Transport in strongly correlated systems

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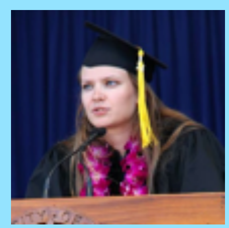

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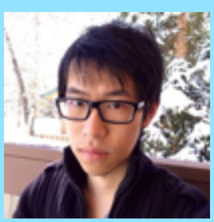

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Transport

$$\boldsymbol{j} = \underline{\sigma} \boldsymbol{E} \qquad \qquad \boldsymbol{j}_e = -\underline{\kappa} \boldsymbol{\nabla} T$$

- Arguably most important aspect of quantum materials: electrical and thermal conductivity (and crossed coefficients)
- Sensitive, versatile
- Probes extreme long wavelength, low frequency

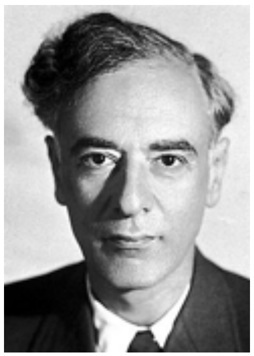
Theory

- *Understanding* of transport mainly through **quasiparticle** picture
  - Boltzmann equation:

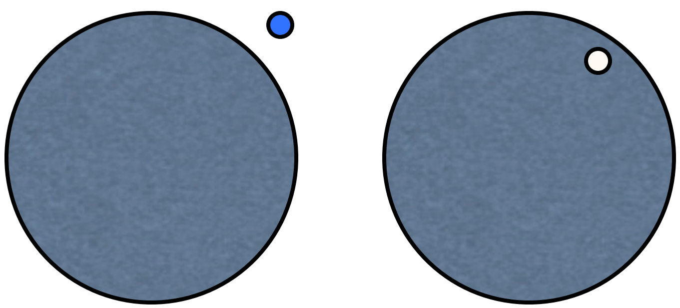
$$\left[\partial_t + \boldsymbol{v}_n(\boldsymbol{k}) \cdot \boldsymbol{\nabla}_r - e\boldsymbol{E} \cdot \boldsymbol{\nabla}_k\right] f_n = \left.\frac{\partial f_n}{\partial t}\right|_{\text{collision}}$$

Linearizing this around equilibrium gives conductivities in terms of band velocities and scattering rates

Fermi Liquid Theory



Landau provided justification for quasiparticle picture in metals when $T \ll E_F$



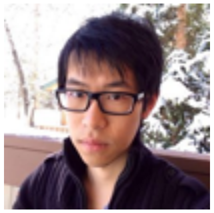
Low energy excitations act like electrons and holes but with wavefunction dressing (Z<1), effective mass, and Landau interactions

$$E = \sum_k \epsilon_k \delta n_k + \frac{1}{2V} \sum_{k,k'} U_{k,k'} \delta n_k \delta n_{k'}$$

scattering is weak because not so many low energy qp states to scatter to

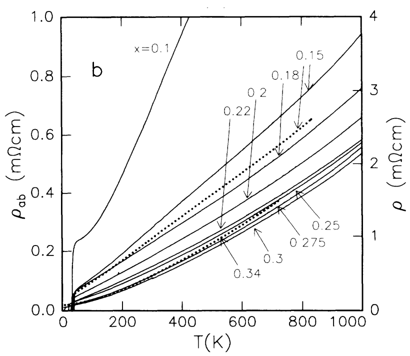
This talk

I. **SYK model of a strongly correlated metal: FL to NFL crossover and a disordered strange metal**

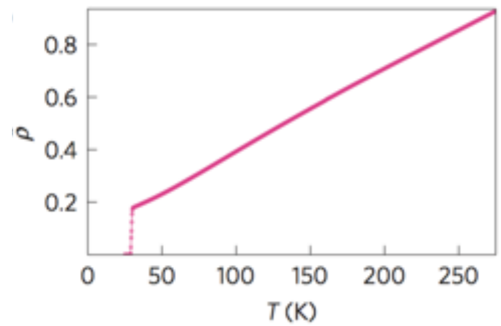


II. Heat transport in spin systems - towards a non-quasiparticle description (progress report)

Non-Fermi Liquids



LSCO Takagi *et al, 1992*



$BaFe_2(As_{1-x}P_x)_2$, Hayes *et al, 2016*

T-linear resistivity is challenging theoretically:

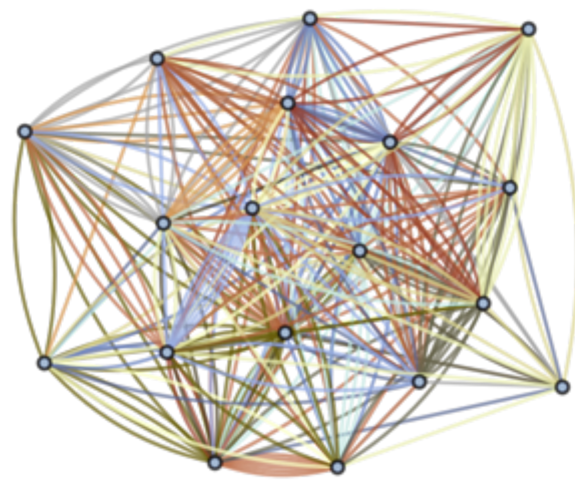
- If even “bad” quasiparticles exist, it is difficult to make them scatter strongly on the *entire* Fermi surface
- If no quasiparticles exist, what is the starting point?

Sachdev-Ye-Kitaev model

A toy *exactly soluble* model
of a non-Fermi liquid

$$H = \sum_{i<j,k<l} U_{ijkl}\, c_i^\dagger c_j^\dagger c_k c_l$$

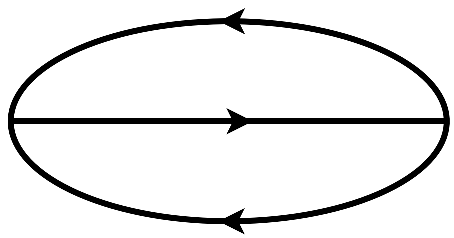
$$\overline{|U_{ijkl}|^2} = \frac{2U^2}{N^3}$$



Like a strongly interacting quantum dot
or atom with complicated Kanamori
interactions between many "orbitals"

SYK Model

Sachdev-Ye, 1993: Model has a soluble large-N limit

$\Sigma =$  $+O(1/N)$

In equations: very similar to DMFT:

$$G(i\omega_n) = \frac{1}{i\omega_n - \Sigma(i\omega_n)} \qquad \Sigma(\tau) = -U^2 G(\tau)^2 G(-\tau)$$

Solution:

