Thermoelectric Transport Coefficients in Correlated Condensed Matter

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APS:

Q:28 Invited Talk

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- Introduction and Motivation
- Formalism and formulas and a bit of history
- Results for $Na_{.68}$ CoO_2 and predictions for a hole doped counterpart.
- Formulation for dynamical heat transport experiments and some suggested experiments.

Introduction and Motivation

Requirements for applications:

Large Seebeck coefficient S

Large figure of merit Z T at 300K

$$Z\ T = \frac{S^2 T\sigma}{\kappa}$$

- Seeking simultaneously :
- High S (thermopower or Seebeck)
- High electrical conductivity σ
- Low Thermal conductivity κ

Semiconductor World

- Bi_2Te_3
- Superlattices

1999-2003 →

Correlated Materials

- Heavy fermions: good metals and large d.o.s.
- Mott Hubbard systems:
- $Na_{.68}CoO_2$: Terasaki, Ong Cava ….

What is new or interesting about all this from the Basic science point of view?

Fundamental interest in Condensed matter physics has moved in a direction away from simple non interacting systems towards strongly interacting systems.

Perturbation theory is inapplicable since there is **nothing small**.

From

Fermi liquid metals (Al, Cu,…the works!) and semiconductors (Bi_2Te_3 ….)

Zone of comfort:

Bloch Boltzmann theory

To

Oxide materials living on the edge.

Mott Insulating state and its doped descendents.

No “standard techniques available”: a great new frontier.

Correlated systems and Thermoelectric effects in them are hugely challenging

In general Mott Hubbard systems have interesting transport near the insulating state:

But:….

Perturbative calculations are hard to do, since there is no small parameter

Bloch Boltzmann Drude theory is suspect since quasiparticles are poorly defined and short lived.

Kubo formulas are exact, but hardly helpful !

E.g. they require a knowledge of the d.c. conductivity σ to compute the thermopower. This is next to impossible today since σ contains the essence of T linear resistivity: the core of High Tc.

This is akin to the directions from your expensive GPS:

“The road to Lhasa from Kathmandu”

Make at left at the Everest and go down the Zanang valley !!.

BADLY NEEDED

A NEW ROAD!!

HINT for a new route comes from the Hall constant.

Shastry Shraiman Singh 1993- Kumar Shastry 2003)

$$\rho_{xy}(\omega) = \frac{\sigma_{xy}(\omega)}{\sigma_{xx}(\omega)^2} \to B R_H^* \text{ for } \omega \to \infty$$

$$R_H^* = R_H(0) \text{ in Drude theory}$$

Perhaps ω dependence of R_H is weak compared to that of Hall conductivity.

$$R_H{}^* = \frac{-i2\pi}{hB} N\mathrm{v} < [J^x, J^y] > / < \tau_{xx} >^2$$

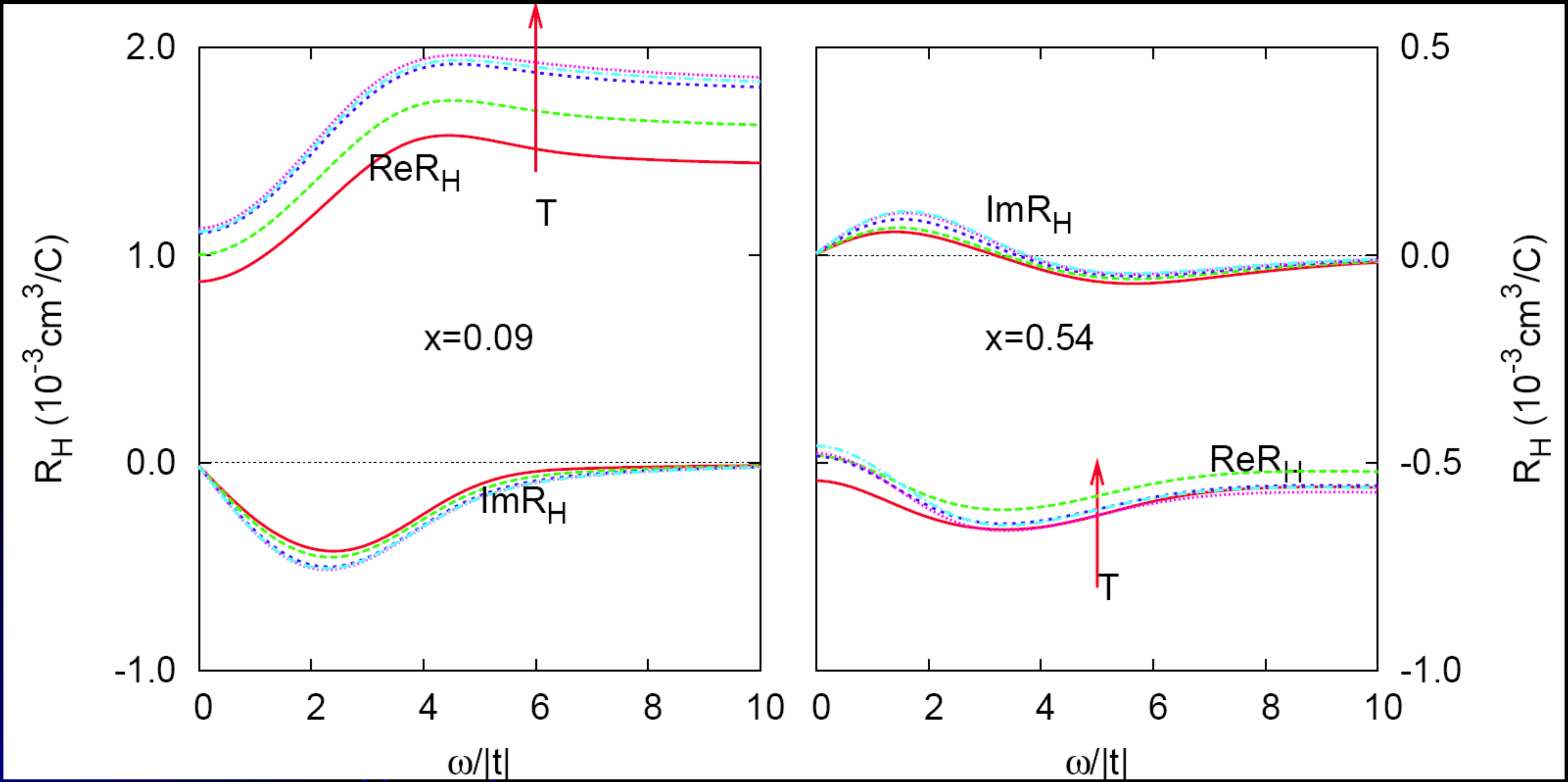
ANALOGY between Hall Constant and Seebeck Coefficients

- **Very useful formula since**
  - **Captures Lower Hubbard Band physics. This is achieved by using the Gutzwiller projected fermi operators in defining J's**
  - **Exact in the limit of simple dynamics (e.g few frequencies involved), as in the Boltzmann eqn approach.**
  - **Can compute in various ways for all temperatures (exact diagonalization, high T expansion etc…..)**
  - **We have successfully removed the dissipational aspect of Hall constant from this object, and retained the correlations aspect.**
  - **Very good description of t-J model.**
  - **This asymptotic formula usually requires ω to be larger than J**

Computation of frequency dependence of Hall constant: NCO (Haerter Shastry)

Worst case dependence

Usual dependence

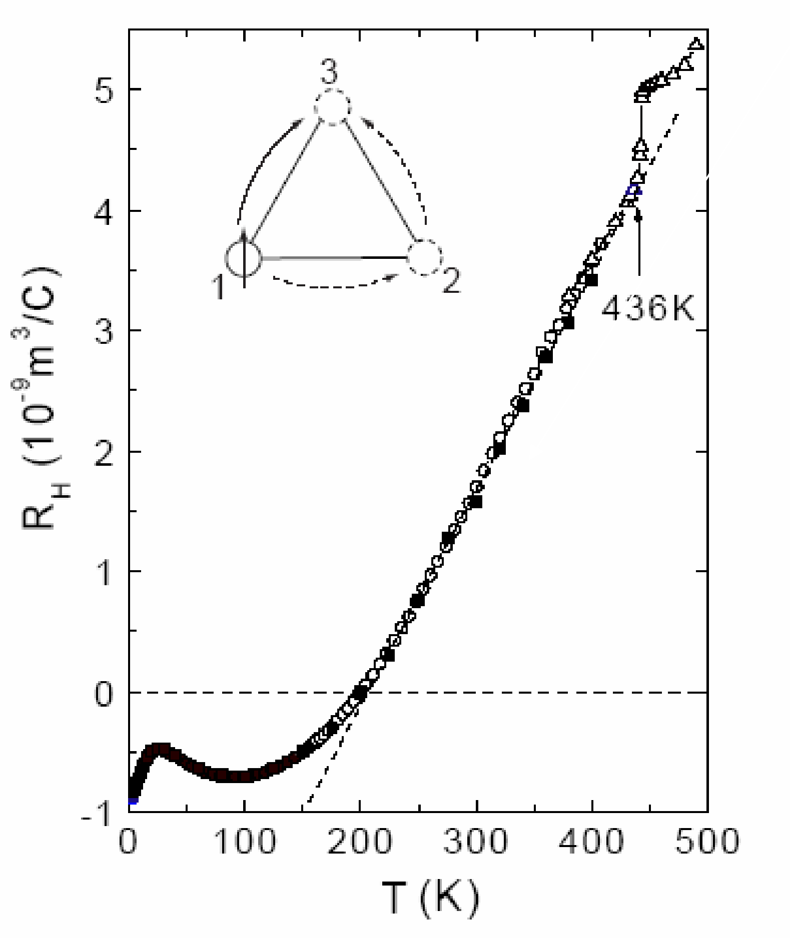


How about experiments? See next:

