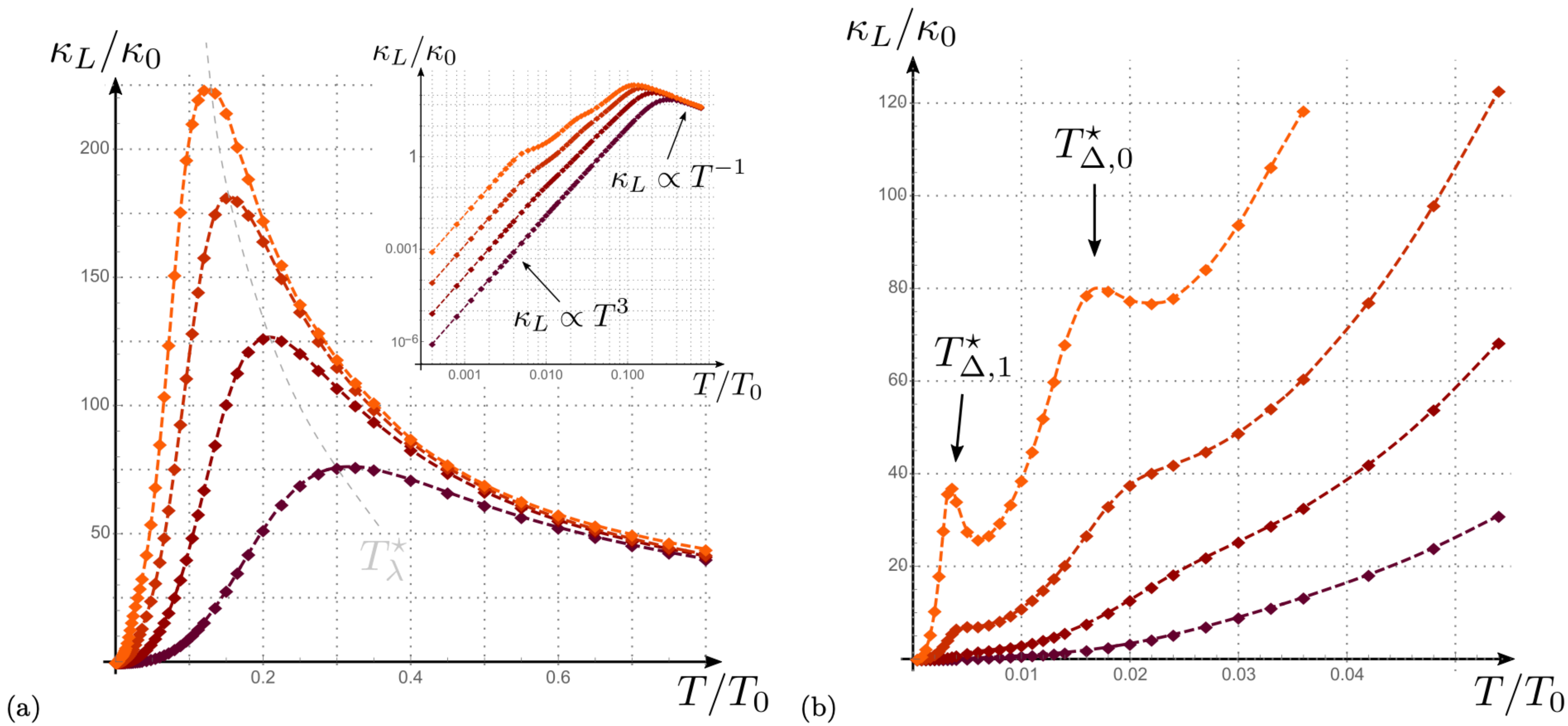
Good match of magnon and phonon phase space

$\frac{v_m}{v_{ph}}$	$\chi\epsilon_0\mathfrak{a}^2$	n_0	$\frac{M_{uc}v_{ph}\mathfrak{a}}{\hbar}$	m_0^x	m_0^y	m_0^z	$\frac{\Delta_0}{\epsilon_0}$	$\frac{\Delta_1}{\epsilon_0}$
2.5	0.19	1/2	$8 \cdot 10^3$	0	0.0 0.05	0.05 0.0	0.2	0.04