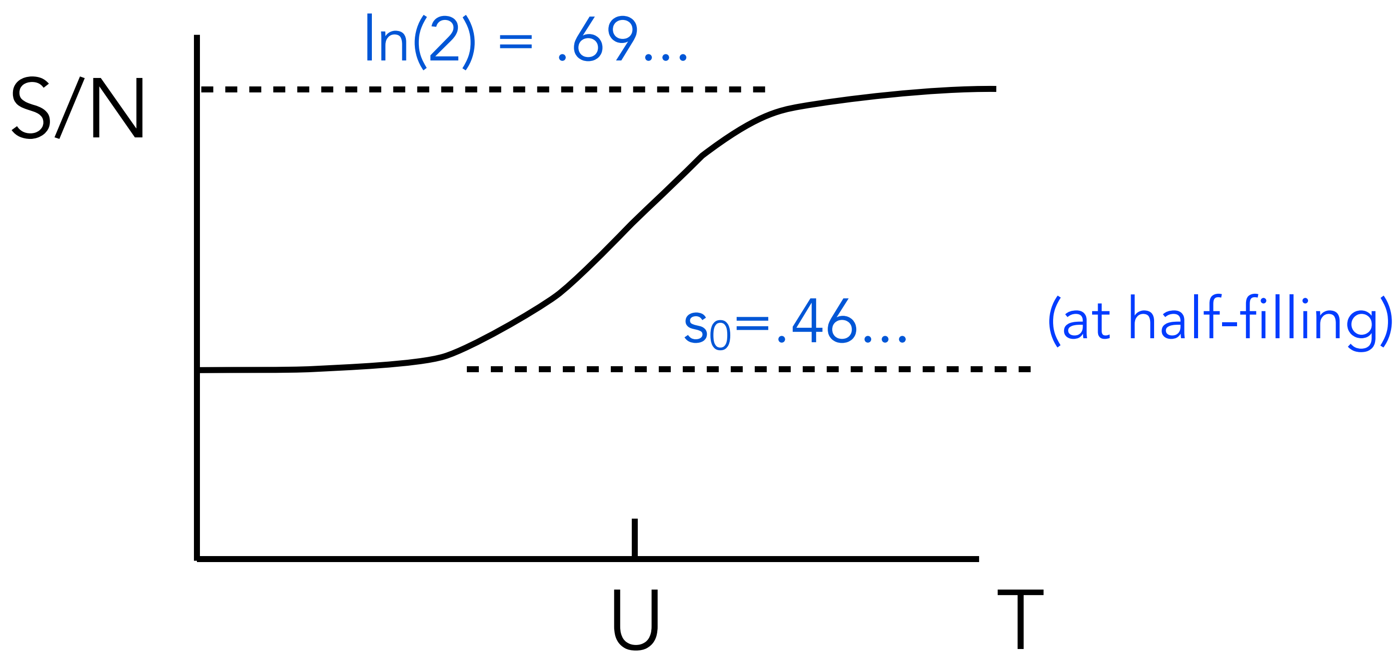
$$G(i\omega) \sim 1/\sqrt{\omega}$$

not a pole: non-Fermi liquid

SYK Model

Why not quasiparticles?

Georges, Parcollet, Sachdev, 2001: **ground state entropy!**



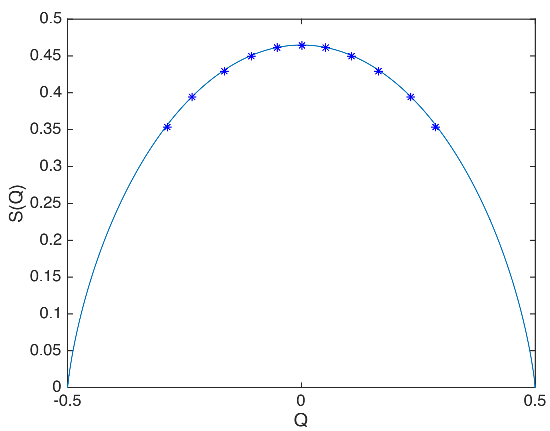
Many states available for scattering

"level spacing" ~ U exp(-Ns_0)

Density dependence

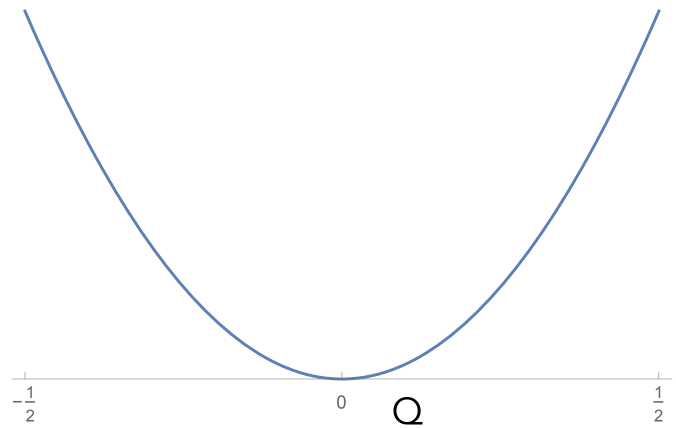
$$H \to H - \mu \mathcal{N} \qquad \mathcal{N} = \sum_i c_i^\dagger c_i \qquad \mathcal{Q} = \frac{\mathcal{N}}{N} - \frac{1}{2}$$

Entropy



Davison *et al*, arXiv:1612.00849

Energy

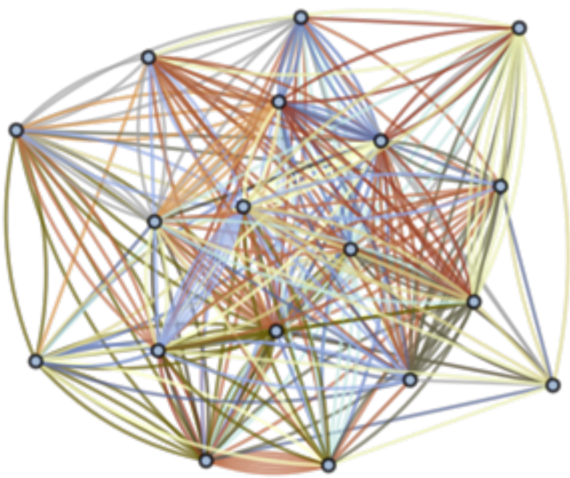


schematic

- Compressibility is constant at T=0

$$K = \left.\frac{\partial \mathcal{Q}}{\partial \mu}\right|_{\mu=0} = \frac{1.04}{U}$$

SYK Summary



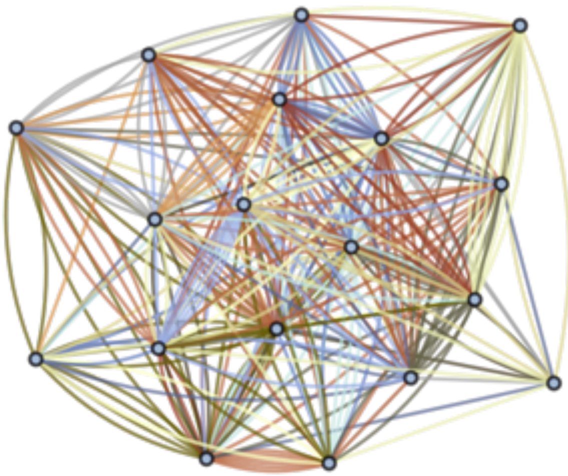
- Compressible
- Ground state entropy
- Non-Fermi liquid

$$K(T=0) = \frac{1.04}{U}$$

$$S(T=0)/N = .46\ldots$$

$$G(i\omega) \sim 1/\sqrt{\omega}$$

SYK Summary



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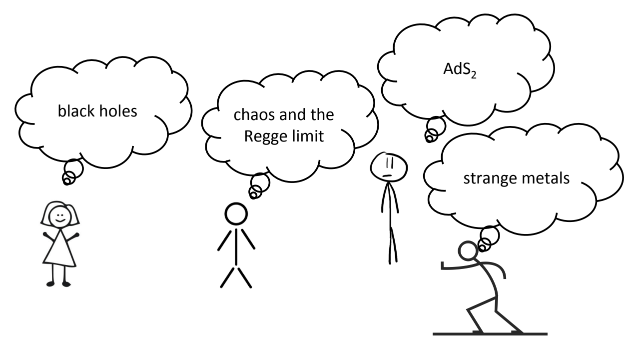
Chaos

$$\left\langle [\mathcal{O}(0), \tilde{\mathcal{O}}^{\dagger}(t)]^2 \right\rangle \sim \frac{1}{N} e^{\lambda_L t}$$

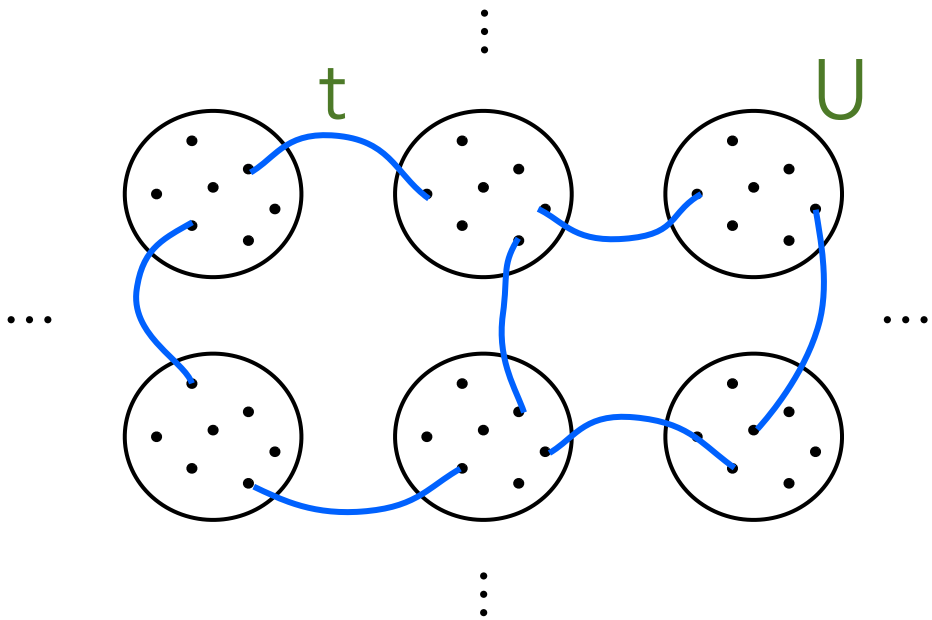
$$\lambda_L = \frac{2\pi k_B T}{\hbar}$$