Anomalous high-temperature Hall effect on the triangular lattice in Na_xCoO_2

Yayu Wang[1], Nyrissa S. Rogado[2], R. J. Cava[2,3], and N. P. Ong[1,3]

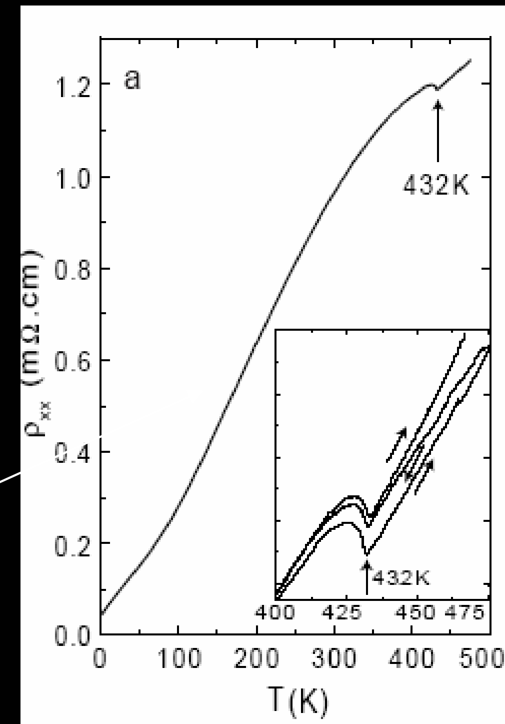
The Hall coefficient R_H of Na_xCoO_2 ($x = 0.68$) behaves anomalously at high temperatures (T) From 200 to 500 K, R_H increases linearly with T to 8 times the expected Drude value, with no sign of saturation. Together with the thermopower Q, the behavior of R_H provides firm evidence for strong correlation. We discuss the effect of hopping on a triangular lattice and compare R_H with a recent prediction by Kumar and Shastry.



Hall constant as a function of T for x=.68 (CW metal). T linear over large range 200^0 to 436^0 (predicted by theory of triangular lattice transport KS)

STRONG CORRELATIONS & Narrow Bands

T Linear resistivity



- Kubo Onsager formulas “without tears”, i.e alternate simple formulas!

- Finite ω response functions:
- New sum rule,
- Two new fundamental operators: Thermal operator ϑ and thermoelectric operator Φ.

New Formalism SS (2006) is based on a finite frequency calculation of thermoelectric coefficients.

Needed in many contexts, e.g. imagine a Si chip at 20 GHZ and its power dissipation. Neglected area with rather surprising new results.

Shastry Phys Rev B 2006

$$S = \frac{L_{12}(\omega)}{L_{11}(\omega) T}$$

$$L = \frac{L_{22}(\omega)}{T^2 L_{11}(\omega)}$$

$$ZT = \frac{(S)^2}{L}$$

Here L_{ij}'s are the Onsager coefficients at finite frequency.

Inspired by the Hall story we suggest taking the limit:

$$\mathrm{Q}^* \equiv \lim_{\omega \to \infty} Q(\omega)$$

All objects to be computed at large frequencies. The answers are finite and analogous to R*

In DC limit these are the transport objects anyway.

Error estimation…? We will see it is very small, much better than Hall constant situation

To address correlations effectively our task is to calculate the following objects. Start with Onsager:

$$\begin{aligned}\frac{1}{\Omega}\langle \hat{J}_x \rangle &= L_{11}E_x + L_{12}(-\nabla_x T/T)\\ \frac{1}{\Omega}\langle \hat{J}^Q_x \rangle &= L_{21}E_x + L_{22}(-\nabla_x T/T),\end{aligned}$$

where $(-\nabla_x T/T)$ is regarded as the *external driving thermal force*, and $\hat{J}^Q_x$ is the heat current operator.

$$\kappa_{zc} = \frac{1}{TL_{11}}(L_{22}L_{11} - L_{12}L_{21}).$$

We want finite frequency versions of these…..Turn to Luttinger

$$K_{tot} = K + \sum_x K(\vec{x})\psi(\vec{x},t).$$

Here $K = \sum_x K(\vec{x})$, and $K(\vec{x}) = H(\vec{x}) - \mu n(\vec{x})$ is the *grand canonical* Hamiltonian

We can define the local temperature through

$$\delta T(\vec{x},t) = \frac{\delta\langle K(\vec{x},t)\rangle}{C(T)}.$$

Luttinger writes

$$\begin{aligned}
\frac{1}{\Omega}\langle \hat{J}_x\rangle &= L_{11}E_x + L_{12}(-\nabla_x T/T) + \hat{L}_{12}(-\nabla_x \psi(\vec{x},t)) \\
\frac{1}{\Omega}\langle \hat{J}^Q_x\rangle &= L_{21}E_x + L_{22}(-\nabla_x T/T) + \hat{L}_{22}(-\nabla_x \psi(\vec{x},t)),
\end{aligned}$$

Let $\psi(\vec{x},t) = \psi_q \exp\{-i(q_x x + \omega t + i0^+ t)\}$, (adiabatic switching implied) and the electric potential $\phi(\vec{x},t) = \phi_q \exp\{-i(q_x x + \omega t + i0^+ t)\}$ thus write

$$\delta J(q) = (iq_x)L_{11}(q_x,\omega)\phi_q + (iq_x)\left[L_{12}(q_x,\omega)\frac{\delta T_q}{T} + \hat{L}_{12}(q_x,\omega)\ \psi_q\right],$$

In equilibrium (i.e. static inhomogeneous limit) there is no net current therefore

$$0 = L_{12}(q,0)\frac{\delta T_q}{T} + \hat{L}_{12}(q,0)\psi_q.$$

However,

$$\lim_{\vec{q}\to 0}\psi(\vec{q},0) = -\lim_{\vec{q}\to 0}\frac{\delta T_q}{T}.$$

Hence We conclude that:

$$\lim_{q\to 0}\left[L_{12}(q,0) - \hat{L}_{12}(q,0)\right] = 0$$

Luttinger's identity

$$L_{ij}(q,\omega) = \hat{L}_{ij}(q,\omega)$$

Basic assumption of our work:

Generalized Luttinger's identity

Can compute RHS mechanically. Extension satisfies Causality, Onsager reciprocity and also Hydrodynamics at small q, w

$$\hat{J}_x^Q = \hat{J}_x^E - \frac{\mu}{q_e}\hat{J}_x,$$

where $\hat{J}_x^E$ is the *energy current* and $\hat{J}_x$ the charge current.

$$\hat{J}_x^Q = \lim_{q_x \to 0} \frac{1}{q_x}\left[K, K(q_x)\right].$$

$$\hat{J}_x^Q(\vec{q}) = \sum_x \hat{J}_x^Q(\vec{x}) \exp(i\vec{q}.\vec{x}), \quad \text{so that } \hat{J}_x^Q = \lim_{q \to 0} \hat{J}_x^Q(\vec{q}).$$

$$\begin{aligned}
\delta \hat{J}_x &= L_{11}(q_x,\omega)(iq_x\phi_q) + L_{12}(q_x,\omega)(iq_x\psi_q) \\
\delta \hat{J}_x^Q &= L_{21}(q_x,\omega)(iq_x\phi_q) + L_{22}(q_x,\omega)(iq_x\psi_q).
\end{aligned}$$

$$K_{tot} = K + [\rho(-q_x)\phi_q + K(-q_x)\psi_q] \exp\left(-i\omega t + 0^+ t\right),$$

We can reduce the calculations of all L_{ij} to essentially a single one, with the help of some notation. Keeping q_x small but non zero, we define currents, densities and forces in a matrix notation as follows:

$$
\begin{array}{ccc}
 & \text{i=1} & \text{i=2} \\
 & \text{Charge} & \text{Energy} \\
\mathcal{I}_i & \hat{J}_x(q_x) & \hat{J}^Q_x(q_x) \\
\mathcal{U}_i & \rho(-q_x) & K(-q_x) \\
\mathcal{X}_i & E^x_q = iq_x\phi_q & iq_x\psi_q .
\end{array}
$$

The perturbed Hamiltonian can then be written as

$$K_{tot} = K + \sum_j Q_j e^{-i\omega_c t}, \quad \text{where} \quad Q_j = \frac{1}{iq_x}\mathcal{U}_j\mathcal{X}_j .$$

$$\langle \mathcal{I}_i \rangle = -\sum_j \chi_{\mathcal{I}_i, Q_j}(\omega_c),$$

$$\begin{aligned}
\chi_{A,B}(\omega_c) &= i\int_0^\infty dt\; e^{i\omega t - 0^+ t} \langle [A(t), B(0)] \rangle \\
&= \sum_{n,m} \frac{p_m - p_n}{\varepsilon_n - \varepsilon_m + \omega_c} A_{nm} B_{mn} \\
&= -\frac{1}{\omega_c}\left[\langle [A, B] \rangle + \sum_{n,m} \frac{p_m - p_n}{\varepsilon_n - \varepsilon_m + \omega_c} A_{nm} ([B, K])_{mn} \right].
\end{aligned}$$

$$L_{ij}(q_x, \omega) = \frac{i}{\Omega \omega_c} \left[-\langle [\mathcal{I}_i, \mathcal{U}_j] \rangle \frac{1}{q_x} - \sum_{n,m} \frac{p_m - p_n}{\varepsilon_n - \varepsilon_m + \omega_c} (\mathcal{I}_i)_{nm} (\mathcal{I}_j^\dagger)_{mn} \right].$$

