Thermoelectric Effects in Correlated Matter

Work supported by
NSF DMR
0408247

Work supported by
DOE, BES DE-FG02-06ER46319

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September , 2008

Intro

- High Thermoelectric power is very desirable for applications.
- Usually the domain of semiconductor industry, e.g. Bi_2Te_3. However, recently correlated matter has found its way into this domain.
- Heavy Fermi systems (low T), Mott Insulator Junction sandwiches (Harold Hwang 2004)
- Sodium Cobaltate NaxCoO2 at x ~ .7 Terasaki, Ong, …..

What is the Seebeck Coefficient S?

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

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

$$\begin{aligned}
\text{Thermopower} \quad S(\omega) &= \frac{L_{12}(\omega)}{TL_{11}(\omega)} \\
\text{Lorentz Number} \quad \mathbf{L}(\omega) &= \frac{\kappa_{zc}(\omega)}{T\sigma(\omega)} \\
\text{Figure of Merit} \quad \mathbf{Z}(\omega)T &= \frac{S^2(\omega)}{\mathbf{L}(\omega)}. \qquad (1)
\end{aligned}$$

Desirable: Large ZT

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

- Need large S
- Large σ
- Small κ

What is S?

Large variety of answers:

Thermodynamic	Kubowallahs	Band Theory …..
Entropy per particle	Kubo formulas	d ρ(μ)/ d μ
Kelvin	Onsager	Mott

$$S_{Kubo} = \left[\frac{\int_0^\infty dt \ \int_0^\beta \ d\tau \ \langle \hat{J}_x^E(t - i\tau)\hat{J}_x(0)\rangle}{\int_0^\infty dt \ \int_0^\beta \ d\tau \ \langle \hat{J}_x(t - i\tau)\hat{J}_x(0)\rangle} - \frac{\mu(0)}{q_e} \right] + \frac{\mu(0) - \mu(T)}{q_e}.$$

S= Transport part + Thermodynamic part Write

$$S_{Kubo} = S_{Tr} + S_{Heikes-Mott},$$

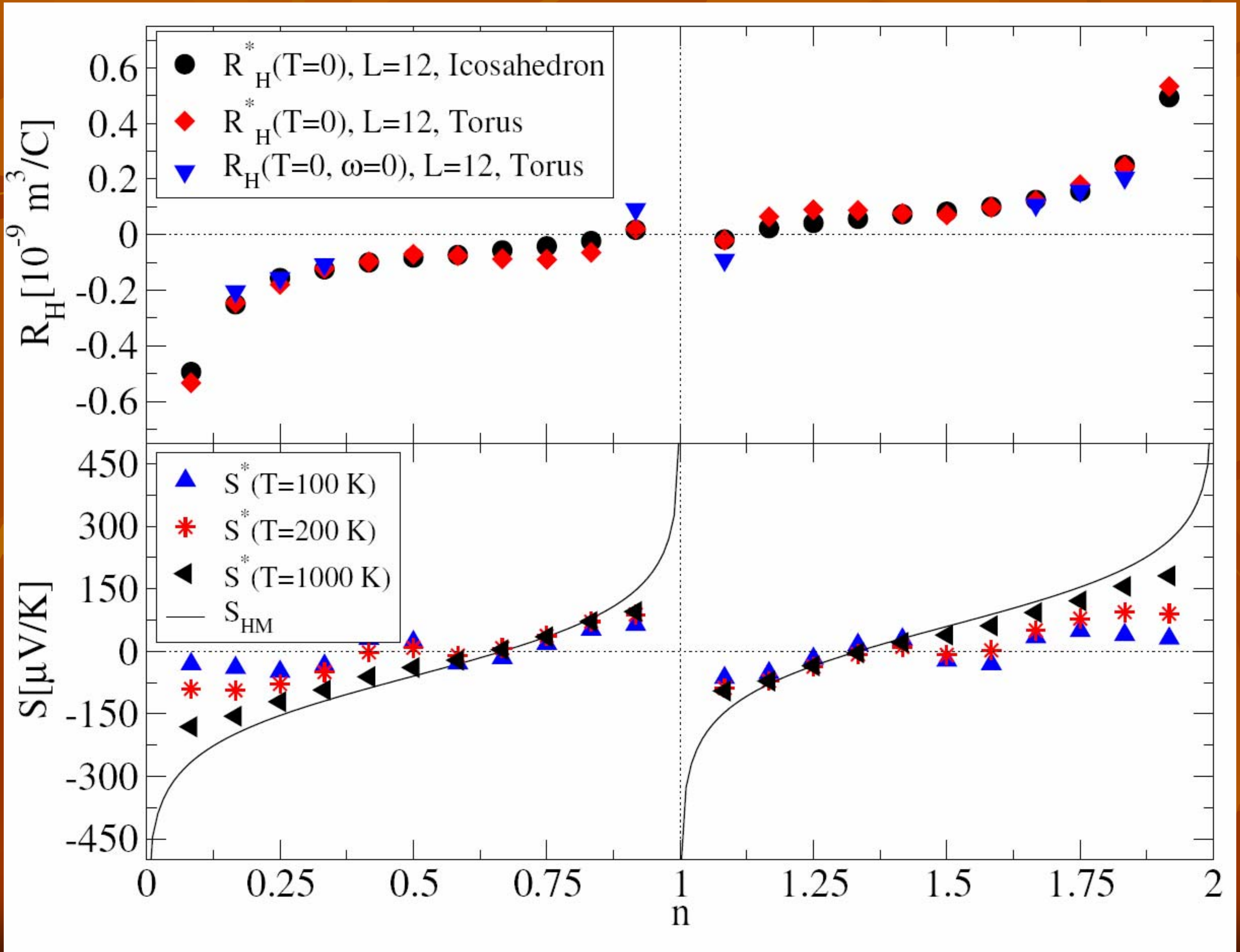
Where the first term is the difficult Transport part of S.

