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**Workshop on
Novel States and Phase Transitions in Highly Correlated Matter**

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Thermal Conductivity of Spin-1/2 Chains and Ladders

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Thermal Conductivity of Spin-1/2 Chains and Ladders

Efrat Shimshoni, Achim Rosch, Edouard Boulat, Pankaj Mehta, N.A.

- Experimental data
  - heat conductivity measurements in spin chains and ladders
  - magnetic contribution to heat transport

- Low energy description (RG)
  - traditional effective theory describes the thermodynamics
  - insufficient for transport : conservation laws lead to anomalous transport
  - restore lattice effects : highly irrelevant operators

- Weakly violated conservation laws and hydrodynamic approach
  - heat current is almost conserved at low temperature
  - computation of heat conductivity

- Results and comparison to experiments

Theoretical background

Heat (charge) conductivity of spin-chains (Luttinger liquids) with Umklapp scattering

- Giamarchi (91), $(4k_F - G)$ -Umklapp in Luttinger liquids

  pertubation theory $\rightarrow \sigma(T > 0) < \infty$

  Luther-Emery transformation $\rightarrow \sigma = \infty$

- many papers: reproduce perturbative results

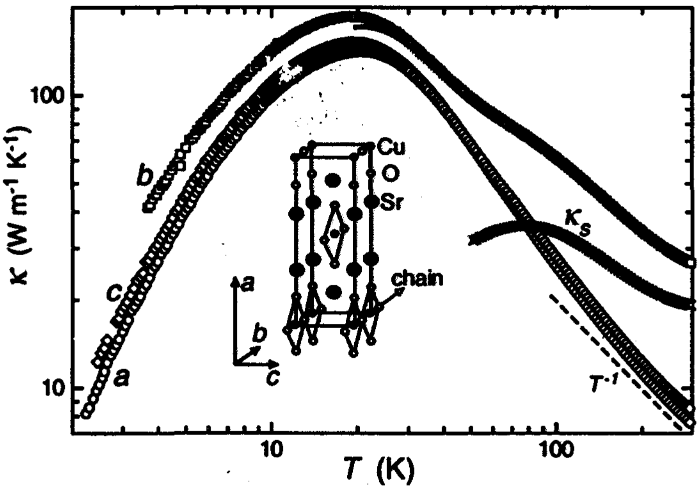
- Castella, Zotos *et al* (95-....):
  in **integrable** systems with ∞-many conservation laws
  $\sigma(T > 0, \omega) = 2\pi D(T)\delta(\omega) + ...$

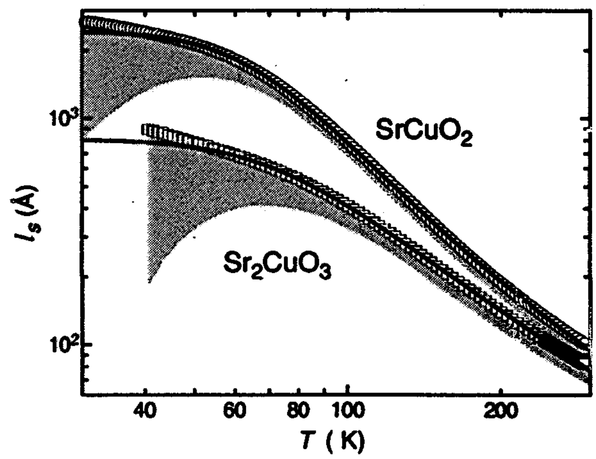
- ∞ heat conductivity in 1d Heisenberg model (Klümper, Sakai (01))

- generic behavior?
  Numerics: Alvarez, Gros (02) always ∞, Heidrich-Meisner *et al.* (03) $\kappa < \infty$

Experiments - spin chain

Heat transport in quasi 1d $S = 1/2$ chain compound $SrCuO_2$, Sr_2CuO_3

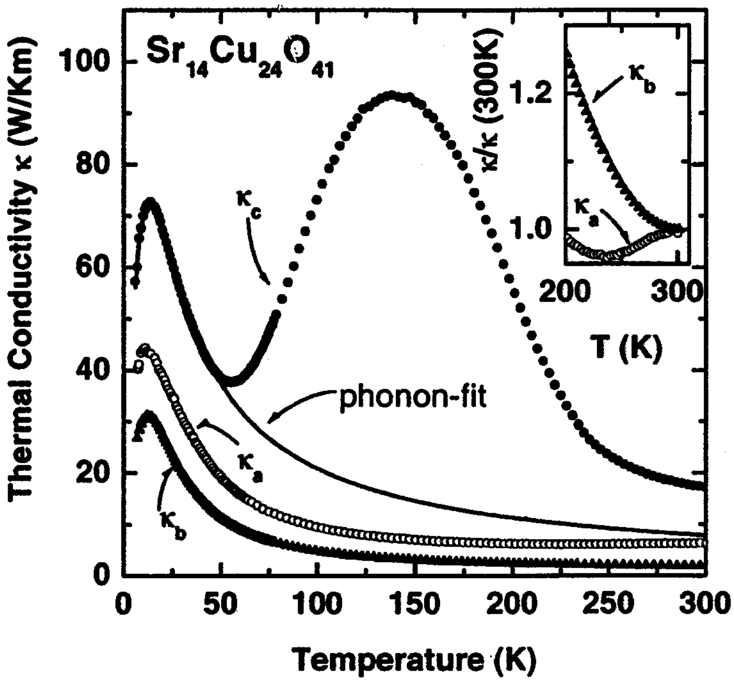


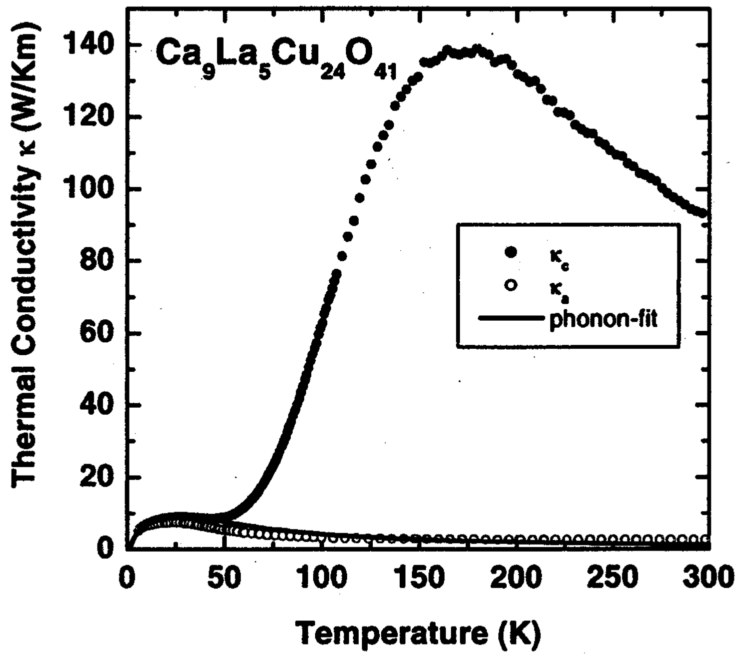


Sologubenko *et al.* (01)

- $\kappa \sim e^{\mathrm{T}^*/T}$ exponentially large
- $\mathrm{T}^* \sim 0.42\Theta_D$ determined by phonons
- Why not by spin-spin interactions, $J \sim 1000K$?