For arbitrary frequencies the Onsager functions read as

High ω limit

$$L_{ij}(\omega) = \frac{i}{\Omega\omega_c}\left[\langle\mathcal{T}_{ij}\rangle - \sum_{n,m}\frac{p_m - p_n}{\varepsilon_n - \varepsilon_m + \omega_c}(\mathcal{I}_i)_{nm}(\mathcal{I}_j)_{mn}\right],$$

$$\langle\mathcal{T}_{ij}\rangle = -\lim_{q_x\to 0}\langle[\mathcal{I}_i, \mathcal{U}_j]\rangle\frac{1}{q_x}.$$

Note apparent divergence of this term: it disappears on closer view. (Shastry 2006)

The operators $\mathcal{T}_{ij}$ are not unique, since one can add to them a ‘gauge operator” $\mathcal{T}_{ij}^{gauge} = [P, K]$ with arbitrary P. These fundamental operators play a crucial role in the subsequent analysis, since they

These important operators are written in a more familiar as follows:

Stress tensor	Thermal operator	Thermoelectric operator
$\mathcal{T}_{11}$	$\mathcal{T}_{22}$	$\mathcal{T}_{12} = \mathcal{T}_{21}$
τ^{xx}	Θ^{xx}	Φ^{xx}
$-\frac{d}{dq_x}\left[\hat{J}_x(q_x), \rho(-q_x)\right]_{q_x\to 0}$	$-\frac{d}{dq_x}\left[\hat{J}_x^Q(q_x), K(-q_x)\right]_{q_x\to 0}$	$-\frac{d}{dq_x}\left[\hat{J}_x(q_x), K(-q_x)\right]_{q_x\to 0}$

The thermoelectric operator can also be written as

$$\Phi^{xx} = \mathcal{T}_{21} = -\frac{d}{dq_x}\left[\hat{J}_x^Q(q_x), \rho(-q_x)\right]_{q_x\to 0},$$

Limiting behaviour:

$$L_{ij}(\omega) \quad \rightarrow \quad \frac{i}{\omega}\langle \mathcal{T}_{ij} \rangle$$

Given these coefficients we can compute S* etc since the frequency dependence goes away.

Using causality and Kramers Kronig relations, we see that the high ω behavior of L implies a sum rule for the real (dissipative part). Hence we get a novel sum rule for the thermal conductivity!

``Sum rule for thermal conductivity and dynamical thermal transport coefficients in condensed matter '', B Sriram Shastry, Phys. Rev. B 73, 085117 (2006)

Plasma sum rule

F sum rule

$$\int_{-\infty}^{\infty} \frac{d\nu}{2} \Re e \sigma(\nu) = \frac{\pi \langle \tau^{xx} \rangle}{2\Omega}$$

$$\int_{-\infty}^{\infty} \frac{d\nu}{2} \Re e \kappa(\nu) = \frac{\pi \langle \Theta^{xx} \rangle}{2T\Omega}, .$$

Thermal sum rule

$$\int_{-\infty}^{\infty} \frac{d\nu}{\pi} \Re e \kappa_{zc}(\nu) = \frac{1}{T\Omega} \left[\langle \Theta^{xx} \rangle - \frac{\langle \Phi^{xx} \rangle^2}{\langle \tau^{xx} \rangle} \right].$$

Zero current thermal conductivity where explicit value of μ is not needed.

$$\int_0^\infty Re\ \kappa_{zc}(\omega)d\omega \;=\; \frac{\pi}{2\hbar T\mathcal{L}}\left\{\langle\Theta^{xx}\rangle - \frac{\langle\Phi^{xx}\rangle^2}{\langle\tau^{xx}\rangle}\right\}, \qquad \text{sum rule}$$

$$S^* \;=\; \frac{\langle\Phi^{xx}\rangle}{T\langle\tau^{xx}\rangle}$$

$$\mathbf{L}^* \;=\; \frac{\langle\Theta^{xx}\rangle}{T^2\langle\tau^{xx}\rangle} - (S^*)^2$$

$$\mathbf{Z}^*T \;=\; \frac{\langle\Phi^{xx}\rangle^2}{\langle\Theta^{xx}\rangle\langle\tau^{xx}\rangle - \langle\Phi^{xx}\rangle^2}$$

Summary of new formulas

The two newly introduced operators Thermal operator Θ^{xx} , and thermo-electric operator Φ^{xx} together with the stress tensor or Kinetic energy operator τ^{xx} can be computed for any given model, and their expectation as above gives all the interesting objects. One small example

Thermo power operator for Hubbard model

$$\Phi^{xx} \;=\; -\frac{q_e}{2}\sum_{\vec{\eta},\vec{\eta}',\vec{r}}(\eta_x+\eta'_x)^2 t(\vec{\eta})t(\vec{\eta}')c^\dagger_{\vec{r}+\vec{\eta}+\vec{\eta}',\sigma}c_{\vec{r},\sigma} - q_e\mu\sum_{\vec{\eta}}\eta_x^2 t(\vec{\eta})c^\dagger_{\vec{r}+\vec{\eta},\sigma}c_{\vec{r},\sigma} +$$
$$\frac{q_eU}{4}\sum_{\vec{r},\vec{\eta}}t(\vec{\eta})(\eta_x)^2(n_{\vec{r},\bar{\sigma}}+n_{\vec{r}+\vec{\eta},\bar{\sigma}})(c^\dagger_{\vec{r}+\vec{\eta},\sigma}c_{\vec{r},\sigma}+c^\dagger_{\vec{r},\sigma}c_{\vec{r}+\vec{\eta},\sigma}).$$

$$
\begin{aligned}
\Theta^{xx} &= \sum_{p,\sigma} \frac{\partial}{\partial p_x} \left\{ v^x_{\vec{p}} (\varepsilon_{\vec{p}} - \mu)^2 \right\} \; c^\dagger_{\vec{p},\sigma} c_{\vec{p},\sigma} + \frac{U^2}{4} \sum_{\eta,\sigma} t(\vec{\eta}) \eta_x^2 (n_{\vec{r},\bar{\sigma}} + n_{\vec{r}+\vec{\eta},\bar{\sigma}})^2 c^\dagger_{\vec{r}+\vec{\eta},\sigma} c_{\vec{r},\sigma} \\
&- \mu U \sum_{\vec{\eta},\sigma} t(\vec{\eta}) \eta_x^2 (n_{\vec{r},\bar{\sigma}} + n_{\vec{r}+\vec{\eta},\bar{\sigma}}) c^\dagger_{\vec{r}+\vec{\eta},\sigma} c_{\vec{r},\sigma} \\
&- \frac{U}{8} \sum_{\vec{\eta},\vec{\eta}',\sigma} t(\vec{\eta}) t(\vec{\eta}') (\eta_x + \eta'_x)^2 \left\{ 3n_{\vec{r},\bar{\sigma}} + n_{\vec{r}+\vec{\eta},\bar{\sigma}} + n_{\vec{r}+\vec{\eta}',\bar{\sigma}} + 3n_{\vec{r}+\vec{\eta}+\vec{\eta}',\bar{\sigma}} \right\} c^\dagger_{\vec{r}+\vec{\eta}+\vec{\eta}',\sigma} c_{\vec{r},\sigma} \\
&+ \frac{U}{4} \sum_{\vec{\eta},\vec{\eta}',\sigma} t(\vec{\eta}) t(\vec{\eta}') (\eta_x + \eta'_x) \eta'_x c^\dagger_{\vec{r}+\vec{\eta},\sigma} c_{\vec{r},\sigma} \left\{ c^\dagger_{\vec{r}+\vec{\eta},\bar{\sigma}} c_{\vec{r}+\vec{\eta}+\vec{\eta}',\bar{\sigma}} + c^\dagger_{\vec{r}-\vec{\eta}',\bar{\sigma}} c_{\vec{r},\bar{\sigma}} - h.c. \right\}.
\end{aligned}
$$

Tough expressions but can be managed !!