ξ	$\Lambda_1^{(\xi)}$	$\Lambda_2^{(\xi)}$	$\Lambda_3^{(\xi)}$	$\Lambda_4^{(\xi)}$	$\Lambda_5^{(\xi)}$	$\Lambda_6^{(\xi)}$	$\Lambda_7^{(\xi)}$
n = 0	12.0	10.0	14.0	10.0	12.0	0.6	0.8
m = 1	−10.0	−12.0	−14.0	−12.0	−10.0	−0.8	−0.6

TABLE I: Numerical values of the fixed dimensionless parameters used in all numerical evaluations. The upper and lower entries for m_0^y and m_0^z correspond to the two cases for calculating ϱ_H^{xy} and ϱ_H^{xz}, respectively. The couplings $\Lambda_i^{(\xi)}$ are given in units of $\epsilon_0/\mathfrak{a}$.

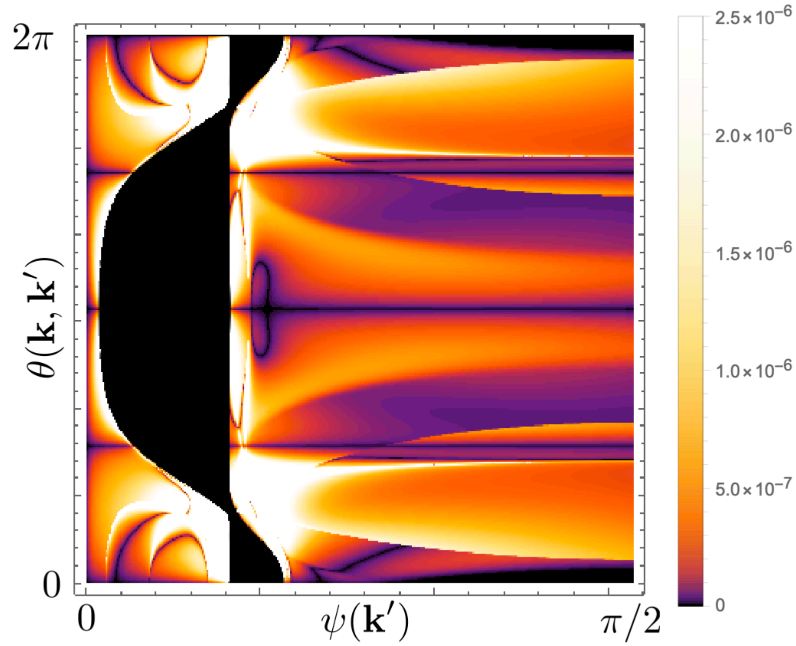
Diagonal conductivity



One can see Heisenberg regimes, anisotropic regime, extrinsic regime

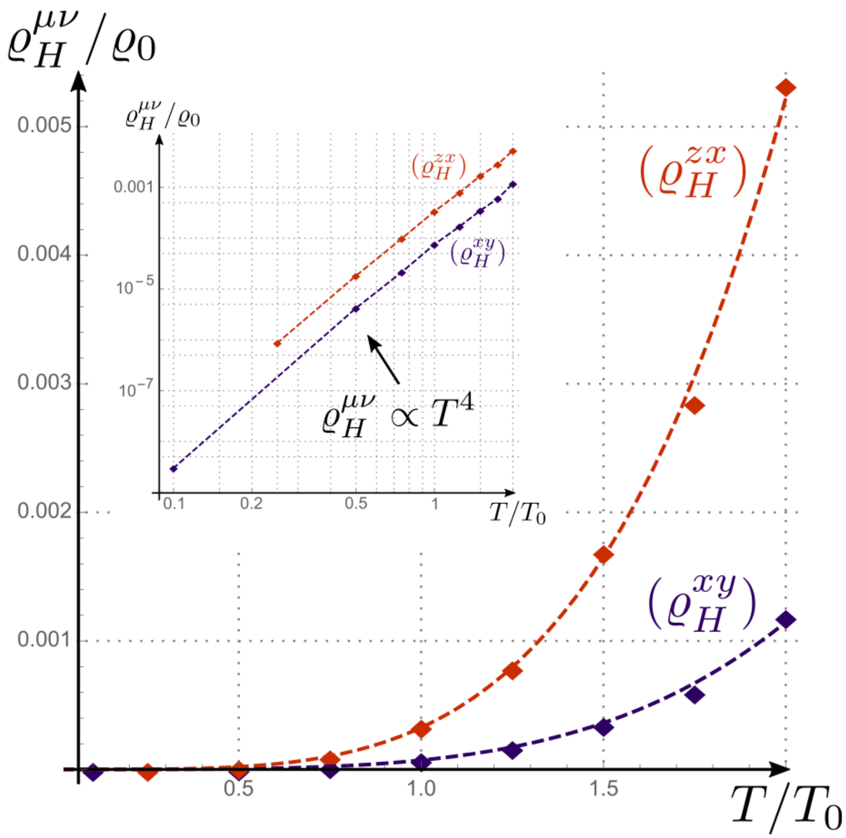
Skew scattering

Cut through the skew scattering rate:



A very complex object, lots of phase space features

Thermal Hall resistivity



Observe T^4 behavior
(Heisenberg regime)

Larger effect with current perpendicular to plane, even though we took the magnetism *strictly* 2d (magnons do not propagate in z direction)

$$\kappa_0 = k_B v_{\mathrm{ph}}/\mathfrak{a}^2$$

$$\varrho_0 = \kappa_0^{-1}$$

$$\kappa_0^{\mathrm{CFTD}} = 0.17\ \mathrm{W{\cdot}K^{-1}{\cdot}m^{-1}}$$

Two types of effects

Phonon Boltzmann equation

- Phonons are good quasiparticles

Convective derivative. Dynamics.

- Non-dissipative effects: modifications of intrinsic dynamics of individual quasiparticles, e.g. Berry phase effects, etc.

$$D_t p = \Gamma[p]$$

- Dissipative effects: modifications of scattering of quasiparticles

Collision term

Work in progress: I can only tell you why this is not so easy

Phonon Hall viscosity