Experiments - spin ladders





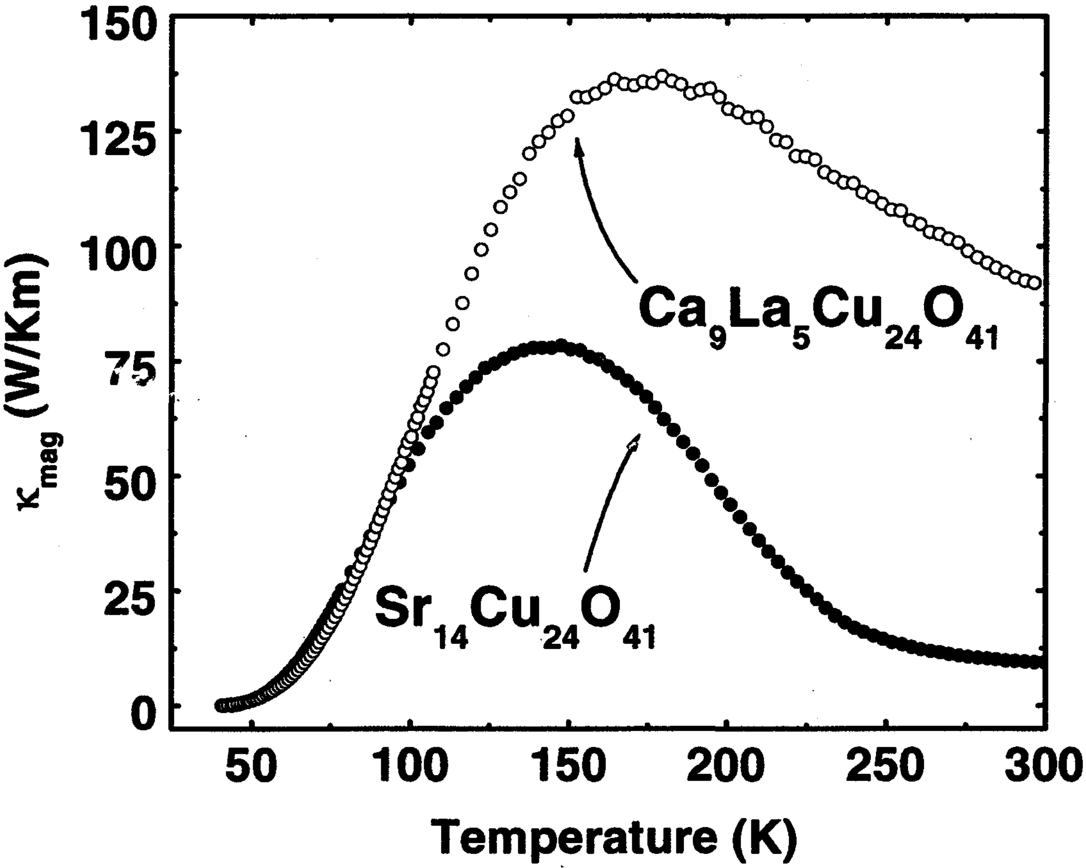
(all data taken from Hess *et al.*, 2001)

$(Sr,Ca,La)_{14}Cu_{24}O_{41}$:

two-leg spin-$\frac{1}{2}$ ladder $\longrightarrow$ Spin gap $m \sim 400°K$

mechanism for finite conductivity ? { disorder, interactions, phonons, **lattice** }

Experiments - spin ladders

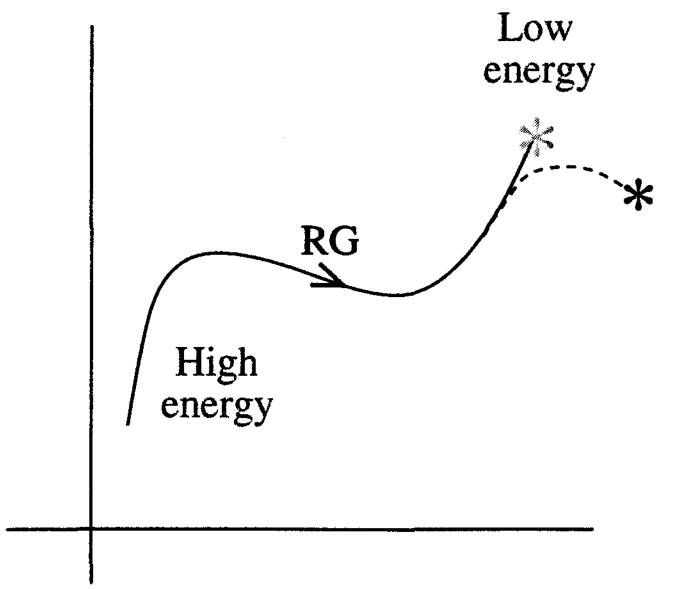


magnetic contribution κ_{mag} to heat conductivity

low energy collective modes (magnons) carry heat

RG approach

identify the low energy effective theory



H_{low} : low energy effective theory

- H_{low} describes the (low energy) spectrum

$\longrightarrow$ **thermodynamics**

- Does H_{low} describe the dynamics of quasi-particles?