These new operators represent exactly the inertial coupling between the external fields and the acceleration of the currents. See later

19th century historical footnote

Seebeck, Peltier, Thomson(=Kelvin)..

$$L_{12} = L_{21}$$

•Famous Reciprocity “proven” by Kelvin using only thermodynamics. 1850’s

•Re-proven by Lars Onsager 1930’s using dynamics:

- **According to Wannier’s book on Statistical Physics “**Opinions are divided on whether Kelvin’s derivation is fundamentally correct or not**”.**

What about Kelvin-Onsager?

$$S = \lim_{\omega \to 0, q_x \to 0} \frac{1}{q_e T} \frac{\chi_{[n_q, H_{-q} - \mu n_{-q}]}(\omega)}{\chi_{[n_q, H_{-q} - \mu n_{-q}]}(\omega)}$$

Onsager-Kubo

Large box then static limit

$$S_{Kelvin} = \lim_{q_x \to 0, \omega \to 0} \frac{1}{q_e T} \frac{\chi_{[n_q, H_{-q} - \mu n_{-q}]}(\omega)}{\chi_{[n_q, H_{-q} - \mu n_{-q}]}(\omega)}$$

Kelvin Thermodynamics

Static limit then large box

$$S^* = \lim_{\omega \gg \omega_c, q_x \to 0} \frac{1}{q_e T} \frac{\chi_{[n_q, H_{-q} - \mu n_{-q}]}(\omega)}{\chi_{[n_q, H_{-q} - \mu n_{-q}]}(\omega)}$$

High Frequency

Large box then frequency larger than characteristic w's

For a weakly interacting diffusive metal, we can compute all three S's. Low T limit :

Here is the result:

Density Of States

Velocity averaged over FS

Energy dependent relaxation time.

$$S = T\frac{\pi^2 k_B^2}{3q_e}\frac{d}{d\,\varepsilon}\ln[\rho(\varepsilon)\langle(v^x)^2\rangle_\varepsilon\tau(\varepsilon)]_{\varepsilon\to\mu} \text{ Onsager- Kubo-Mott formula}$$

"Exact"

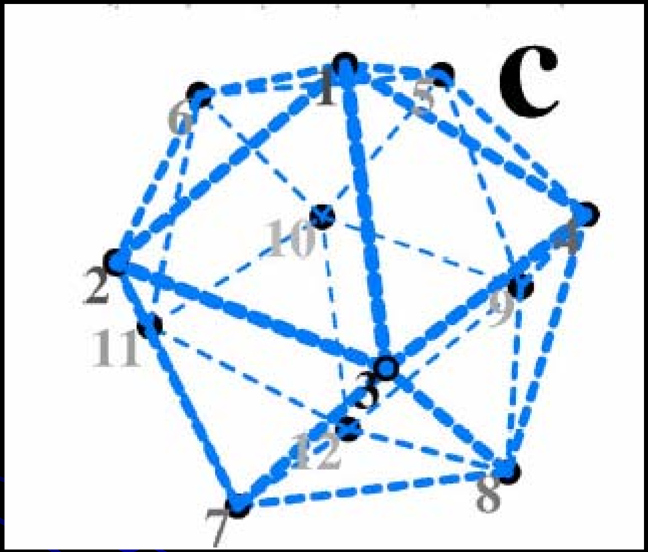
$$S = T\frac{\pi^2 k_B^2}{3q_e}\frac{d}{d\varepsilon}\ln[\rho(\varepsilon))]_{\varepsilon\to\mu} \text{ Kelvin inspired formula}$$

Easy to compute for correlated systems, since transport is simplified!

But S* is better in this limit

$$S^* = T\frac{\pi^2 k_B^2}{3q_e}\frac{d}{d\varepsilon}\ln[\rho(\varepsilon)\langle(v^x)^2\rangle_\varepsilon]_{\varepsilon\to\mu} \text{ High frequency formula}$$

Clusters of t-J Model + Exact diagonalization: all states all matrix elements.



Data from paper with Mike Peterson and Jan Haerter Phs Rev 2007

$Na_{\{.68\}}$ Co O_2

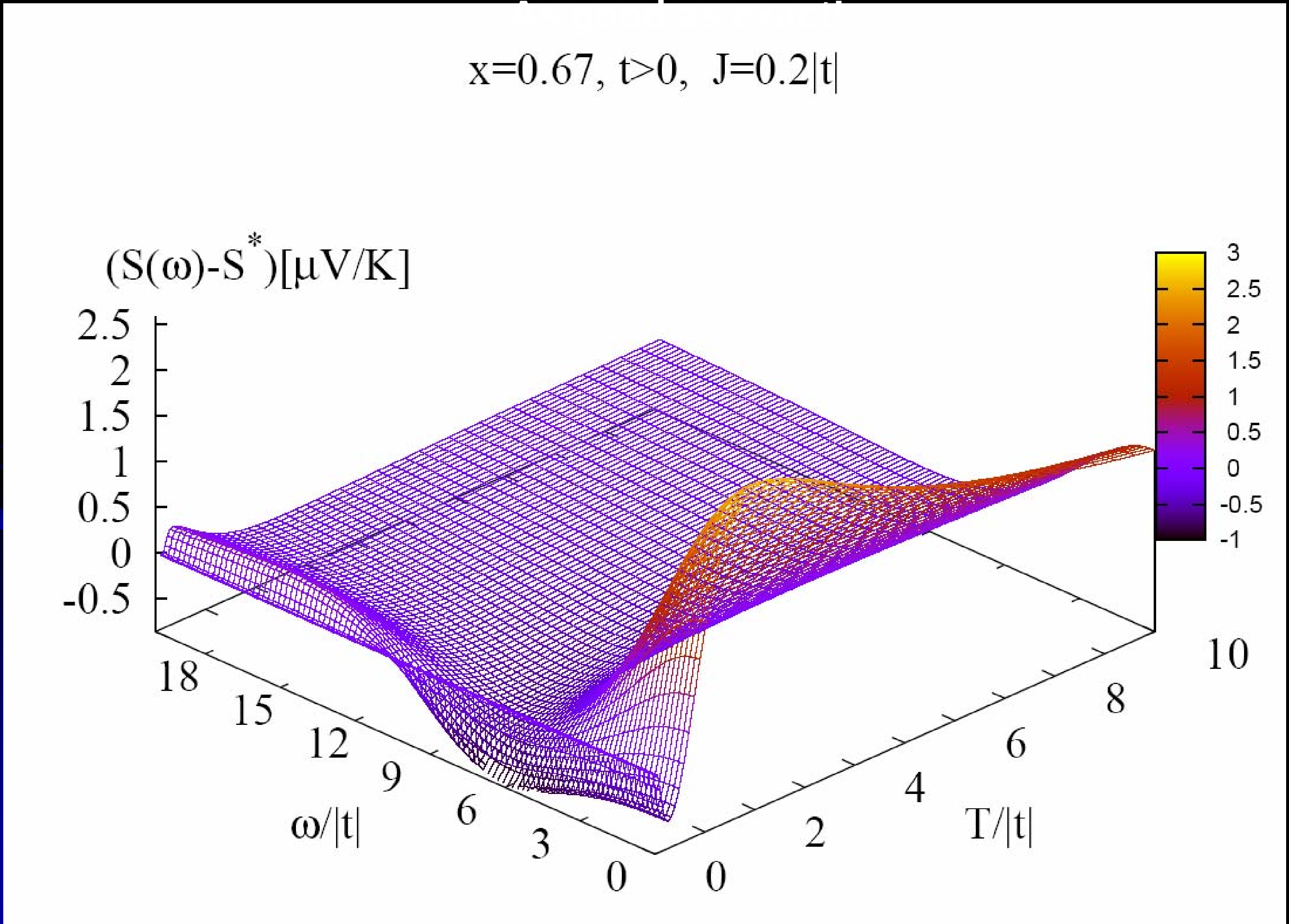
Modeled by t-J model with only two parameters "t=100K" and "J=36K". Interested in Curie Weiss phase. Photoemission gives scale of "t" as does Hall constant slope of R_H and a host of other objects.

REMARK: Low value of t is taken from Photoemission of Zahid Hasan et al (Princeton). This is crucially and surprisingly smaller than LDA by factor of 10!!

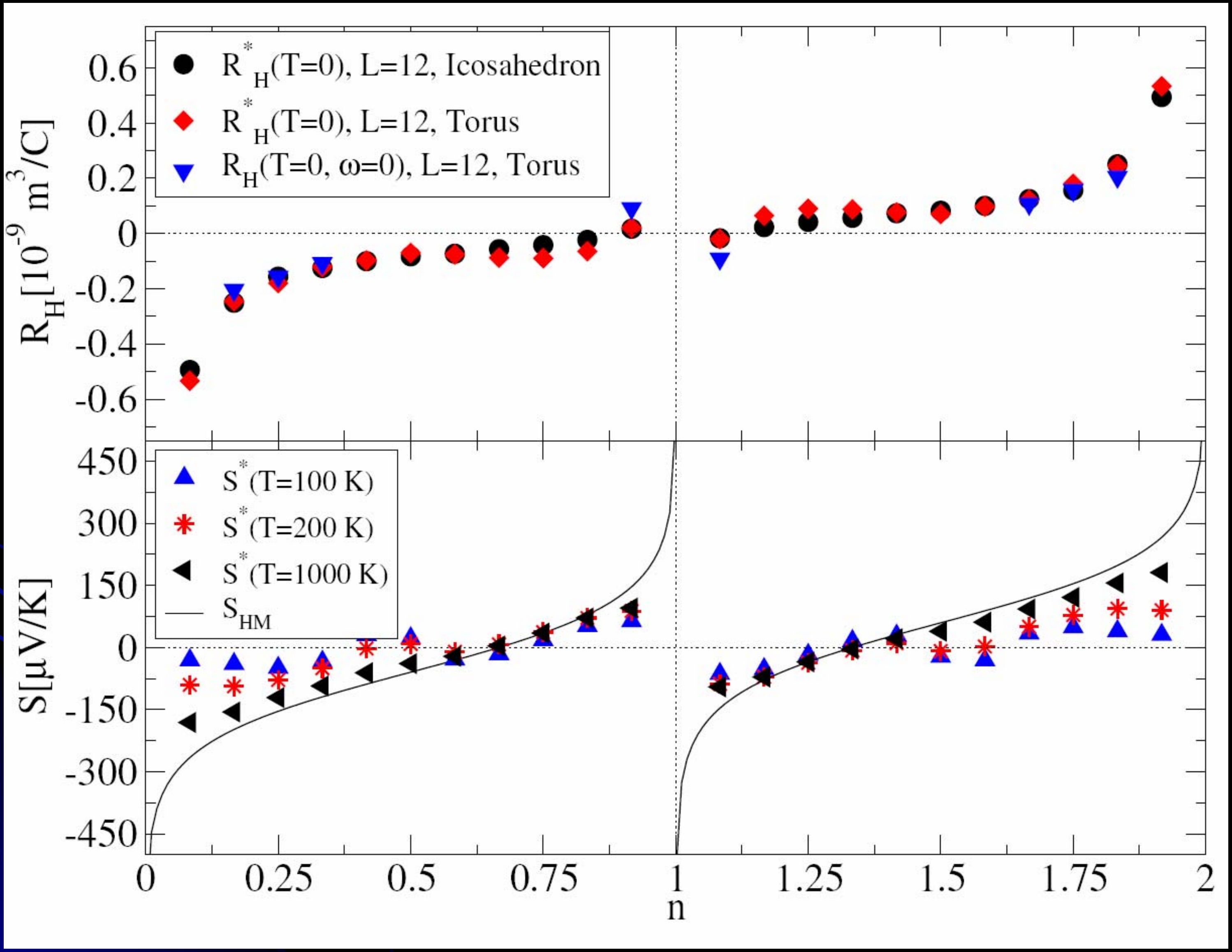
One favourite cluster is the platonic solid Icosahedron with 12 sites made up of triangles. Also pbc's with torii. Sizes upto 15 sites.