Holography



slide from D. Stanford, IAS, 2017

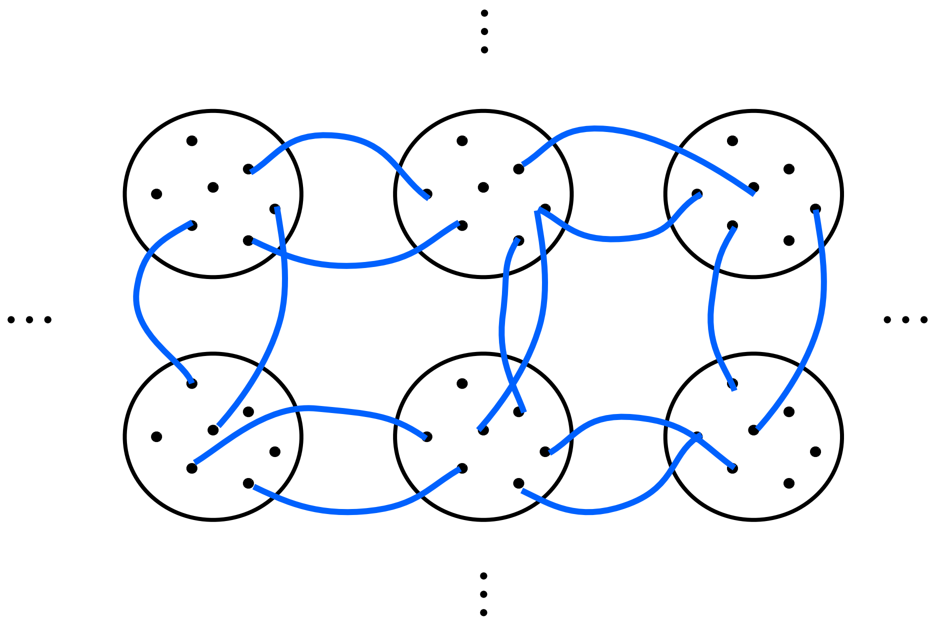
Building a metal



$$H = \sum_x \sum_{i<j,k<l} U_{ijkl,x} c^\dagger_{ix} c^\dagger_{jx} c_{kx} c_{lx} + \sum_{\langle xx' \rangle} \sum_{i,j} t_{ij,xx'} c^\dagger_{i,x} c_{j,x'}$$

$$\overline{|t_{ij,x,x'}|^2} = t_0^2/N.$$

Building a metal



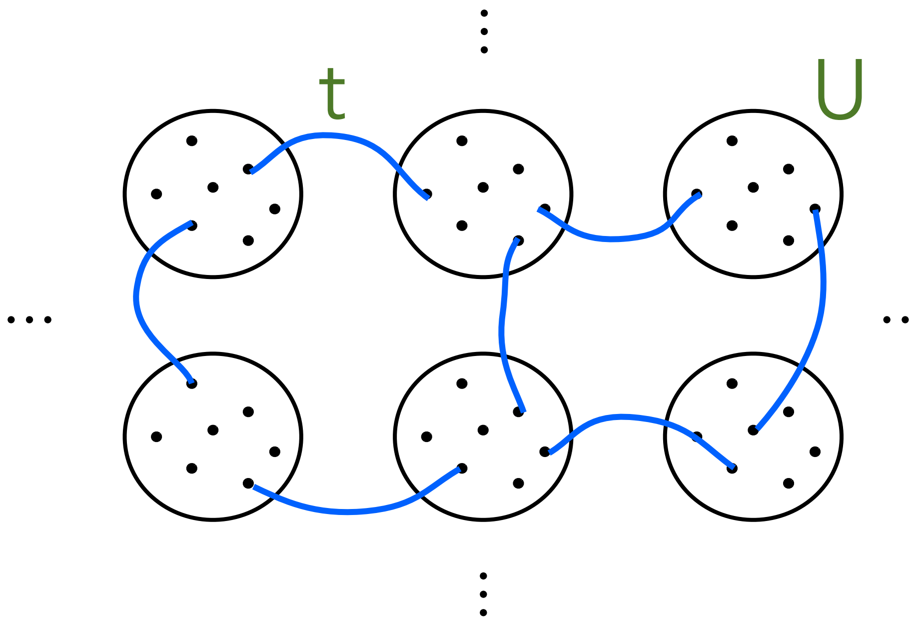
Other work: 2-electron hopping

Y.Gu *et al*, arXiv:1609.07832
R. Davison *et al*, arXiv:1612.00849

$$H = \sum_x \sum_{i<j,k<l} U_{ijkl,x} c^\dagger_{ix} c^\dagger_{jx} c_{kx} c_{lx} + \sum_{\langle xx' \rangle} \sum_{i,j} t_{ijkl,xx'} c^\dagger_{i,x} c^\dagger_{j,x} c_{k,x'} c_{l,x'} + \text{h.c.}$$

Omitting *relevant* 1-electron hopping leaves system NFL even at T=0

Building a metal

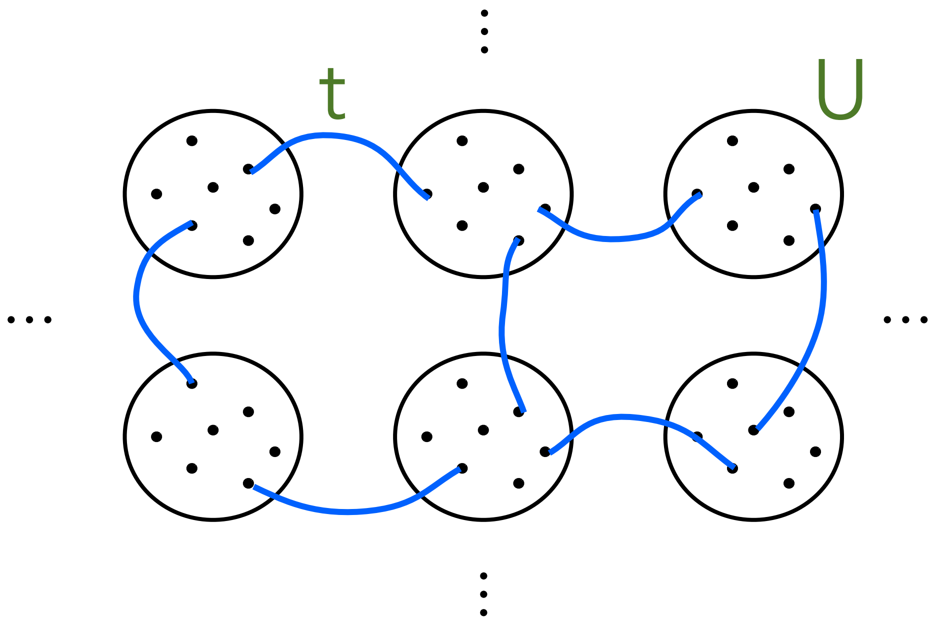


$$H = \sum_{x} \sum_{i<j,k<l} U_{ijkl,x} c^{\dagger}_{ix} c^{\dagger}_{jx} c_{kx} c_{lx} + \sum_{\langle xx' \rangle} \sum_{i,j} t_{ij,xx'} c^{\dagger}_{i,x} c_{j,x'}$$

competition!