$\longrightarrow$ **transport ??**

Spin chain system

Lattice hamiltonian

$$H = J \sum_{j=1}^{N} \mathbf{S}_j^{\perp} \cdot \mathbf{S}_{j+1}^{\perp} + J_z \sum_{j=1}^{N} \mathbf{S}_j^{z} \cdot \mathbf{S}_{,j}^{z}$$

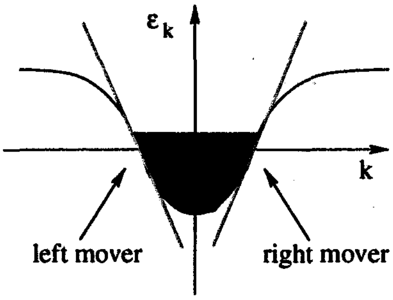
(in a real material, H is more complicated : next nearest neighbour couplings ...)

Low energy description

$$H_{low} = H^* + \cdots$$

$$\begin{aligned} H^* &= v \int \left(\Psi_R^\dagger i\partial_x \Psi_R - \Psi_L^\dagger i\partial_x \Psi_{L\sigma} \right) + g \int \rho_R \rho_L \\ &= v \int \frac{dx}{2\pi} \left(K(\pi\Pi)^2 + \frac{1}{K}(\partial_x \phi)^2 \right) \end{aligned}$$

Reminder:



$$\Psi(x) = \Psi_L(x) e^{-ik_F x} + \Psi_R(x) e^{ik_F x}$$
$$\rho_R(x) = \Psi_R^\dagger(x) \Psi_R(x)$$
$$\rho_L(x) = \Psi_L^\dagger(x) \Psi_L(x)$$

also need add: PHONONS

The 3D Spin - Phonon System

- Array 1d **spin** chains coupled to 3d phonons

$$H = \sum_{\alpha} H_{\mathrm{s},\alpha} + H_{\mathrm{p}}^{3D} + H_{\mathrm{s,p}}$$

- Anisotropic Heisenberg model with finite range interactions

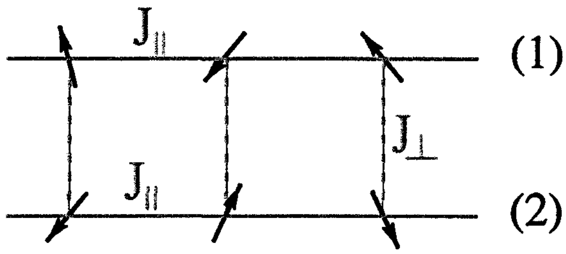
$$H_{\mathrm{s}} = \sum_{i,j=1}^{N} J_{ij} \left(S_i^x S_j^x + S_i^y S_j^y \right) + \sum_{i,j=1}^{N} J_{ij}^z S_i^z S_j^z - h \sum_{i=1}^{N} S_i^z$$

- H_{p}^{3D}: 3d acoustic phonons

- $H_{\mathrm{s,p}}$ coupling of phonons to **spin** chains (symmetry!)

Spin ladder system

Lattice hamiltonian



$$H = \mathrm{J}_{\parallel} \sum_{j=1}^{N} \sum_{\alpha=1,2} \mathbf{S}_{\alpha,j} \cdot \mathbf{S}_{\alpha,j+1} + \mathrm{J}_{\perp} \sum_{j=1}^{N} \mathbf{S}_{1,j} \cdot \mathbf{S}_{2,j}$$

(in a real material, H is more complicated : diagonal / next nearest neighbour couplings ...)

Low energy description $\quad H_{\mathrm{low}} = H^* + \cdots$

$$H^* = \int dx \sum_{a=0}^{3} \left[\frac{iv_a}{2} \left(\xi^a_{\mathrm{L}} \partial_x \xi^a_{\mathrm{L}} - \xi^a_{\mathrm{R}} \partial_x \xi^a_{\mathrm{R}} \right) + i\, m_a\, \xi^a_{\mathrm{R}} \xi^a_{\mathrm{L}} \right]$$

(Shelton *et al.*, 1996)

Spectrum at weak coupling ($\mathrm{J}_{\perp} \ll \mathrm{J}_{\parallel}$)

- Triplet $\left(\xi^a_{\mathrm{R,L}}\right)_{a=1,2,3}$ — gap $m_t \propto J_{\perp}$
- Singlet $\xi^0_{\mathrm{R,L}}$ — gap $m_s \propto 3J_{\perp}$

also need add: PHONONS

Spurious conservation laws of H^*

H^* insufficient for transport

For example: Spin Ladder

- H^*(spin ladder) – free field theory
  $\Rightarrow$ infinite number of conservation laws
- heat current conserved

$$J_E = \sum_a v_a^2 \int dx \; (\xi_{\mathrm{L}}^a \partial_x \xi_{\mathrm{L}}^a + \xi_{\mathrm{R}}^a \partial_x \xi_{\mathrm{R}}^a)$$

But on the lattice:

spin ladder *not* integrable
heat current *not* conserved

ffective theory possesses **spurious** conservation laws
$\Rightarrow$ anomalous transport:

$$\sigma(\omega) = D(T)\delta(\omega) + \sigma_{\mathrm{reg.}}(\omega)$$

$D(T) \neq 0 \Leftrightarrow$ anomalous (dissipationless) transport

Adding leading irrelevant operators to H^* - not enough!

Transport and conservation laws

When is $D(T)$ non zero ?

- Conserved current $[H, J] = 0$

$$\boxed{D(T) = \left\langle J^2 \right\rangle / T^2} \longrightarrow \text{Drude weight } (\delta \text{ peak})$$

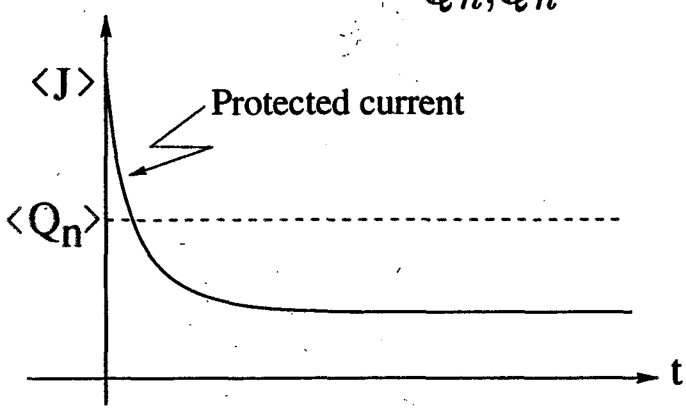
- Current not conserved but protected by a conserved quantity Q_n : $\chi_{J,Q_n} \neq 0$