How good is the S* formula compared to exact Kubo formula?

A numerical benchmark: Max deviation 3% anywhere !!



Notice that these variables change sign thrice as a band fills from 0->2. Sign of Mott Hubbard correlations.



Results from this formalism:

PRL 97, 226402 (2006) PHYSICAL REVIEW LETTERS week ending 1 DECEMBER 2006

Strong Correlations Produce the Curie-Weiss Phase of Na_xCoO_2

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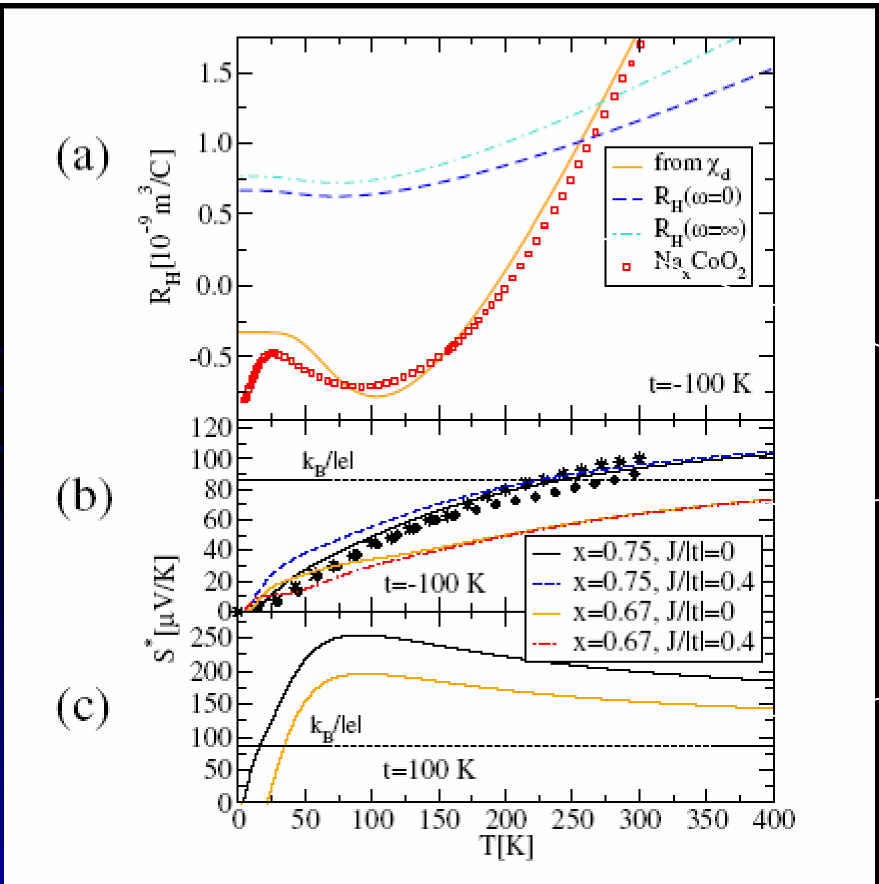
(Received 21 July 2006; published 28 November 2006)



T linear Hall constant for triangular lattice predicted in 1993 by Shastry Shraiman Singh! Quantitative agreement hard to get with scale of "t"

Comparision with data on absolute scale!

Prediction for t>0 material

The various formulas

$$\mathrm{S}_{Heikes-Mott} = \frac{\mu(0)-\mu(T)}{q_e T}$$

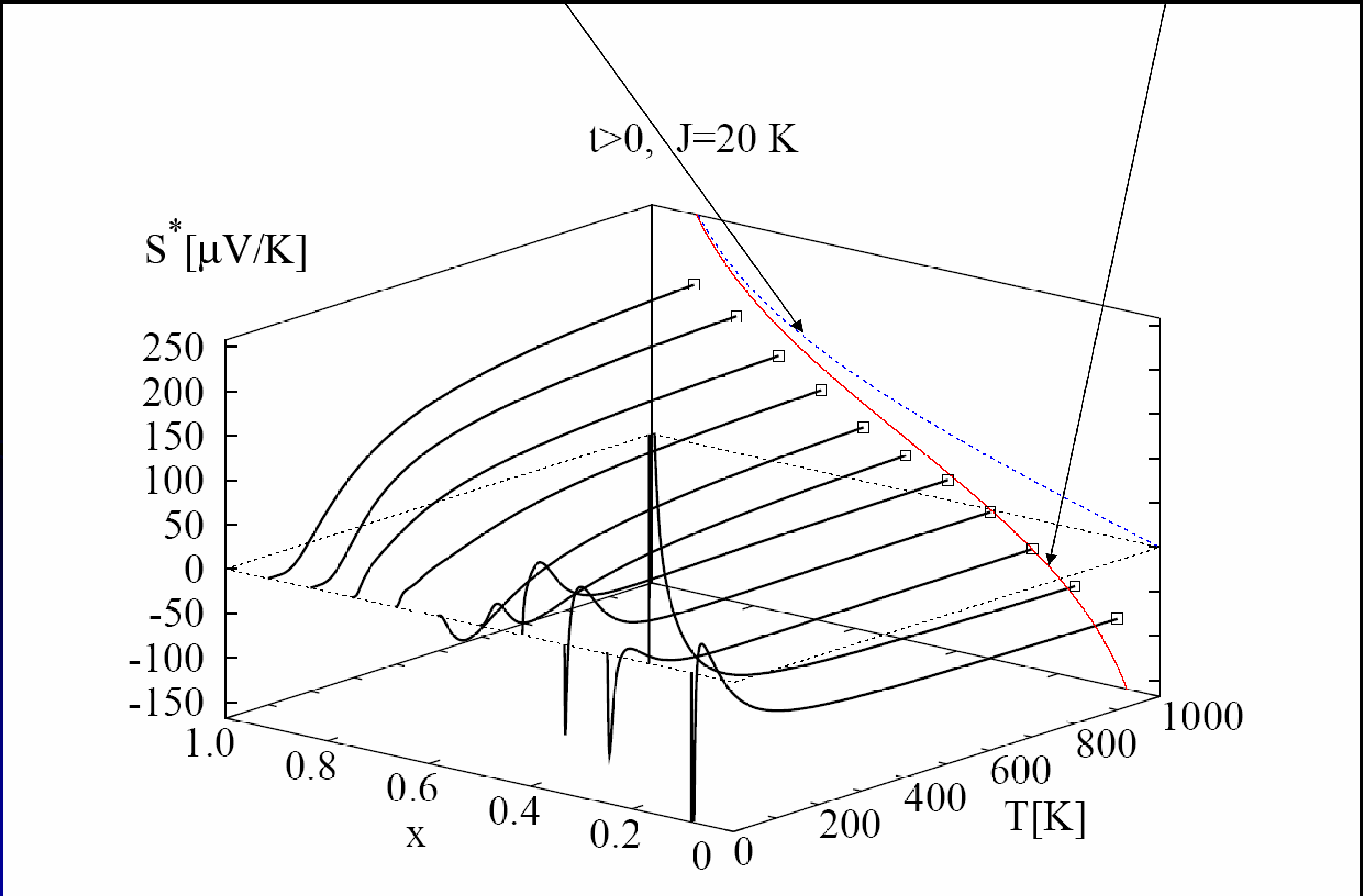
Throws out " transport part" and keeps only a thermodynamic contribution.

$$\mathrm{S}^* = \frac{\langle \Phi^{xx} \rangle}{T\langle \tau^{xx} \rangle} - \frac{\mu(T)}{q_e T}$$

"Transport part"