t/U≪1 interesting

Self-consistent equations



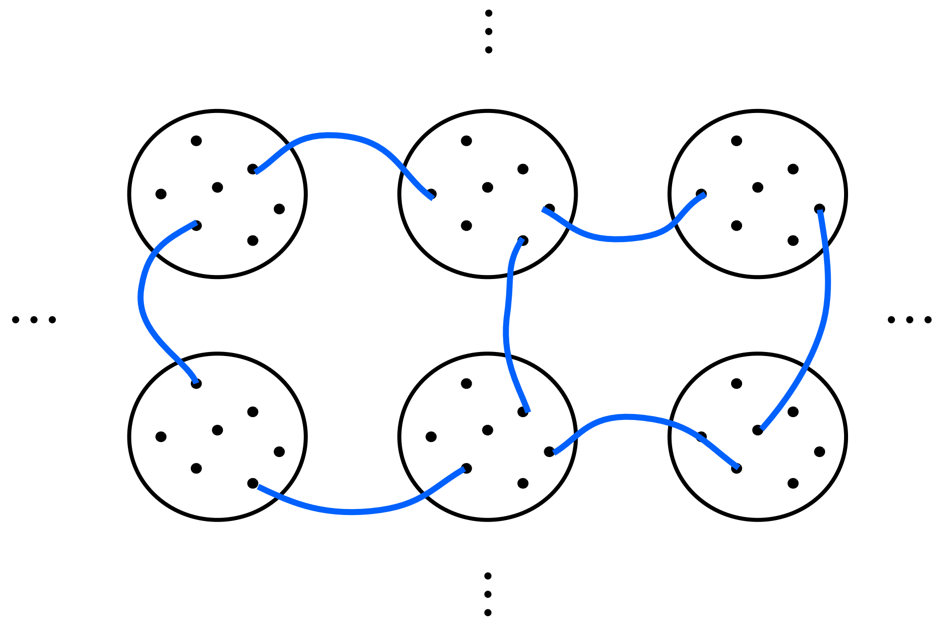
$$G(i\omega_n)^{-1} = i\omega_n + \mu - \Sigma_4(i\omega_n) - zt_0^2 G(i\omega_n),$$
$$\Sigma_4(\tau) = -U_0^2 G(\tau)^2 G(-\tau),$$

$$\bar{G}(i\bar{\omega}) = \tilde{t}G(i\omega)$$

strong similarities to DMFT equations

mathematical structure appeared in early study of doped t-J model with *double* large N and infinite dimension limits: O. Parcollet+A. Georges, 1999

Coherence scale



$$G(i\omega_n)^{-1} = i\omega_n + \mu - \Sigma_4(i\omega_n) - z t_0^2 G(i\omega_n),$$
$$\Sigma_4(\tau) = -U_0^2 G(\tau)^2 G(-\tau),$$

$$\bar{G}(i\bar{\omega}) = \tilde{t} G(i\omega)$$

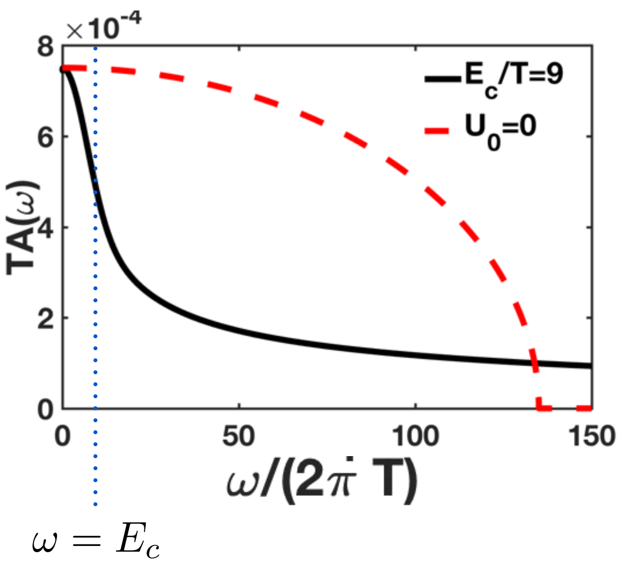
Rescaling $\bar{\omega} = \frac{\omega}{\tilde{E}_c}, \quad \bar{\tau} = \tau \tilde{E}_c, \qquad \bar{G}(i\bar{\omega}) = \tilde{t} G(i\omega) \quad \bar{\Sigma}(i\bar{\omega}) = \Sigma(i\omega)/\tilde{t} \qquad \tilde{t} = \left(\frac{z}{2}\right)^{\frac{1}{2}} t$

$$\bar{G}(i\bar{\omega}) = \frac{\tilde{t}}{U} i\bar{\omega} - \bar{\Sigma}(i\bar{\omega}) \qquad \bar{\Sigma}(\bar{\tau}) = -\bar{G}(\bar{\tau})^2 \bar{G}(-\bar{\tau}) + 2\bar{G}(\bar{\tau}),$$

For t≪U, a single universal coherence scale appears $\tilde{E}_c = \frac{\tilde{t}^2}{U}$

Coherence scale

We solve these equations in a real time Keldysh formulation numerically and determine asymptotics analytically.

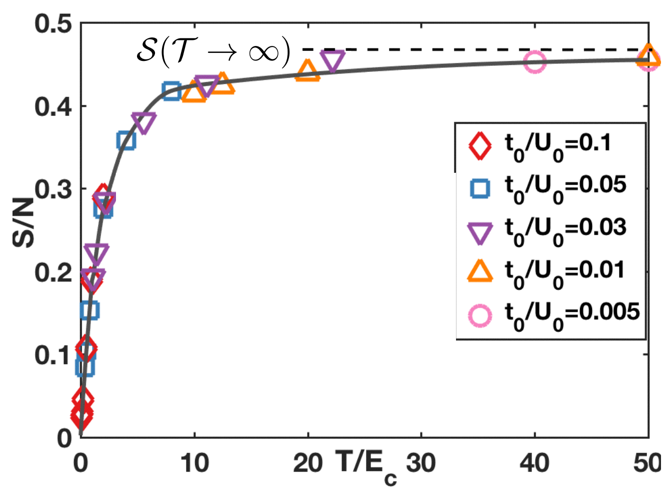


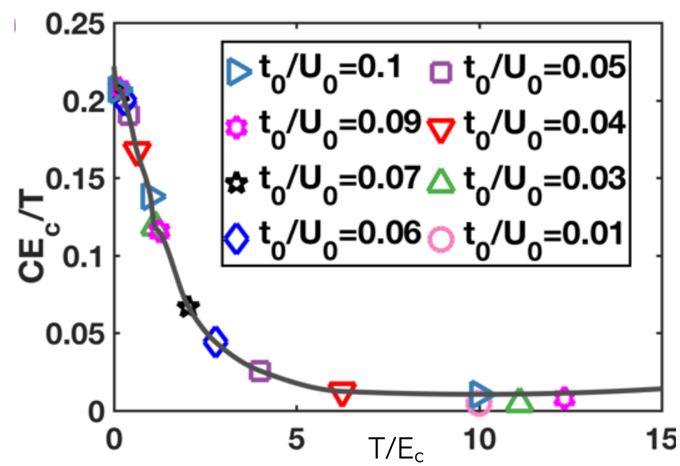
Narrow "coherence peak" appears in spectral function: heavy quasiparticles form for $T \ll E_c$

Quasiparticle weight $Z \sim t/U$

Entropy

Level repulsion: entropy is released for $T<E_c$!





Universal scaling forms

$$S/N = \mathcal{S}(T/E_c)$$

$$C/N = T/E_c \mathcal{S}'(T/E_c)$$

$$\gamma \equiv \lim_{T \to 0} \frac{C}{T} = \frac{\mathcal{S}'(0)}{E_c}$$

Sommerfeld enhancement

$$m^*/m \sim U/t$$

Compressibility

For $t \ll U$, compressibility is almost unaffected by hopping

$$K = \left.\frac{\partial \mathcal{Q}}{\partial \mu}\right|_{\mu=0} = \frac{1.04}{U} \quad \ll \gamma \sim \frac{U}{t^2}$$

??How to reconcile with Sommerfeld enhancement??