($\chi_{A,B} = \frac{\partial^2 \langle H \rangle}{\partial A \partial B}$ cross susceptibility)

$$\lim_{\mathcal{T}\to\infty} \frac{1}{\mathcal{T}} \int_0^{\mathcal{T}} \langle J(t) J(0) \rangle \, dt \geq \mathcal{B} = \sum_n \frac{\chi^2_{J,Q_n}}{\chi_{Q_n,Q_n}}$$

(Mazur 1969)

$$\longrightarrow \boxed{D(T) \geq \mathcal{B}/T}$$

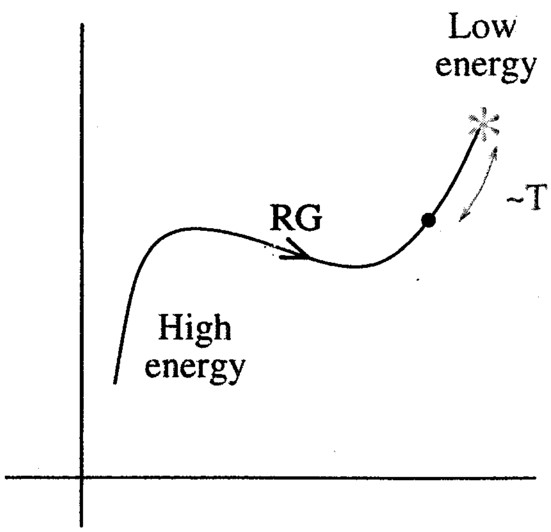


- Particular case - INTEGRABLE MODELS

- infinite number of conservation laws $\longrightarrow D(T) > 0$

- anomalous transport

Irrelevant operators - breaking of conservation laws.



$$H_{\mathsf{low}} = H^* + H_{\mathsf{irr}} + \delta H$$

Classification of irrelevant operators

1 H_{irr} : all translation invariant operators.

Along with H^*, determines the thermodynamics.

example : $$\sum_a \int dx \left(\xi^a_{\mathsf{R}} \partial^2_x \xi^a_{\mathsf{R}} + \xi^a_{\mathsf{L}} \partial^2_x \xi^a_{\mathsf{L}} \right)$$

"conventional" field theory description

$$H^* + H_{\mathsf{irr}} = \int dx\, \mathcal{H}(x) , \quad \mathcal{H}(x) \text{ - translation invariant}$$

H_{irr} breaks many spurious conservation laws
but continuous translation symmetry unbroken

Irrelevant operators - breaking of conservation laws

2 $\delta H \equiv$ Umklapp processes

$\longrightarrow$ necessarily present for a lattice model

$\longrightarrow$ **breaks translation invariance**

$\longrightarrow$ infinitely irrelevant in the RG sense

example :
leading Umklapp operator for the spin ladder

$$\delta H \sim \int dx\, e^{2ik_F x} \prod_{a=0}^{3} \sigma^a(x)$$

- SU(2) invariant $\delta H = \int dx\, \vec{J}(x) \cdot \vec{n}(x) \cos\left(2ik_F x\right)$
- all other Umklapp operators have greater scaling dimension

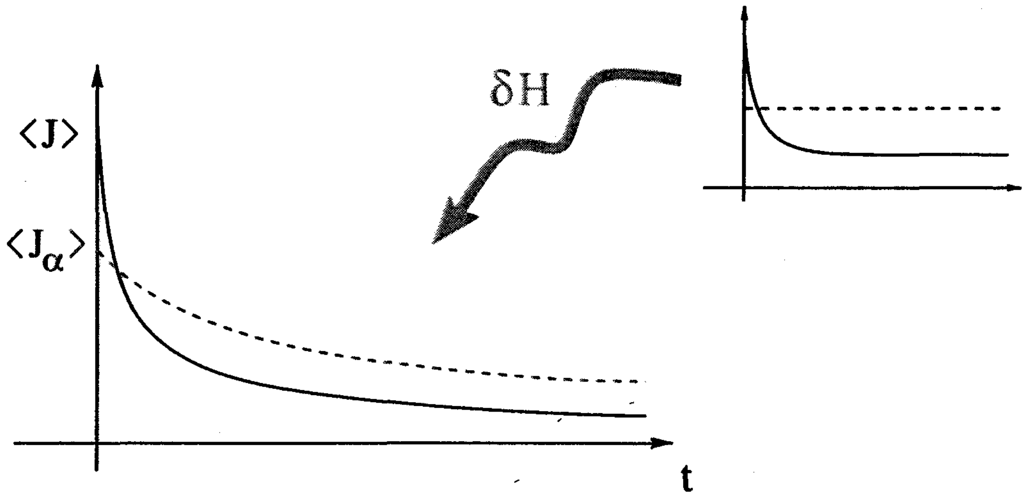
Heat transport determined by δH

Weakly violated conservation laws

amongst the spurious conservation laws of the effective theory :

- most are violated by $H_{\text{irr}} \longrightarrow$ strongly violated
- the rest is violated by $\delta H \longrightarrow$ weakly violated
  $\Rightarrow$ the associated approximately conserved quantities J_α are slow modes (slowly decaying)

$\longrightarrow$ the slow modes determine long time asymptotics of protected current correlations



- The translation operator is a slow mode (translation invariance broken by Umklapp operators)

- The heat current is ALWAYS protected by the translation operator

$\Rightarrow$ it is therefore a slow mode itself

$\Rightarrow$ the heat current is degraded by δH

The Spin-phonon system - (Approximately) conserved charges

The low-E Hamiltonian possesses (approximately) conserved "charges":

$$
\begin{aligned}
J_s &= vK\int dx\,[\psi_R^\dagger\psi_R - \psi_L^\dagger\psi_L] = vK\int dx\Pi \\
P_T &= \int dx\Pi\partial_x\phi \quad + \int d^3xP\partial_x q \\
J_Q &= -\int dx\,v^2\Pi\partial_x\phi - \int d^3x\,v_p^2P\partial_x q
\end{aligned}
$$

Where

- J_s = spin current
- P_T = momentum operator
- J_Q = heat current

These are the "slow modes":

- J_s, P_T commute with $H^* = H_{LL}$ and with δH
- do *not* commute with $H^U \Rightarrow$ slow current decay
- J_s, P_T "protect" J_Q
- other conserved charges decay fast

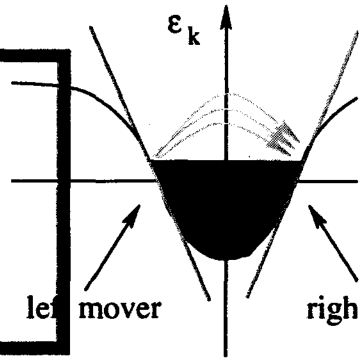
(approximately) conserved charges strongly affect dynamics