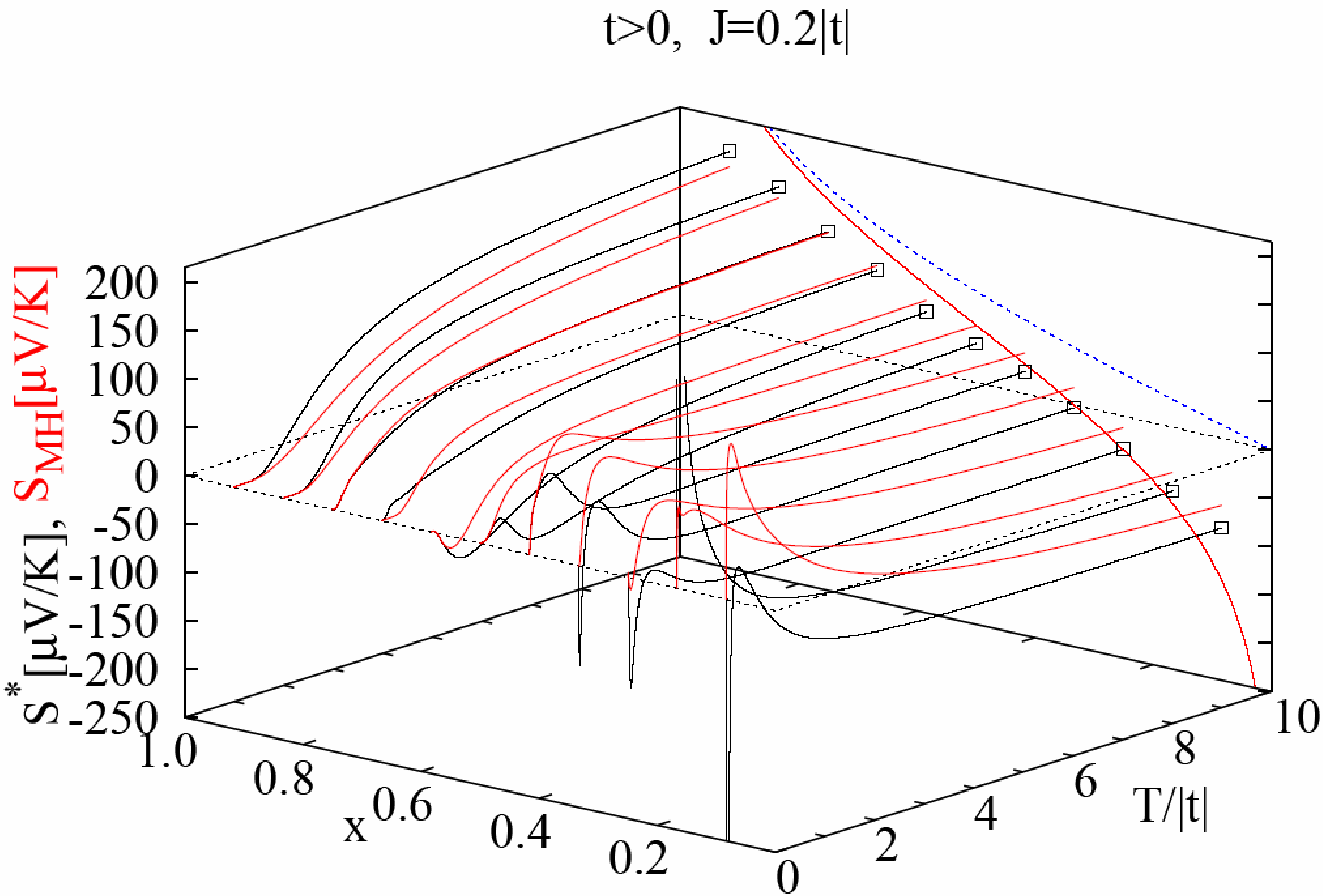
$$\mathrm{S}_{Kubo} = \frac{\langle\langle J^E(t) J(0) \rangle\rangle}{\langle\langle J(t) J(0) \rangle\rangle} - \frac{\mu(T)}{q_e T}$$

Typical results for S* for NCO type case. Low T problems due to finite sized clusters. The blue line is for uncorrelated band, and red line is for t-J model at High T analytically known.

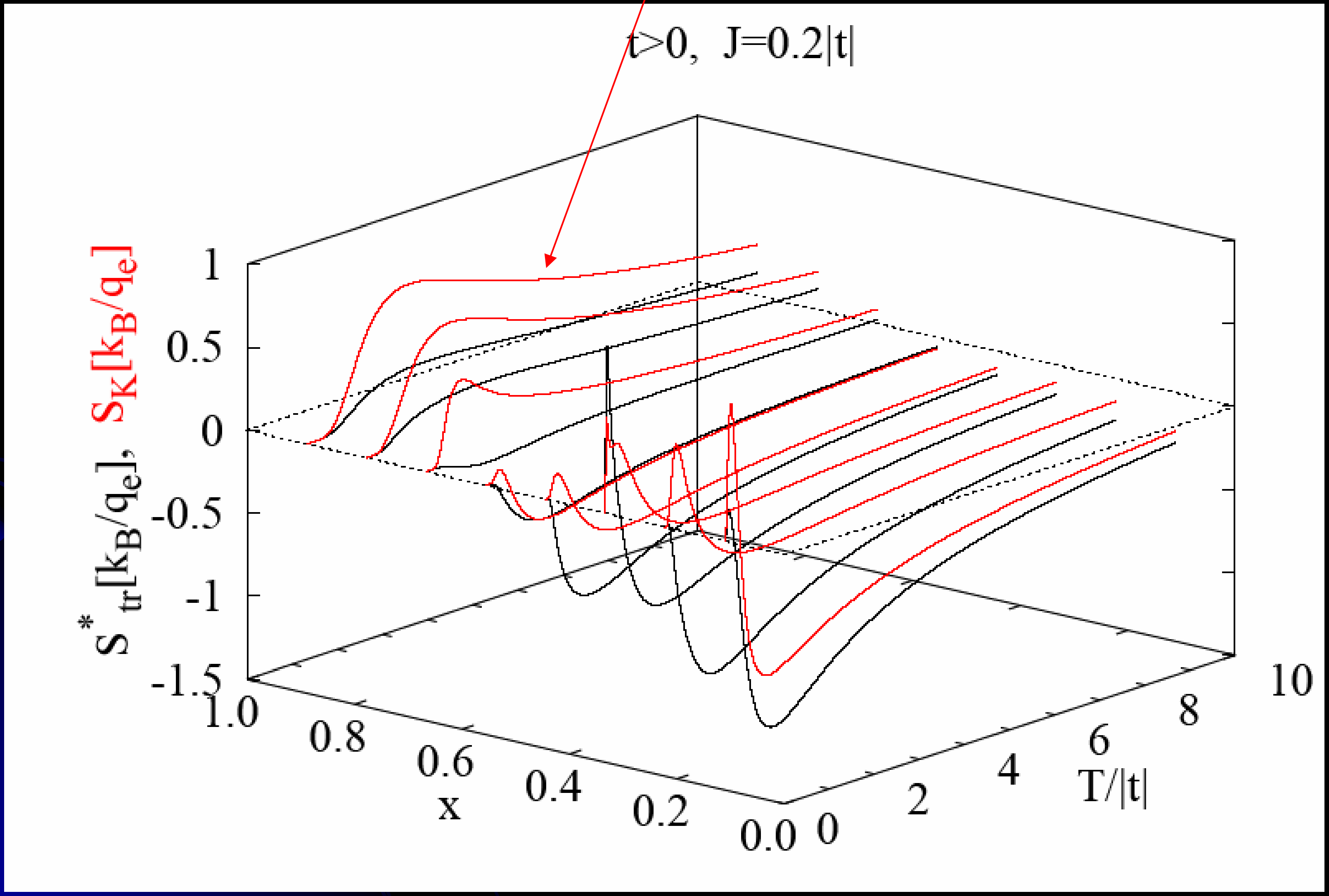


S* and the Heikes Mott formula (red) for Na_xCo O2.