- Fermi liquid theory: compressibility is renormalized by Fermi liquid parameter $F = g(E_F)\, U_{FL}$

$$\gamma / K = \frac{\pi^2}{3}(1 + F)$$

$$\gamma / K \sim (U/t)^2$$

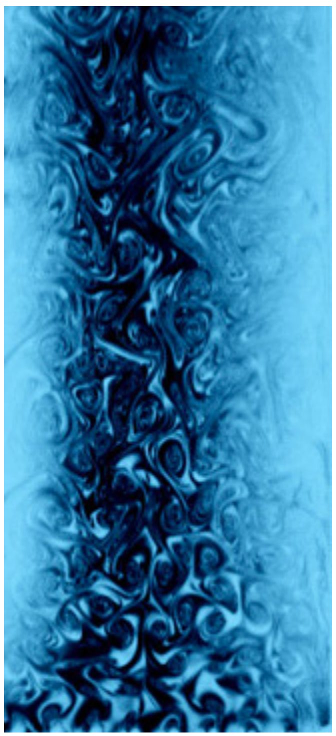
⇒

$$F \sim \left(\frac{U}{t}\right)^2 \gg 1$$

Transport

Quasiparticle picture applies only for $T \ll E_c$

More generally, we use hydrodynamics



$$\sigma = \lim_{\omega \to 0} \lim_{p \to 0} \frac{-i\omega}{p^2} D_{Rn}(p,\omega)$$

✦ Calculate density response using Keldysh method.

✦ Do analogously for thermal conductivity

N.B. Because of randomness, momentum is not a hydrodynamic variable

Transport

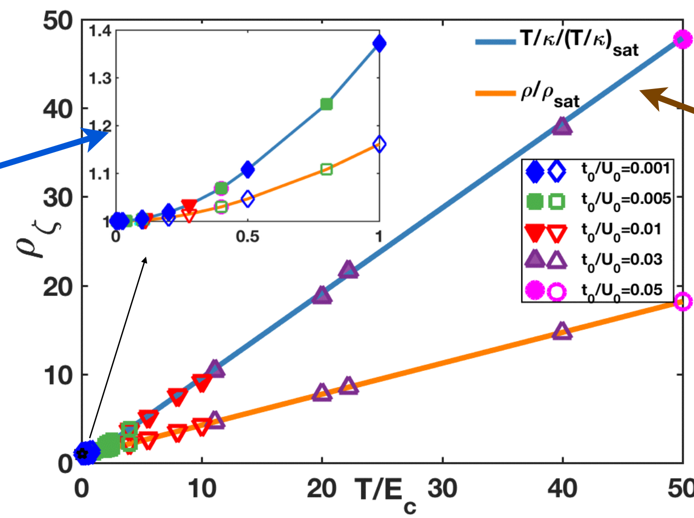
Generalized resistivity

$$\rho_c = 1/\sigma \qquad \rho_e = T/\kappa$$

scaling

$$\rho_\zeta(t_0, T \ll U_0) = \frac{1}{N} R_\zeta\left(\frac{T}{E_c}\right)$$

Fermi liquid
$R = R_0 + AT^2$
for $T \ll E_c$



Linear in T for
$E_c \ll T \ll U$

Crossover from heavy FL to strange metal

Transport ratios

<u>Kadowaki-Woods</u>

$$\rho_\zeta(T \ll E_c) \approx \rho_\zeta(0) + A_\zeta T^2,$$

$$A \sim 1/(NE_c^2)$$

recall $\gamma \sim 1/E_c$

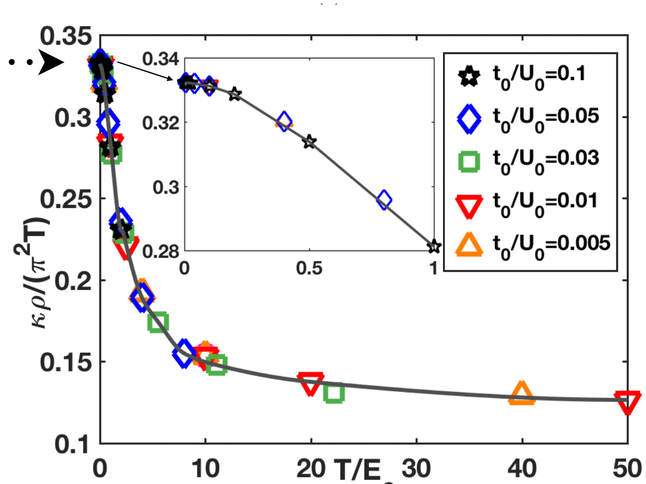
$$KW = A/(N\gamma)^2 \sim 1/N^3$$

independent of t,U!

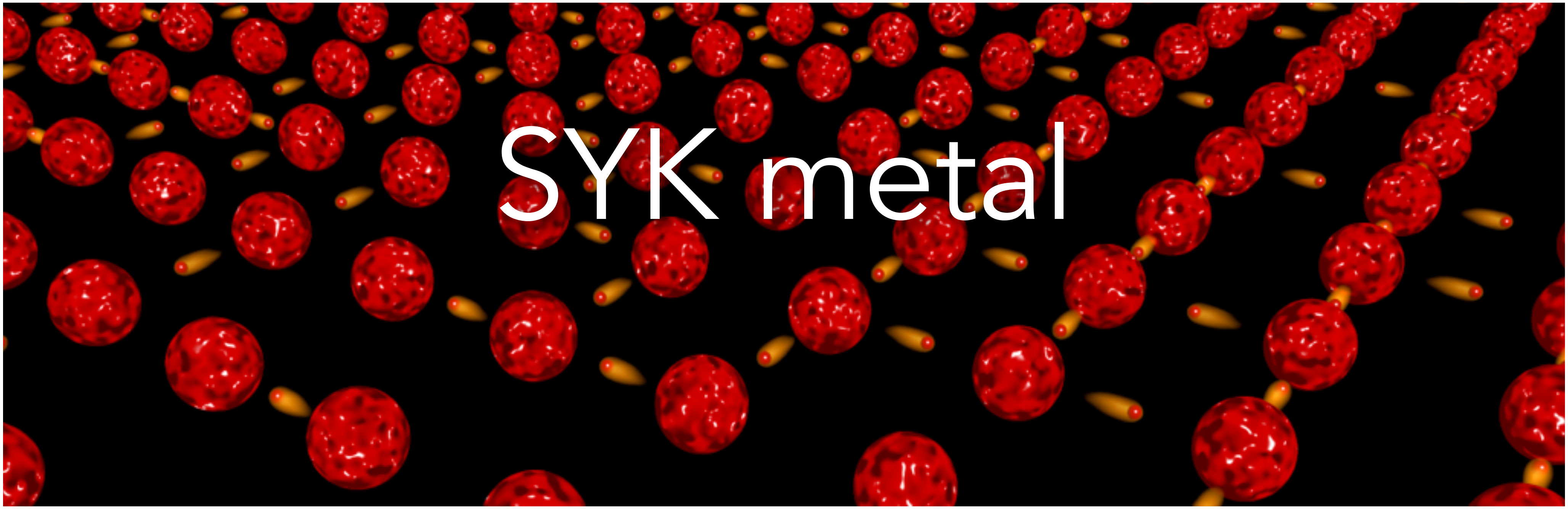
<u>Lorenz</u>

$$L = \frac{\kappa}{\sigma T} = \mathcal{L}(T/E_c)$$

FL $\frac{\pi^2}{3}$



$\frac{\pi^2}{8}$ NFL



SYK metal

- Small coherence scale $E_c=t^2/U$
- Heavy mass $\gamma \sim m^*/m \sim U/t$
- Small QP weight $Z \sim t/U$
- Kadowaki-Woods A/γ^2 = constant
- Linear in T resistivity and T/κ
- Lorenz ratio crosses over from FL to NFL value

Where is this going?

Similarity with DMFT is encouraging: can we bootstrap this to a more realistic treatment of incoherent metals?

- Translational invariant SYK lattice model

$$H = \sum_x \sum_{i<j,k<l} U_{ijkl} c^\dagger_{ix} c^\dagger_{jx} c_{kx} c_{lx} - t \sum_{\langle xx' \rangle} \sum_i c^\dagger_{i,x} c_{i,x'}$$

- Large N equations

$$\begin{aligned} G(\boldsymbol{k}, i\omega_n)^{-1} &= i\omega_n - \epsilon(\boldsymbol{k}) - \Sigma(\boldsymbol{k}, i\omega_n), \\ \Sigma(\boldsymbol{x}, \tau) &= -U_0^2 G(\boldsymbol{x}, \tau)^2 G(-\boldsymbol{x}, -\tau), \end{aligned}$$

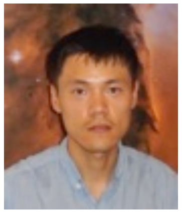
describes NFL to FL crossover.
Similarities to DCA?