- *low energy processes cannot relax the heat current*

Irrelevant operators

- Spin Umklapp:

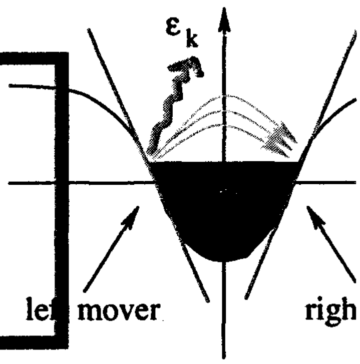
$$H^U_{\mathrm{n,m}} = \begin{cases} n \text{ Fermions from L to R} \\ + \text{ m lattice - momenta} \\ \Delta k_{\mathrm{n,m}} = \mathrm{n}2k_F - \mathrm{m}G \end{cases}$$



$$\begin{aligned} H^U_{n,m} &= g^U_{nm} \int dx e^{i\Delta k_{nm}x} \prod_{j=0}^{n} \psi^\dagger_R(x+ja)\psi_L(x+ja) \\ &= \frac{g^U_{nm}}{(2\pi a)^n} \int dx e^{i\Delta k_{nm}x} e^{i2n\phi(x)} \end{aligned}$$

- Spin-Phonon Umklapp:

$$H^U_{\mathrm{n,m}} = \begin{cases} n \text{ Fermions from L to R} \\ + \text{ m lattice - momenta} \\ + \text{ phonons} \end{cases}$$



$$H^{U,s-p}_{n,m} = \frac{g^{U,p}_{nm}}{(2\pi a)^n} \int dx [e^{i\Delta k_{nm}x} e^{i2n\phi} \partial_x q + h.c.]$$

- Some non Umklapp operators:

$$\begin{aligned} H^{nonU}_s &= \int \psi^\dagger_R \partial^2 \psi_R \\ H^{nonU}_{s,p} &= \int (\partial\phi)^2 \partial_x q \end{aligned}$$

The Calculation

Pertubation theory for, $\kappa(\omega, T)$?

- perturbations are irrelevant operators

$$\kappa = \langle J_Q,\ J_Q \rangle_{H^* + H_{irr} + \delta H}$$

But:

$\kappa(\omega, T)$ - singular function of perturbations:

$$\kappa = \langle J_Q,\ J_Q \rangle_{H^* + H_{irr}} = \infty$$

What to calculate?:

Memory Matrix - Matrix of slow decay rates

Mori (65), Zwanzig (61)

Philosophy: Conservation laws weakly violated

→ slow modes:

→ "hydrodynamic" description possible

→ *asymptotically exact for small perturbations*

if time-scales well separated

Transport and the Memory Function Formalism I

-Transport in the presence of several approximately conserved - "slow" - variables: $J_1, J_2 ... J_N$

- Scalar product in *operator* space

$$(A(t)|B) \equiv \frac{1}{\beta}\int_0^\beta d\lambda \langle A(t)^\dagger B(i\lambda)\rangle$$

- Dynamic Correlation function

$$\begin{aligned} C_{AB}(\omega) &= \int_0^\infty dt e^{i\omega t}(A(t)|B) \\ &= \left(A\left|\frac{i}{\omega-\mathcal{L}}\right|B\right), \quad \mathcal{L}A=[H,A] \\ &= \frac{iT}{\omega}\int_0^\infty dt e^{i\omega t}\langle[A(t),B]\rangle - \frac{(A|B)}{i\omega} \end{aligned}$$

- Matrix of conductivities (Kubo)

$$\hat{\sigma}_{pq}(\omega,T) = \frac{1}{TV}C_{J_p J_q}(\omega)$$

- Thermal Conductivity

$$\boxed{\kappa(\omega,T) = \frac{1}{T}\sigma_{QQ}(\omega,T)}$$

Transport and the Memory Function Formalism II

The conductivity has no good perturbative expansion -
($\sigma \sim 1/\Gamma$, singular in PT in presence of slow modes.)

Define: $\hat{M}(\omega, T)$ - Memory Matrix

- The conductivity

$$\hat{\sigma}(\omega, T) = \hat{\chi}(T) \left(\hat{M}(\omega, T) - i\omega\hat{\chi}(T) \right)^{-1} \hat{\chi}(T)$$

- The susceptibility matrix

$$\hat{\chi}_{pq} = \frac{1}{TV} (J_p | J_q)$$

- The memory matrix ($\sim$ matrix of Relaxation Rates)

$$\hat{M}_{pq}(\omega) = \frac{1}{T} \left(\partial_t J_p \middle| \mathcal{Q} \frac{i}{\omega - \mathcal{Q}\mathcal{L}\mathcal{Q}} \mathcal{Q} \middle| \partial_t J_q \right)$$

- The projection away from slow modes

$$\mathcal{Q} = 1 - \sum_{pq} |J_p) \frac{1}{T} (\hat{\chi}^{-1})_{pq} (J_q|$$

Philosophy: $\hat{M}$ non-singular in P.T.

- P.T. valid for short-time behavior

- P.T. also valid for long-time behavior of slowest modes (provided slow modes dynamics projected out - $\mathcal{Q}$.)

The Thermal conductivity - I

Compute (to lowest order in irrelevant perturbation) for $aT \ll v_p, v$:

$$\kappa(T) \approx v^2 T^3 \left[(\hat{M}^{-1})_{TT} + 2(\hat{M}^{-1})_{QT} + (\hat{M}^{-1})_{QQ}\right]$$

where:

$$\hat{M} = \sum_{nm} \left(\hat{M}^{s-s}_{nm} + \hat{M}^{s-p}_{nm}\right)$$

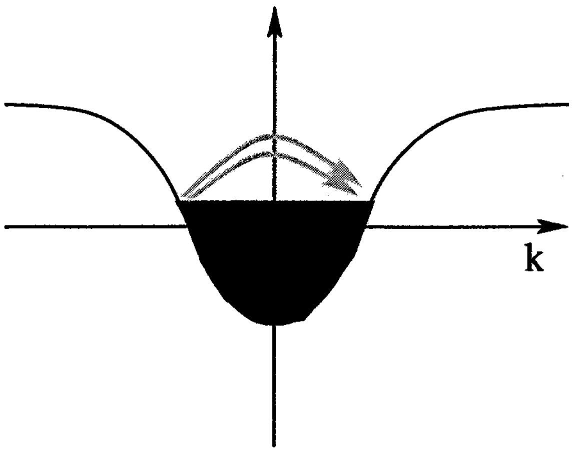
$$\begin{aligned} \hat{M}^{s-s}_{nm} &= (\Delta k_{nm})^{(n^2K-2)} e^{-v\Delta k_{nm}/2T} \\ \hat{M}^{s-p}_{nm} &= T^{(2n^2K-1)} e^{-v_p\Delta k_{nm}/2T} \end{aligned}$$