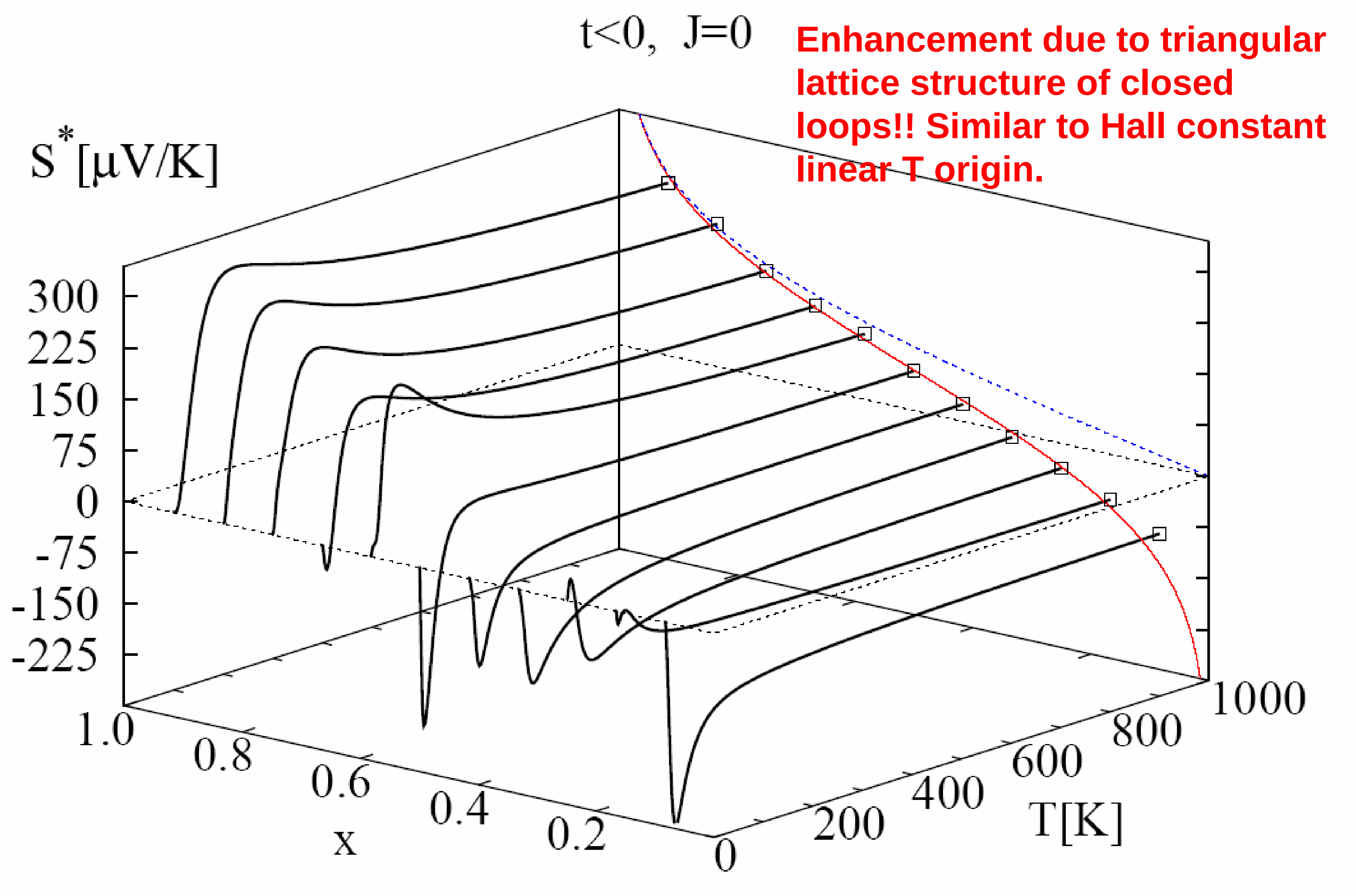
Close to each other for t>o i.e. electron doped cases



Kelvin Inspired formula is somewhat off from S* (and hence S) but right trends. In this case the Heikes Mott formula dominates so the final discrepancy is small.

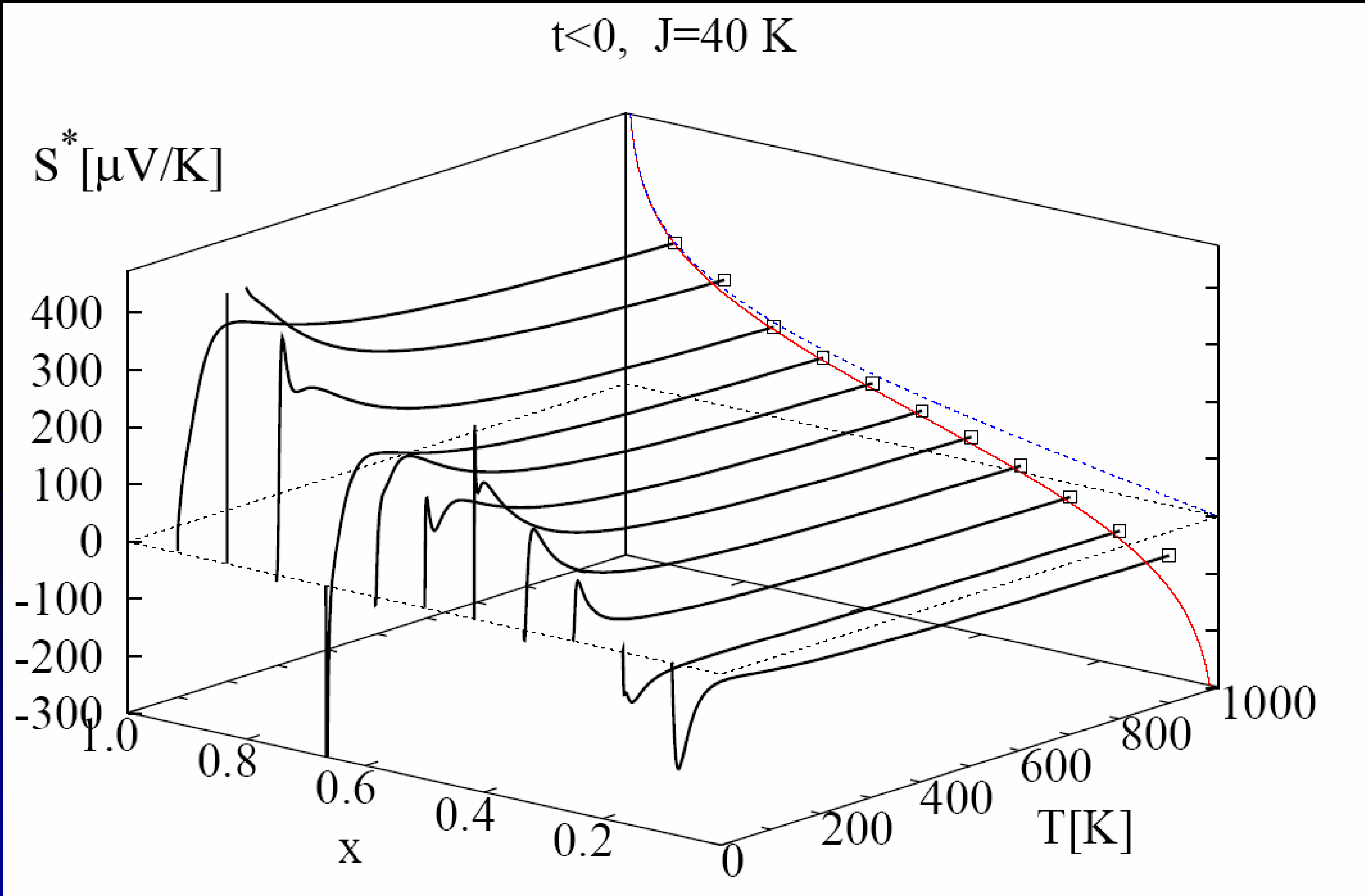


Predicted result for t<0 i.e. fiducary hole doped CoO_2 planes. Notice much larger scale of S* arising from transport part (not Mott Heikes part!!).



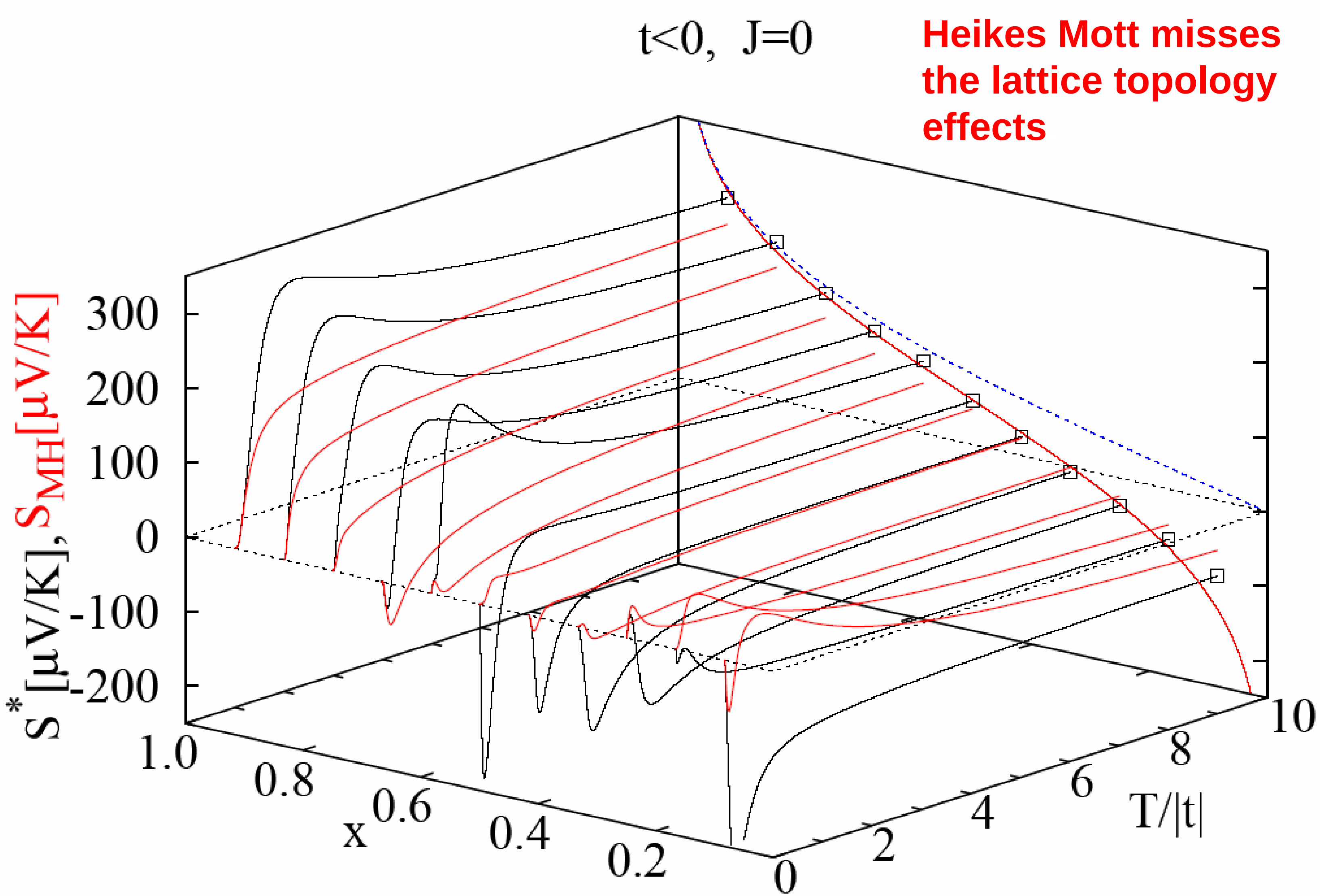
Predicted result for t<0 i.e. fiducary hole doped CoO_2 planes.