$$\mathcal{L}_E = \frac{\rho}{2}\left(\partial_\tau u_\mu\right)^2 + \frac{1}{2}c_{\mu\nu\gamma\lambda}\partial_\mu u_\nu \partial_\gamma u_\lambda + i\eta_{\mu\nu\gamma\lambda}\partial_\tau u_\mu \partial_\nu \partial_\gamma u_\lambda .$$

Leading effect of TRS breaking for phonons

- Originates from electronic, spin contributions
- Hamiltonian:

$$\mathcal{H}(x) = \frac{1}{2\rho}\left(\Pi_\mu - A_\mu[u]\right)^2 + \frac{1}{2}c_{\mu\nu\gamma\lambda}\partial_\mu u_\nu \partial_\gamma u_\lambda \qquad A_\mu[u] = \eta_{\mu\nu\gamma\lambda}\partial_\nu \partial_\gamma u_\lambda$$

  - Induces Berry curvature of phonon states
  - Intrinsic thermal Hall effect is allowed

Phonon Hall viscosity

PHYSICAL REVIEW B **86**, 104305 (2012)

Berry curvature and the phonon Hall effect

Tao Qin,[1] Jianhui Zhou,[1] and Junren Shi[2]

$$\kappa_{xy}^{\mathrm{tr}} = -\frac{(\pi k_B)^2}{3h} Z_{\mathrm{ph}} T - \frac{1}{T}\int d\epsilon \epsilon^2 \sigma_{xy}(\epsilon) \frac{dn(\epsilon)}{d\epsilon},$$

where

$$\sigma_{xy}(\epsilon) = -\frac{1}{V\hbar}\sum_{\hbar\omega_{ki}\leqslant\epsilon} \Omega_{ki}^z$$

$$\kappa_{xy} \sim \eta T^3$$

- Simple formula seems semi-classical but subtle
- c.f. electrical Hall effect

- Contributions far from chemical potential $\sigma_{\mu\nu}^a = -2e^2\left[\sum_n \int \frac{d^d \boldsymbol{k}}{(2\pi)^d} n_{\mathrm{F}}(\epsilon_{n\boldsymbol{k}})\Omega_{n\boldsymbol{k}}^{\lambda}\right]\epsilon_{\lambda\mu\nu}$
- Driven by anomalous velocity due to *force* on electrons $\boldsymbol{v}_{\mathrm{anom}} = -\frac{d\boldsymbol{k}}{dt} \times \boldsymbol{\Omega} = e\boldsymbol{E} \times \boldsymbol{\Omega}$