- Process with smallest Δk_{nm} dominates at low - T (Δk_{nm} determined by commesurabilty).
- For $h = 0$, (half-filling), dominant process $\Delta k_{2,1} = 0$, but ineffectual (conserves pseudo-momentum).
- The second strongest process $\Delta k_{1,1} = G/2$ determines rate.
- $v_p \ll v \quad \Rightarrow \quad \hat{M}^{s-p}_{nm} \gg \hat{M}^{s-s}_{nm}$, spin-phonon Umklapp processes dominate.

$$\boxed{\kappa \approx \kappa_0 \left(\frac{T}{\mathrm{T}^*}\right)^{2(1-K)} \exp\left[\frac{\mathrm{T}^*}{T}\right], \quad \mathrm{T}^* = \frac{v_{\mathrm{p}}G}{4}}$$

The Thermal conductivity - II

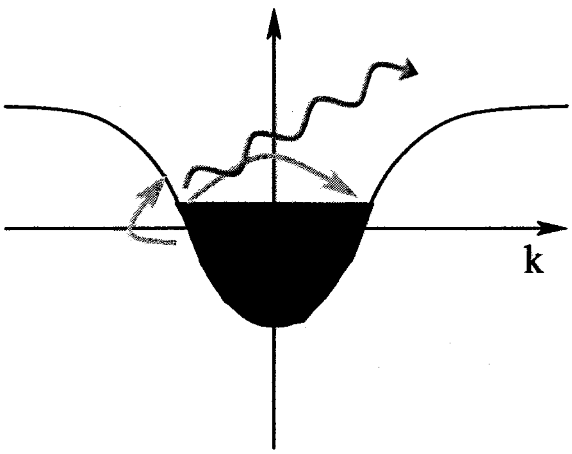
- The second strongest process determines the rate



dominant process:
Umklapp **spinon-spinon** scattering
$\Delta k_{2,1} = 4k_F - G = 0$

$$H^U_{2,1} = \int dx\, \Psi^\dagger_R \Psi^\dagger_R \Psi_L \Psi_L e^{i(4k_F - G)x}$$

but: conserves pseudo momentum



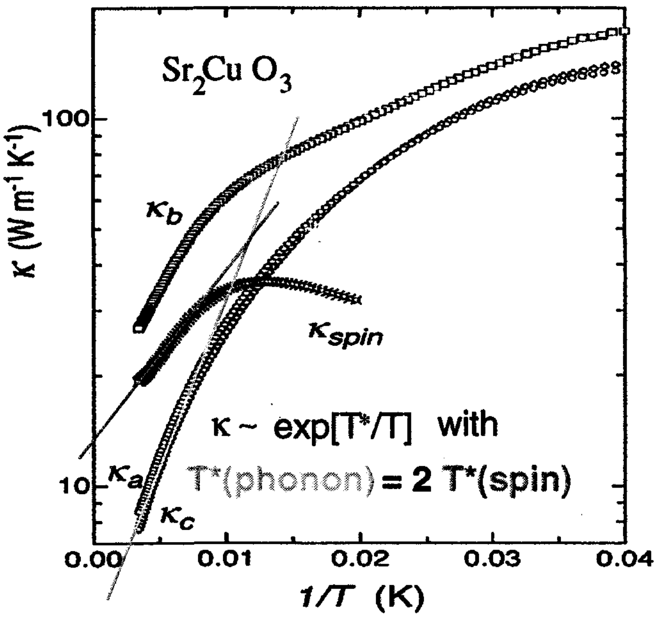
second strongest process:
mixed phonon-**spinon** scattering
$\Delta k_{1,1} = G - 2k_F = \Delta k_{1,0} = 2k_F$

$$H^U_{1,0} = \int dx\, \Psi^\dagger_L \Psi^\dagger_R \Psi_L \Psi_L (a + a^\dagger) e^{i2k_F x}$$

The Thermal conductivity - III

$$\kappa \approx \kappa_0 \left(\frac{T}{\mathrm{T}^*}\right)^{2(1-K)} \exp\left[\frac{\mathrm{T}^*}{T}\right], \quad \mathrm{T}^* = \frac{v_{\mathrm{p}} G}{4}$$

- Comparison to experiment (no parameters!)
  - isotropic $\Theta_D \approx v_p(6\pi^2/a^3)^{1/3} \approx 0.6\, v_p G$
  - $\mathrm{T}^* \approx 0.41\Theta_{\mathrm{D}}$ (theory)
  - $\mathrm{T}^* \approx 0.42\Theta_{\mathrm{D}}$ (experiment)



Sologubenko *et al.* (01)

- Why exponential?
  pseudo-momentum conservation, $G - 4k_F$ Umklapp cannot relax heat current completely
- Why phonons?
  cheapest way to absorb extra momentum, ($v_{\text{phonon}} \ll v_{\text{spin}}$)
- Why $T^*_{\text{phonon}} = 2\mathrm{T}^*_{\text{spin}}$?
  small mixed spinon-phonon Umklapp, $\Delta k = G - 2k_F = G/2$

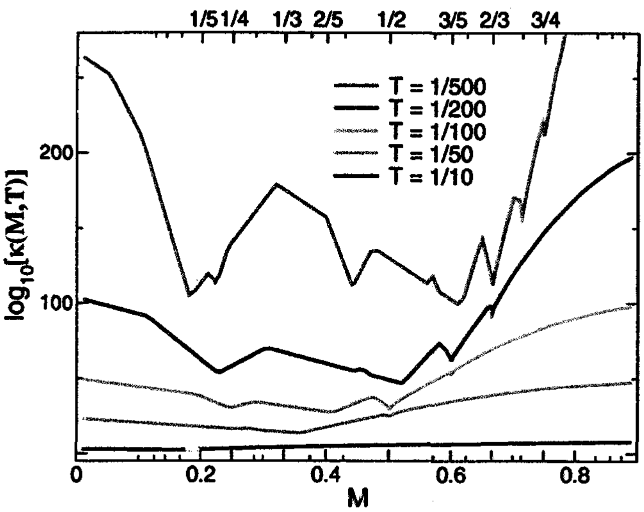
Heat conductivity in a magnetic field - I