Different J higher S.



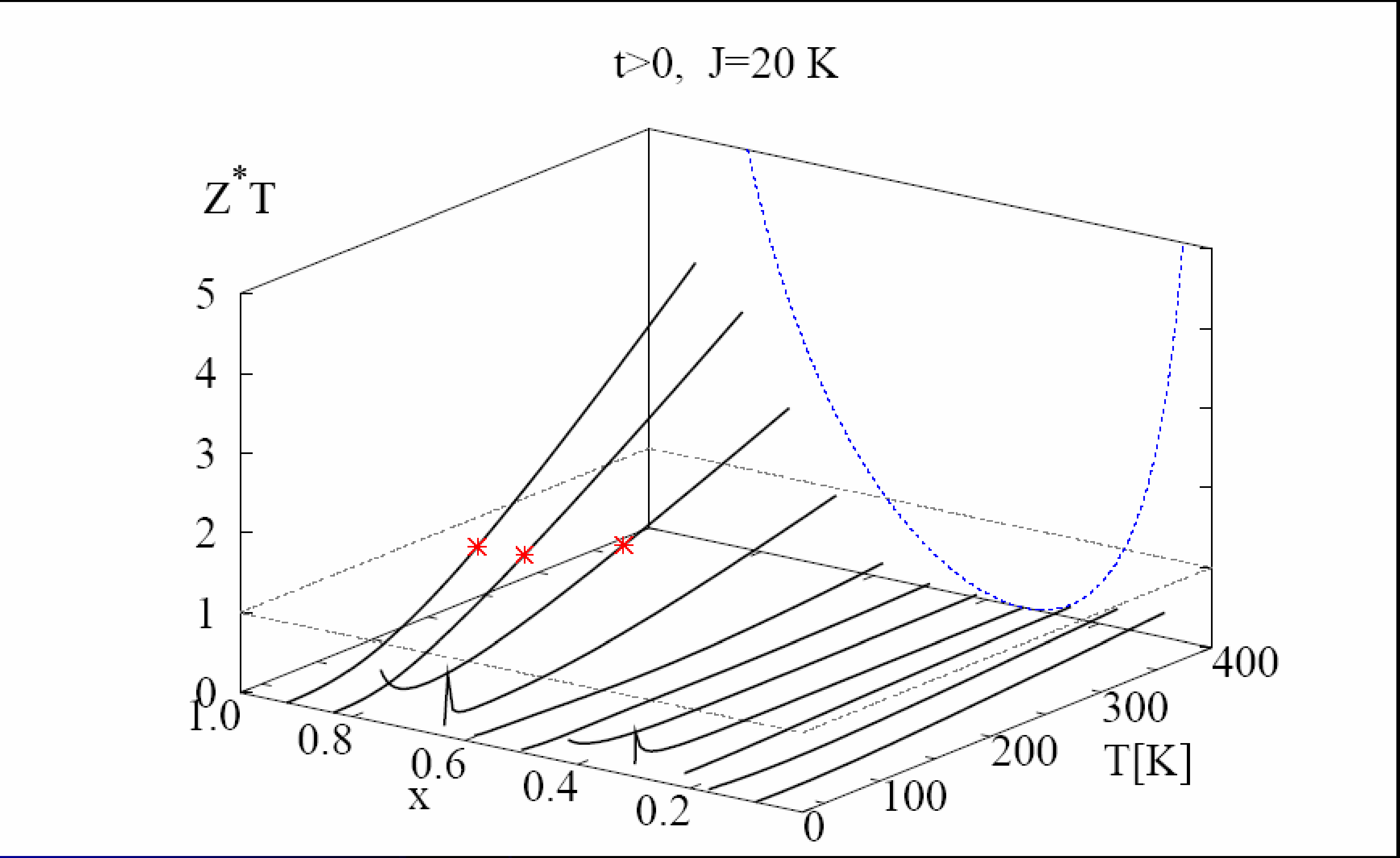
Predictions of S* and the Heikes Mott formula (red) for fiducary hole doped CoO2.

Notice that S* predicts an important enhancement unlike Heikes Mott formula



Z*T computed from S* and Lorentz number. Electronic contribution only, no phonons. Clearly large x is better!!

Quite encouraging.



Phenomenological eqns for coupled charge heat transport

- Meaning of the new operators becomes clear.
- Some interesting experiments using laser heating are suggested.

$$
\begin{aligned}
\left[\frac{1}{\tau}+\frac{d}{dt}\right]\langle\hat{J}^{Q}_{x}(\vec{r},t)\rangle &= -\frac{D_Q}{\tau}\nabla\langle K(\vec{r}t)\rangle-\frac{c_1}{\tau}\nabla\langle\rho(\vec{r}t)\rangle \\
&\quad -\left\{\frac{\langle\Theta^{xx}\rangle_0}{\Omega}\nabla\psi(\vec{r}t)+\frac{\langle\Phi^{xx}\rangle_0}{\Omega}\nabla\phi(\vec{r}t)\right\}
\end{aligned}
$$

and

$$
\begin{aligned}
\left[\frac{1}{\tau}+\frac{d}{dt}\right]\langle\hat{J}_{x}(\vec{r},t)\rangle &= -\frac{c_2}{\tau}\nabla\langle K(\vec{r}t)\rangle-\frac{D_c}{\tau}\nabla\langle\rho(\vec{r}t)\rangle \\
&\quad -\left\{\frac{\langle\tau^{xx}\rangle_0}{\Omega}\nabla\phi(\vec{r}t)+\frac{\langle\Phi^{xx}\rangle_0}{\Omega}\nabla\psi(\vec{r}t)\right\}
\end{aligned}
$$

Hydrodynamics of energy and charge transport in a band model:

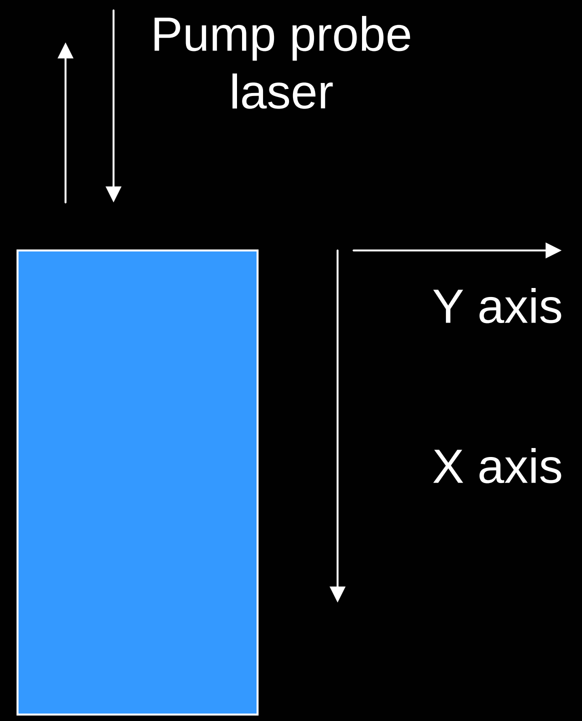
This involves the fundamental operators in a crucial way:

Continuity

$$\frac{\partial \rho}{\partial t} + \nabla J(r) = 0$$

$$\frac{\partial K(r)}{\partial t} + \nabla J^Q(r) = p_0 \delta(x)$$

Input power density



These eqns contain energy and charge diffusion, as well as thermoelectric effects. Potentially correct starting point for many new nano heating expts with lasers. Work in progress. Preprint soon

The inertial terms contribute for initial rise of the energy and heat current.

Exact coupling term term

$$\left\{ \frac{\partial}{\partial t} + \frac{1}{\tau_E} \right\} \delta J^Q(r) = -\frac{1}{\Omega} \langle \Theta^{xx} \rangle \left[\nabla \Psi \right] + \mathrm{rest}$$

Hence a δ(t) heat pulse gives an initial jump in current that is a **measure of the sum rule**.

Also energy density responds inertially initially. Initial response to pulses of heat and charge are a good measure of these coefficients.

Conclusions

- Hole doping prediction of large S
- Low bandwidth in NCO is the big factor leading to enhanced S (not orbital degeneracy).
- Dynamical heating experiments can address interesting and fundamental questions “what is energy and what is temperature”.