- Apply to realistic band structures

This talk

I. SYK model of a strongly correlated metal: FL to NFL crossover and a disordered strange metal

II. Heat transport in spin systems - towards a non-quasiparticle description (progress report)



What’s in there?
a QSL…or a chicken?

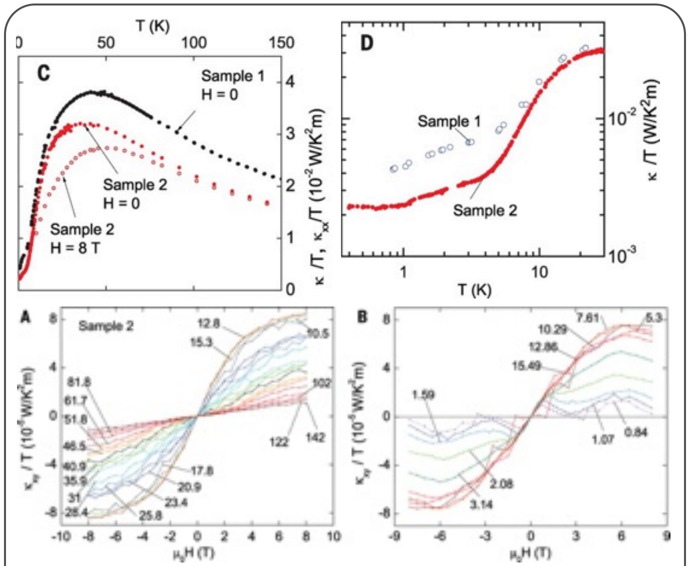
Heat transport in magnets

Insulating magnet: typically heat is the only possible transport measurement

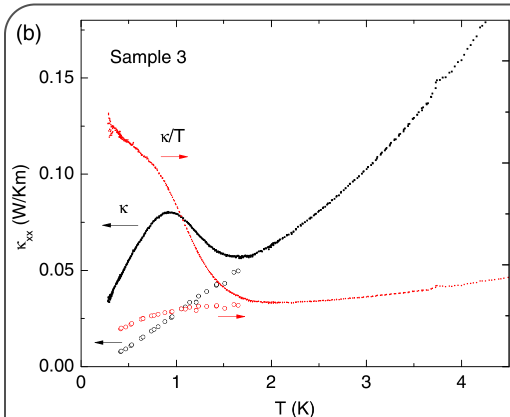
- Probes extended nature of excitations at ultra-low frequency
- Automatically removes contributions from localized nuclei and isolated defects, which may carry large entropy

Heat transport in magnets

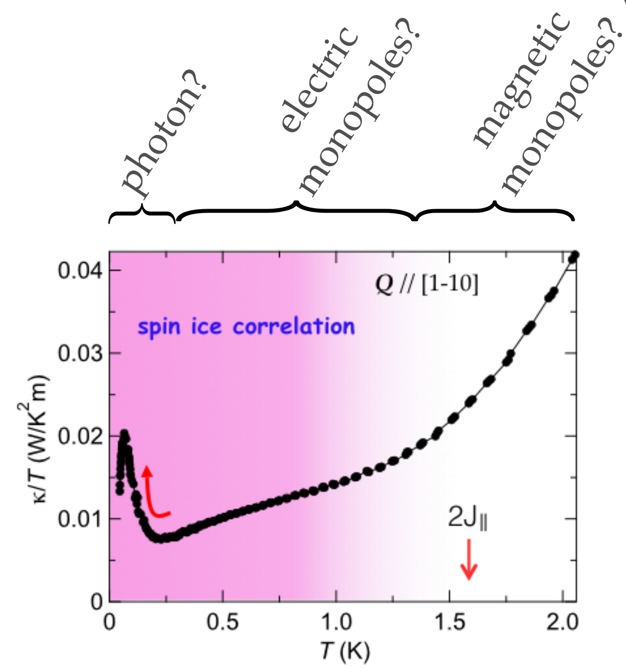
Insulating magnet: typically heat is the only possible transport measurement



$Tb_2Ti_2O_7$
Ong's group 2015

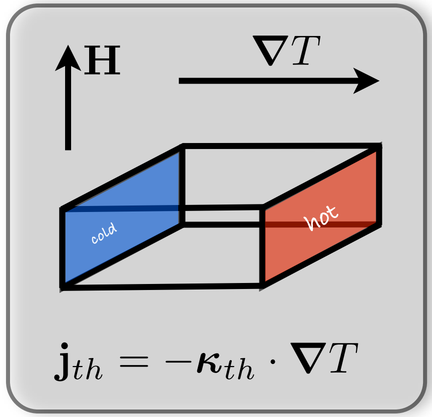


Hirschberger *et al.* 2015
Cu(1,3-benzenedicarboxylate)



$Pr_2Zr_2O_7$
Tokiwa, Matsuda *et al.* (2017?)

Heat transport in magnets



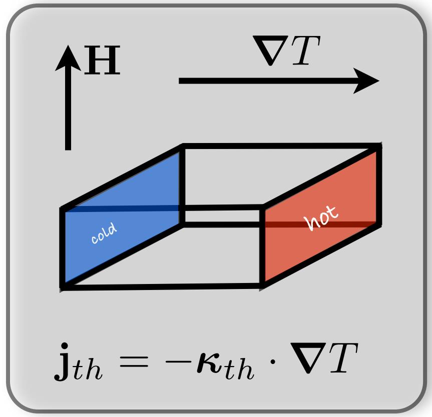
Two types of heat current

$$\boldsymbol{j} = \boldsymbol{j}_{\text{spins}} + \boldsymbol{j}_{\text{lattice}}$$

Two important effects of spins

1. Spin heat current j_{spins} induced by thermal gradient
2. Scattering of heat-carrying phonons off of spins

Heat transport in magnets



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Two important effects of spins

1. Spin heat current j_{spins} induced by thermal gradient
2. Scattering of heat-carrying phonons off of spins

Quasiparticles?

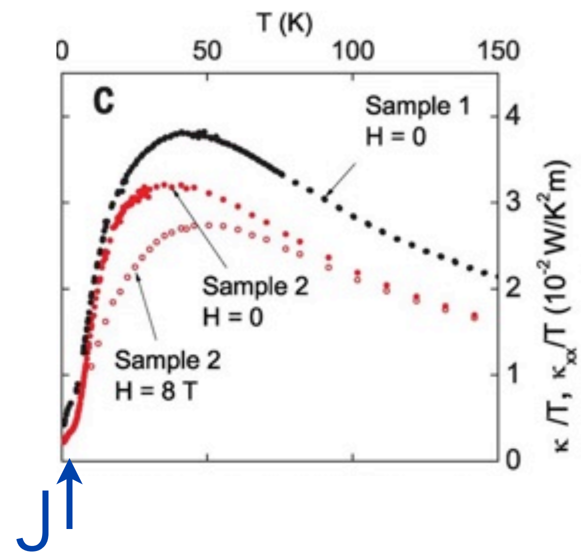
Spin Hamiltonian

$$H = \frac{1}{2} \sum_{\langle ij \rangle} \sum_{\mu\nu} J_{ij}^{\mu\nu} S_i^{\mu} S_j^{\nu}$$

- no obvious free particle starting point
- $E_F \rightarrow J$ much smaller

Many (most?) measurements have T>J
and are not in the QP regime

e.g. $Tb_2Ti_2O_7$



Luttinger theory

Luttinger (1964) formulated thermal conductivity as response to a fictional "gravitational field"

$$\kappa^{\mu\nu}(\omega) = \frac{-1}{N_{uc}\,\omega\,T}\int_0^{+\infty} dt\, e^{i\omega t}\langle[j^\mu(t), j^\nu(0)]\rangle$$

Challenging: even when equal-time correlations are fully short-range, e.g. $\beta J \ll 1$,

the long-time dynamics enters, and this is still hard because $Ht >> 1$

Spectral representation

longitudinal

$$\frac{1}{2}(\kappa^{\mu\nu} + \kappa^{\nu\mu}) = \frac{\pi}{Z N_{uc} k_{\mathrm{B}} T^2} \sum_{m,n} \langle m | j^\mu | n \rangle \langle n | j^\nu | m \rangle e^{-\beta E_n} \delta(E_n - E_m)$$

Hall

$$\frac{1}{2}(\kappa^{\mu\nu} - \kappa^{\nu\mu}) = \frac{-i}{Z N_{uc} T} \sum_{m,n} \langle m | j^\mu | n \rangle \langle n | j^\nu | m \rangle \frac{e^{-\beta E_n} - e^{-\beta E_m}}{(E_n - E_m)^2}$$