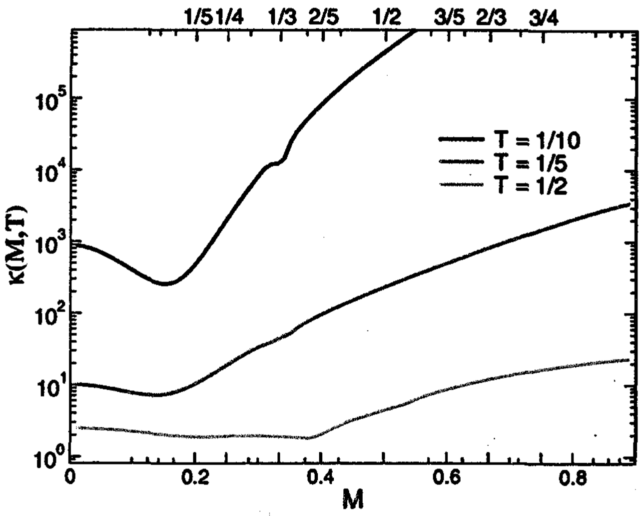
Magnetization dependence of the spin chain heat conductivity κ:

- phonons and spinons start to mix (linear coupling)
- more important: $k_F = \frac{\pi}{a}(1 + \mathrm{M})$ changes modifies interplay of Umklapps
- strongest Umklapp is strongest for almost commensurate M
  but cannot relax heat current fully
- second strongest **weakest** for almost commensurate M
- $\Rightarrow$ peaks for commensurate $\mathrm{M} = \frac{2\mathrm{m}_0}{\mathrm{n}_0} - 1$
  with $\kappa \sim \exp\left[\frac{vG}{2\mathrm{n}_0 T}\right]$

Heat conductivity in a magnetic field - II

schematic magnetization dependence of heat conductivity κ





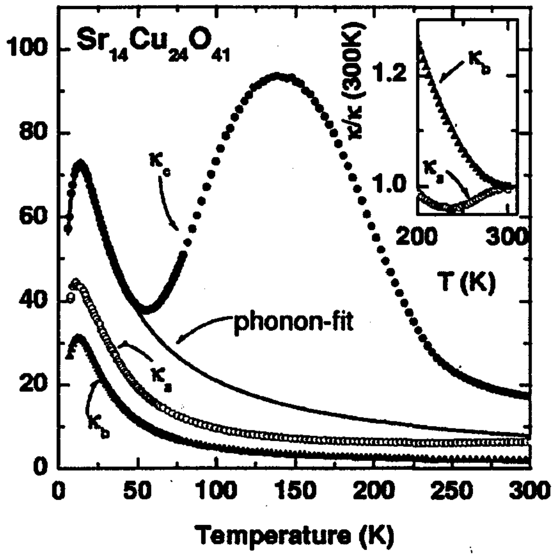
peaks: $\kappa \sim \exp\left[\frac{vG}{2n_0T}\right]$

background: $\kappa \sim \exp\left[(T^*/T)^{2/3}\right]$

Results - spin ladders

Low temperature $T \ll m_t$

$$\kappa(T) = \kappa_{\text{mag}}(T) + \kappa_{\text{ph}}(T)$$



$$\kappa_{\text{ph}}(T) \sim e^{T^*_{ph}/T}$$

$$\kappa_{\text{mag}}(T) \sim e^{-\alpha m_t/T}$$

$\longrightarrow \quad T^*_{ph} = \frac{v_{ph}G}{2}$

$\longrightarrow \quad \alpha = 3/2$

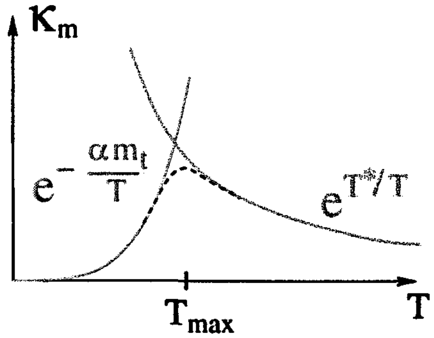
Note that:

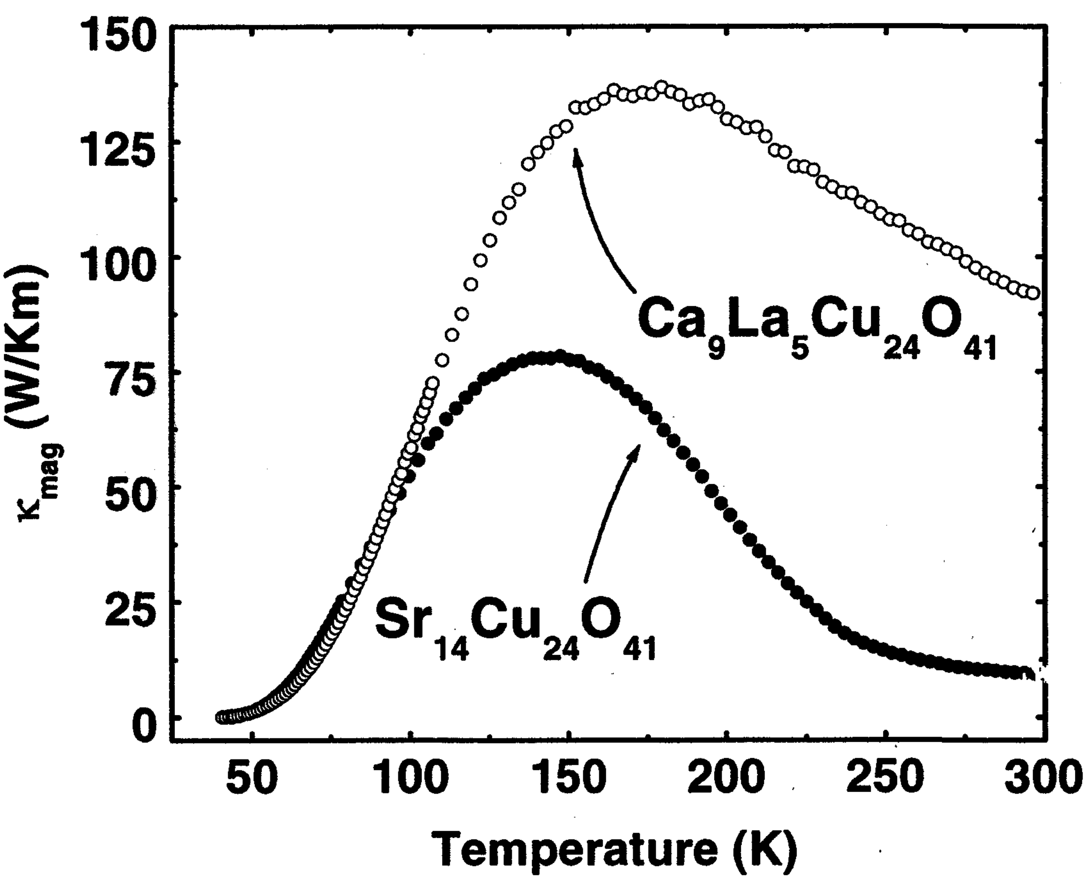
$\longrightarrow \quad \kappa_{\text{ph}}(T) \gg \kappa_{\text{mag}}(T)$, *(for very low* T*)*