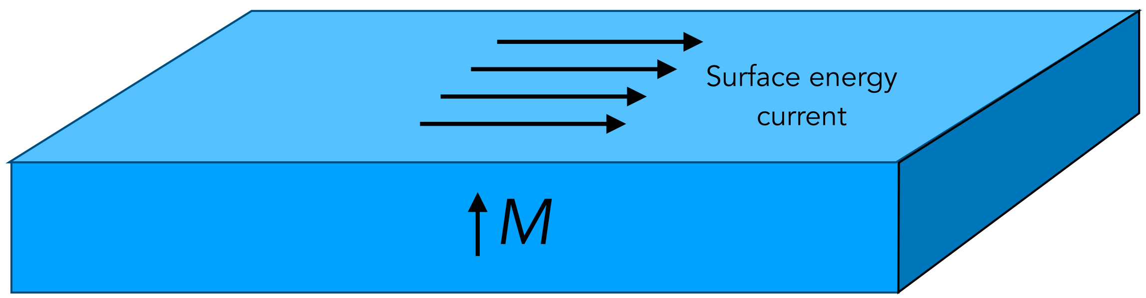
These subtleties are related to “energy magnetization”, taking into account “local equilibrium” currents

Energy magnetization

N. Cooper *et al*, 1997; T. Qin *et al*, 2011; A. Kapustin+L. Spodyneiko, 2020

Equilibrium energy current $\boldsymbol{J}_\epsilon^{\mathrm{eq}} = \boldsymbol{\nabla} \times \boldsymbol{M}_\epsilon$

M=0 outside



Magnetization current becomes non-zero in bulk out of equilibrium

$$\boldsymbol{\nabla} \times \boldsymbol{M}_\epsilon = \boldsymbol{\nabla} T \times \frac{\partial \boldsymbol{M}_\epsilon}{\partial T}$$

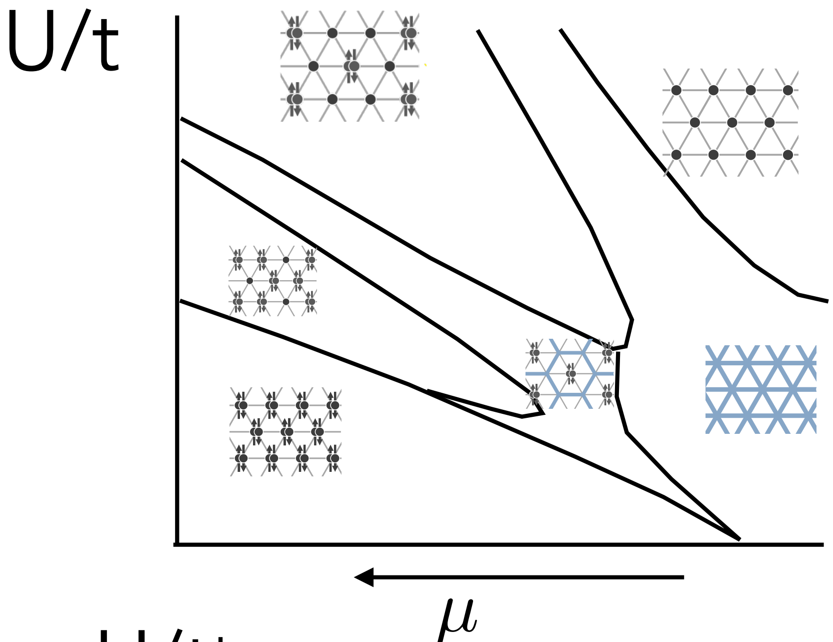
This is a physical current but it is always cancelled by a boundary contribution and does not contribute in any transport measurement