- Useful for ED calculations
- Can prove thermal Hall vanishes unless TRS is broken *and* SOC present
- Can derive scaling relations

Definition of energy current

see also: H. Lee, J.H. Han, P.A. Lee 2015

similar setup based on Luttinger energy density defined on a bond

Break Hamiltonian into sum of local terms

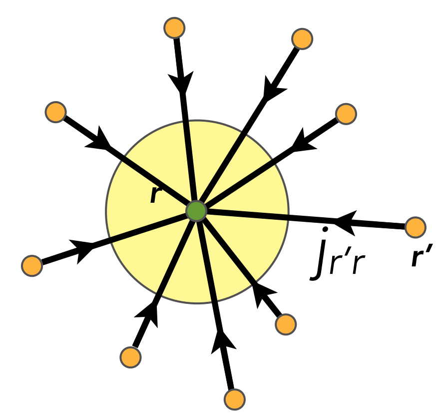
$$\hat{H} = \sum_{\mathbf{r}} \hat{\rho}_{\mathbf{r}}$$

Continuity equation defines the current

Noether current (energy conservation): $\partial_\mu \hat{j}^\mu = 0$ i.e. $\mathrm{div}\hat{\mathbf{j}} + \partial_t \hat{\rho} = 0$

Heisenberg equation of motion:

$$\partial_t \hat{\rho}_{\mathbf{r}} = -i[\hat{H}, \hat{\rho}_{\mathbf{r}}] = -i \sum_{\mathbf{r}'} [\hat{\rho}_{\mathbf{r}'}, \hat{\rho}_{\mathbf{r}}] \equiv \sum_{\mathbf{r}'} j_{\mathbf{r}'\mathbf{r}}$$



in the Kubo formulas, $j = j_{tot}$

Definition of energy current

$$j_{r'\to r} = -i\,[\hat{\rho}_{r'}, \hat{\rho}_r]$$

What does this look like?

$$\hat{\rho} \sim J\boldsymbol{S}\boldsymbol{S} + B\boldsymbol{S}$$

$$j \sim JS \times (JSS + BS)$$

"velocity" "energy"

explicit forms depend heavily on lattice structure and interactions

Scaling

- Knowing form of current and Luttinger response formulae, we find

$$C^{jj}(t) = \langle j(t)j(0)\rangle \sim J^4/T f(Jt, T/J, B/T) = BJ^3/T \tilde{f}(Jt, T/J)$$

$$\kappa_H \sim BJ^2/T^2 \int dt\, f(t, T/J)$$

$$\kappa_{\text{long}} \sim J^3/T^2 \int dt\, f(t, T/J)$$

Scaling

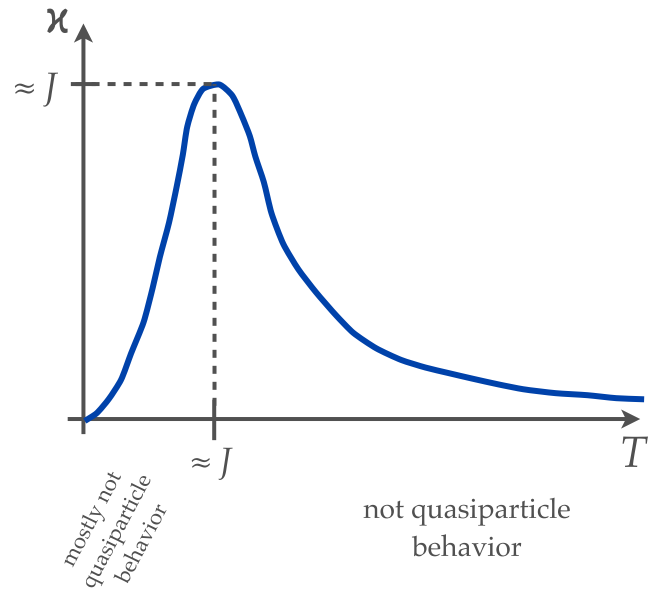
- Knowing form of current and Luttinger response formulae, we find

$$C^{jj}(t) = \langle j(t)j(0)\rangle \sim J^4/T f(Jt, T/J, B/T) = BJ^3/T\tilde{f}(Jt, T/J)$$

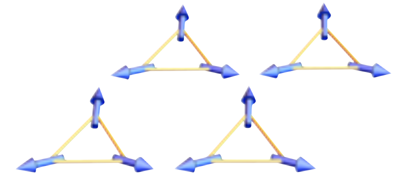
$$\kappa_H \sim BJ^2/T^2$$

$$\kappa_{\text{long}} \sim J^3/T^2$$

expect constant at high T



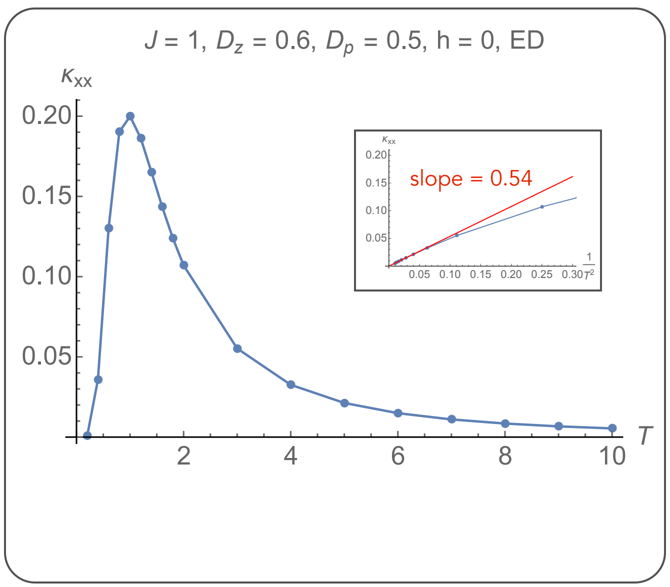
Calculations



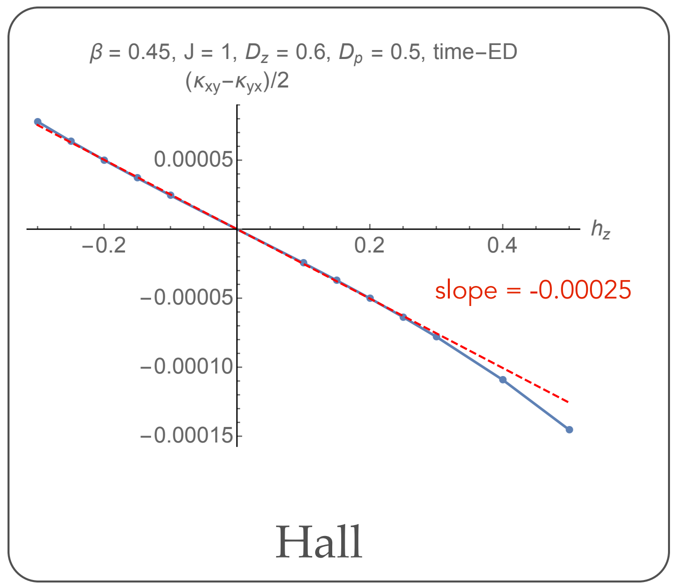
- 2x2 system (12 spins)

set $J = 1$, $D_z = 0.6$, $D_\perp = 0.5$

- First ED calculations for the kagomé lattice



longitudinal H=0



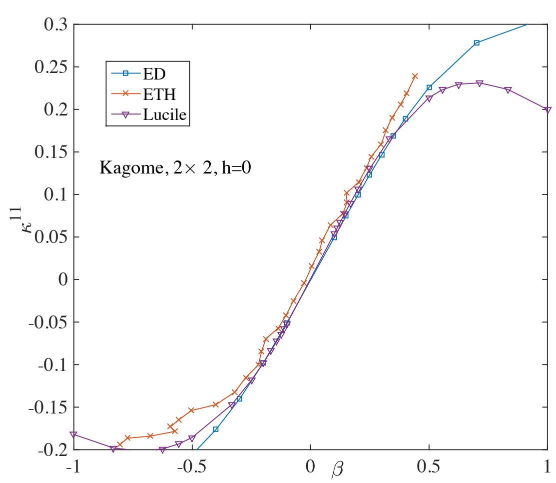
linear in H at small H

Features promising but *finite size effects??*

Typical states method

$$\kappa^{\mu\nu}(\omega) = \frac{-1}{N_{uc}\,\omega\,T}\int_0^{+\infty} dt\, e^{i\omega t}\langle[j^\mu(t), j^\nu(0)]\rangle$$

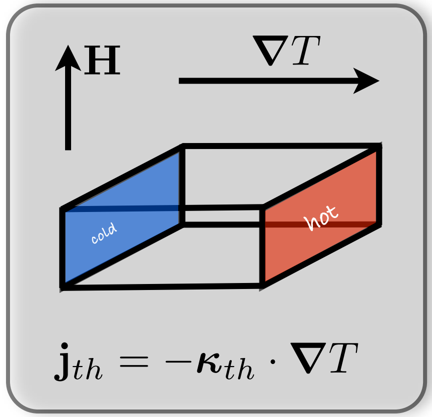
- Based on ETH, we expect that the thermodynamic average can be replaced by an average over a small number of "typical states"within some energy window
- Time evolve these states directly
- This method does not require full diagonalization.