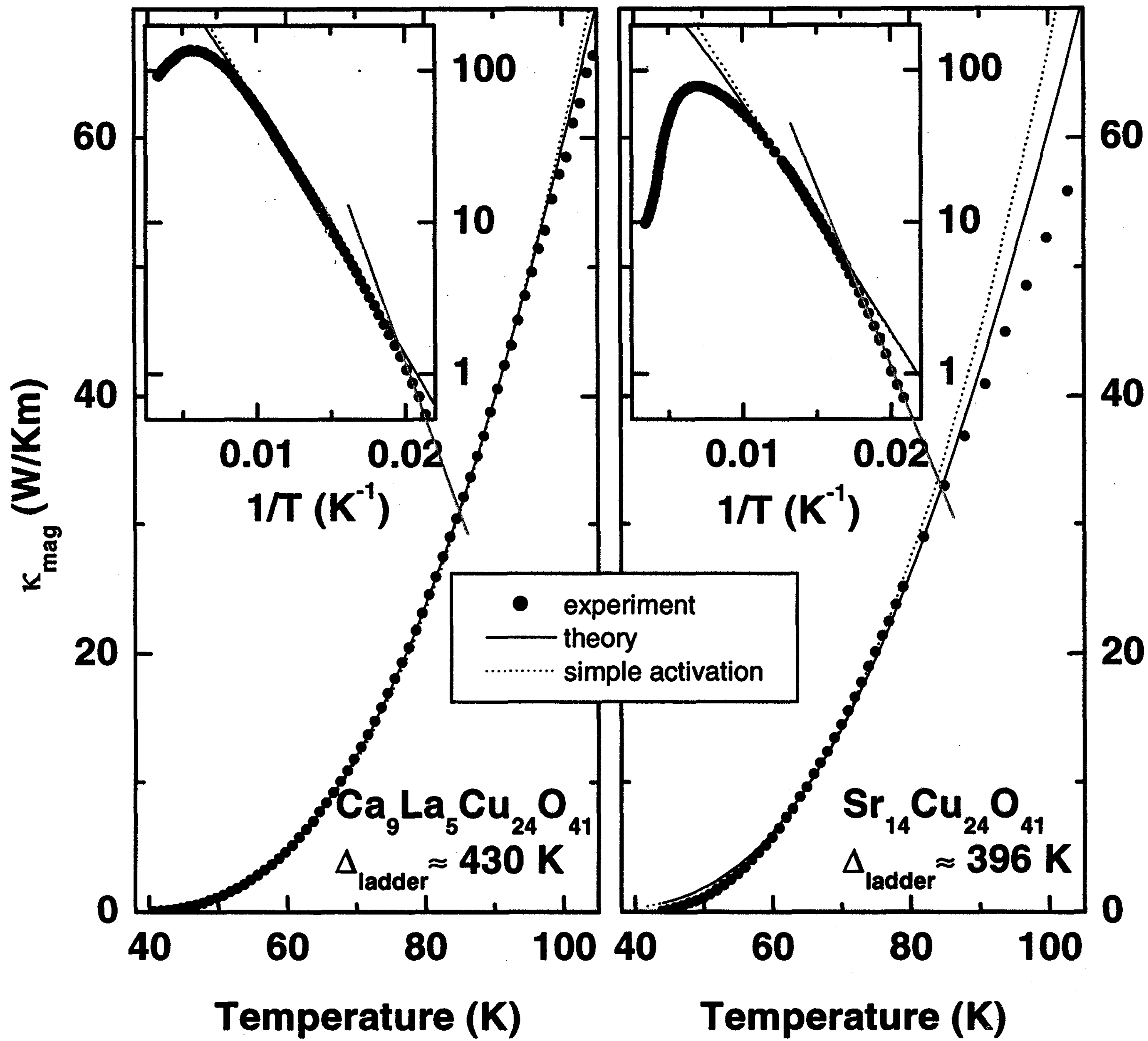
Results - spin ladders

Putting together low and high temperature results, with phonons, for **magnetic contribution** :

existence of a maximum in $\kappa_{mag}(T)$ for $T \sim m_t$







κmag (W/Km)
Temperature (K)
Temperature (K)
1/T (K-1)
1/T (K-1)
experiment
theory
simple activation
Ca9La5Cu24O41
Δladder ≈ 430 K
Sr14Cu24O41
Δladder ≈ 396 K

Low Temperature Transport - General Approach

- RG flow of Hamiltonian H (typically on a lattice), $H \to H_{lowE} = H^* + \sum_i g_i O_i$

  - The fixed point H^*.
  - Insufficient to describe transport ($\kappa = \infty$)
  - The irrelevant operators around it O_i.
  (all operators consistent with symmetries of H.)

- Classify irrelevant operaors:
  - O_i^U Umklapp operators - break translation invariance of H^*
  - O_i^{nonU} non Umklapp operators - do not directly lead to current degradation

- Identify "slow modes" $J_1 \cdots J_N$
  - (approximately) conserved operators P,
  (conservation violated only by Umklapp operators)
  - those protected by them $\chi_{JP} \neq 0$

- Use hydrodynamic approach (Memory Matrix formalism) to computed conductivities of slow modes.

$$\kappa(\omega, T) = \langle J_Q,\ J_Q \rangle(\omega, T)$$