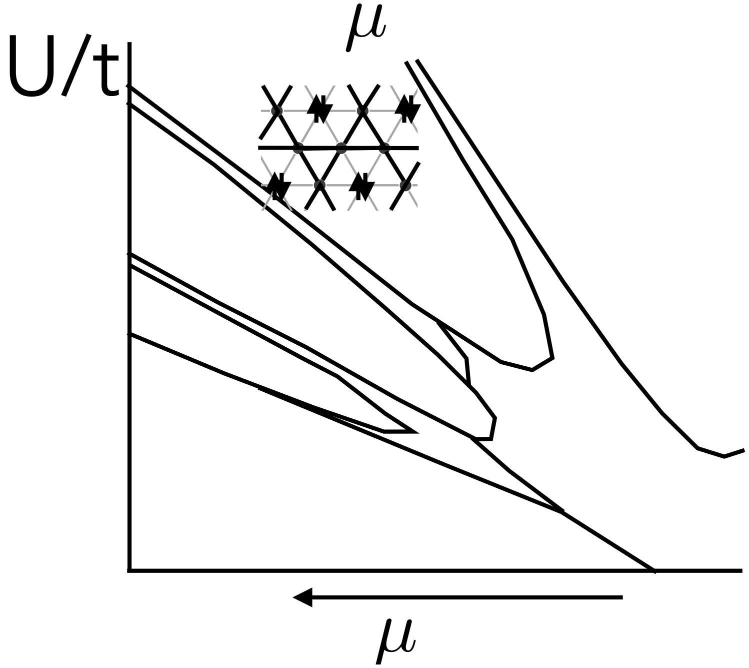
"Transport current" $\boldsymbol{J}_\epsilon^{\mathrm{tr}} = \boldsymbol{J}_\epsilon - \boldsymbol{\nabla} \times \boldsymbol{M}_\epsilon$

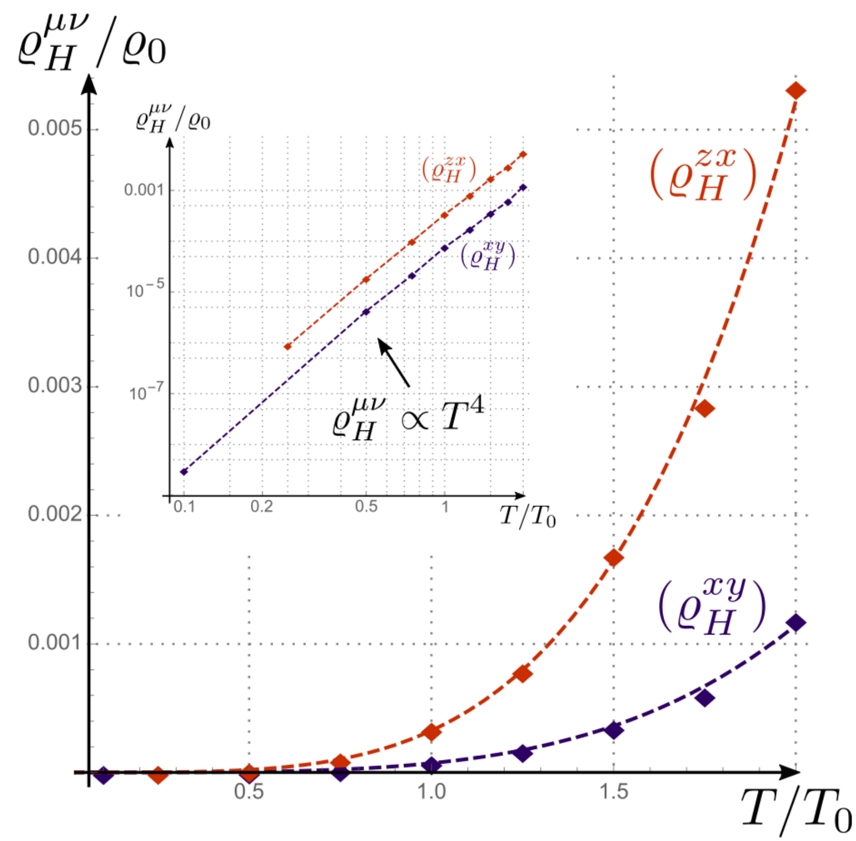
In progress

- Quasi-classical (kinetic equation) derivation of energy magnetization
- Combination with Berry phase dynamics in quantum kinetic equation (c.f. Sachdev *et al* on Hall viscosity+scattering)
  - Corrections to the current operator in a gravitational field
- Keldysh formulation to include both effects
  - We'd like to learn Son's new coadjoint orbit approach!

Thanks







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