<u>Benchmark</u>: reproduces ED results for upper temperature range

will allow up to 18-21 spins

Heat transport in magnets



Two types of heat current

$$\boldsymbol{j} = \boldsymbol{j}_{\text{spins}} + \boldsymbol{j}_{\text{lattice}}$$

Two important effects of spins

1. Spin heat current j_{spins} induced by thermal gradient
2. Scattering of heat-carrying phonons off of spins

Phonon heat transport

Can use Boltzmann eqation for phonons

$$\partial_t \overline{N}_{n,\mathbf{k}} + \mathbf{v}_{n,\mathbf{k}} \cdot \boldsymbol{\nabla}_{\mathbf{r}} \overline{N}_{n,\mathbf{k}} = \left.\frac{\partial \bar{N}_{n,\mathbf{k}}}{\partial t}\right|_{\text{coll.}}$$

scattering from spins

Spin-lattice interactions

$$H_{\text{int}} \sim a^\dagger \left(S^\mu + S^\mu S^\nu + \cdots\right) + a^\dagger a \left(S^\mu + S^\mu S^\nu + \cdots\right) + a^\dagger a^\dagger \left(S^\mu + S^\mu S^\nu + \cdots\right) + \text{h.c.} + \cdots$$

Jahn-Teller coupling: non-Kramers ions

Phonon heat transport

Can use Boltzmann equation for phonons

$$\partial_t \overline{N}_{n,\mathbf{k}} + \mathbf{v}_{n,\mathbf{k}} \cdot \boldsymbol{\nabla}_{\mathbf{r}} \overline{N}_{n,\mathbf{k}} = \left. \frac{\partial \bar{N}_{n,\mathbf{k}}}{\partial t} \right|_{\text{coll.}}$$

scattering from spins

Spin-lattice interactions

$$H_{\text{int}} \sim a^\dagger \left(S^\mu + S^\mu S^\nu + \cdots \right) + a^\dagger a \left(S^\mu + S^\mu S^\nu + \cdots \right) + a^\dagger a^\dagger \left(S^\mu + S^\mu S^\nu + \cdots \right) + \text{h.c.} + \cdots$$

$$H_{\text{int}} = \sum_{\mathbf{k},n} \sum_{\mathbf{r},\alpha} \lambda_{n\alpha}(\mathbf{k},\mathbf{r}) a^\dagger_{\mathbf{k},n} \mathcal{O}_{\mathbf{r},\alpha} + \text{h.c.}$$

Born approximation

spin-phonon product states

transition amplitude

transition probability

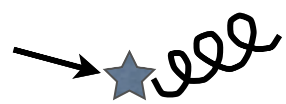
$$\Gamma_{\mathtt{if}} = \frac{2\pi}{\hbar}|T_{\mathtt{if}}|^2\delta(E_{\mathtt{f}} - E_{\mathtt{i}})p_{\mathtt{i}}$$

transition amplitude

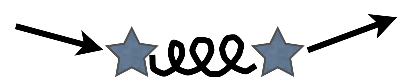
$$T_{\mathtt{if}} = \langle \mathtt{f}|H_{\mathrm{int}}|\mathtt{i}\rangle + \sum_{\mathtt{n}} \frac{\langle \mathtt{f}|H_{\mathrm{int}}|\mathtt{n}\rangle\langle \mathtt{n}|H_{\mathrm{int}}|\mathtt{i}\rangle}{E_{\mathtt{n}} - E_{\mathtt{i}}}$$

first Born approximation

second Born approximation



does not lead to a Hall effect



trace over spins

$$\Gamma_{i_p,f_p} = \sum_{i_s,f_s} p(E_{i_s})\Gamma_{i_p,i_s;f_p,f_s}$$

First Born Approximation

$$\left.\frac{\partial \bar{N}_{n,\mathbf{k}}}{\partial t}\right|_{\text{coll.}} = -\Gamma_{n,\mathbf{k}} \left(\frac{\bar{N}_{n,k}}{N^{\text{eq}}_{n,k}} - 1 \right)$$

$$\Gamma_{n,\mathbf{k}} = 2\pi \sum_{\alpha\alpha'} \lambda_{n\alpha}(\mathbf{k}) \lambda^*_{n\alpha'}(\mathbf{k}) G_{\alpha\alpha'}(\mathbf{k}, \omega_{n,k})$$

$$G_{\alpha\alpha'}(\mathbf{k}, \omega) = \frac{1}{2\pi} \sum_{rr'} e^{ik\cdot(r-r')} \int_{-\infty}^{\infty} dt\, e^{-i\omega t} \left\langle \mathcal{O}^\dagger_{r',\alpha'}(t) \mathcal{O}_{r,\alpha}(0) \right\rangle_\beta$$

Single-phonon emission/absorption rate measures dynamical structure factor of spin-lattice operator along the phonon dispersion relation

$$\Rightarrow \quad \kappa^{\text{ph}}_{\mu\nu} = \frac{1}{V} \sum_{n,\mathbf{k}} \Gamma^{-1}_{n,\mathbf{k}} v^\mu_{n\mathbf{k}} v^\nu_{n\mathbf{k}} \frac{\epsilon^2_{n\mathbf{k}}}{4T^2} \frac{1}{\sinh^2(\beta\epsilon_{n\mathbf{k}}/2)}$$

symmetric: no Hall effect

2nd Born Approximation

Second order scattering violates *detailed* balance: allows "skew-scattering" processes that induce Hall effect.

c.f. Mori, Spencer-Smith, Sushkov, Maekawa 2014

General expression is complicated, but

$$\Gamma_{nk,n'k'} \sim FT\left[\left\langle \mathcal{O}_{r_4}(t_4)\mathcal{O}^\dagger_{r_3}(t_3)\mathcal{O}_{r_2}(t_2)\mathcal{O}^\dagger_{r_1}(t_1)\right\rangle\right]$$

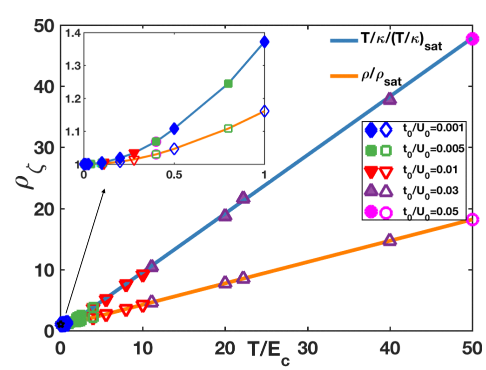
intriguing "out of time ordered" correlator of spin system controls phonon skew scattering

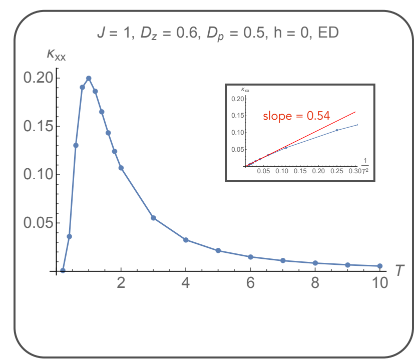
challenging to calculate but in progress...

Summary

I. SYK model of a strongly correlated metal: FL to NFL crossover and a disordered strange metal

II. Heat transport in spin systems - towards a non-quasiparticle description (progress report)





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