Similarly thermal conductivity and resitivity are defined with appropriate current operators. The computation of these transport quantities is brutally difficult for correlated systems.

Hence seek an escape route……….That is the rest of the story!

Triangular lattice Hall and Seebeck coeffs: (High frequency objects)

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



Considerable similarity between Hall constant and Seebeck coefficients.

Both gives signs of carriers---(Do they actually ???)

Zero crossings tell a tale. These objects are sensitive to half filling and hence measure Mott Hubbard hole densities.

Brief story of Hall constant to motivate the rest.

The Hall constant at finite frequencies: S Shraiman Singh- 1993

High T_c and triangular lattices---

Consider a novel dispersion relation

(Shastry ArXiv.org 0806.4629)

$$\Re e R_H(0) = R_H^*(\Omega) + \frac{2}{\pi}\int_0^{\Omega} \frac{\Im m R_H(\nu)}{\nu}\, d\nu \ .$$

•Here Ω is a cutoff frequency that determines the RH*. LHS is measurable, and the second term on RHS is beginning to be measured (recent data exists).

• The smaller the Ω, closer is our RH* to the transport value.

•We can calculate RH* much more easily than the transport value.

•For the tJ model, it would be much closer to the DC than for Hubbard type models. This is obvious since cut off is max{t,J} rather than U!!

$$\begin{aligned} \hbar\omega &\gg \{|t|, U\}_{max} \\ \hbar\omega &\gg \{|t|, J\}_{max}. \end{aligned}$$

ANALOGY between Hall Constant and Seebeck Coefficients

New Formalism SS (2006) is based on a finite frequency calculation of thermoelectric coefficients. Motivation comes from Hall constant computation (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.

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

•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.

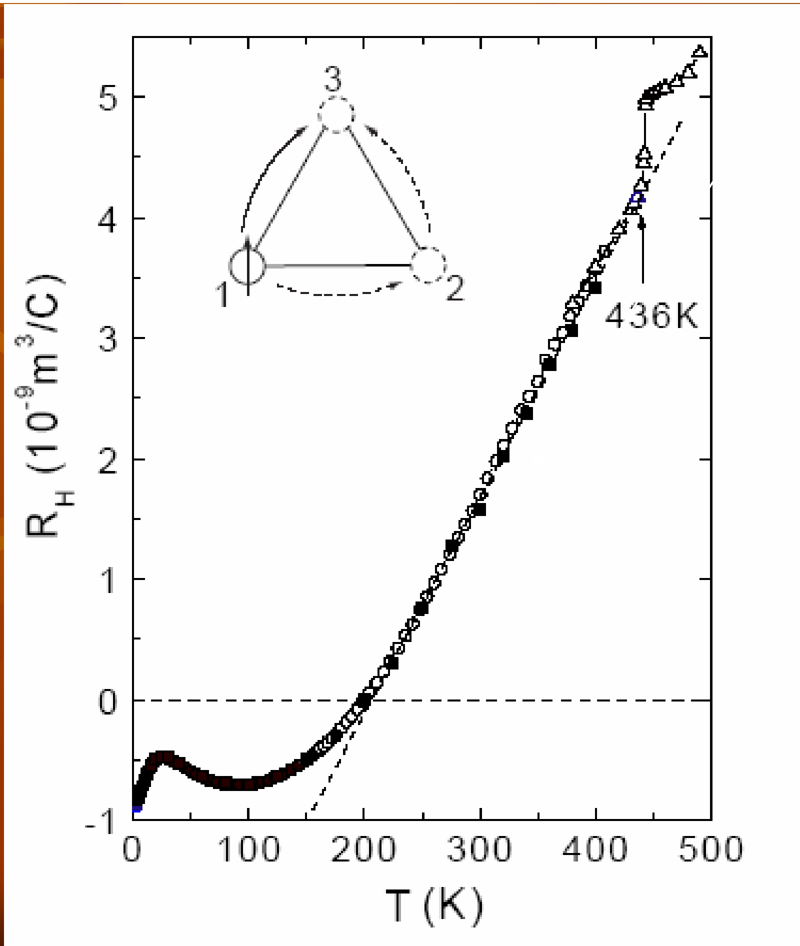
•Very good description of t-J model.

•This asymptotic formula usually requires ω to be larger than J

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]

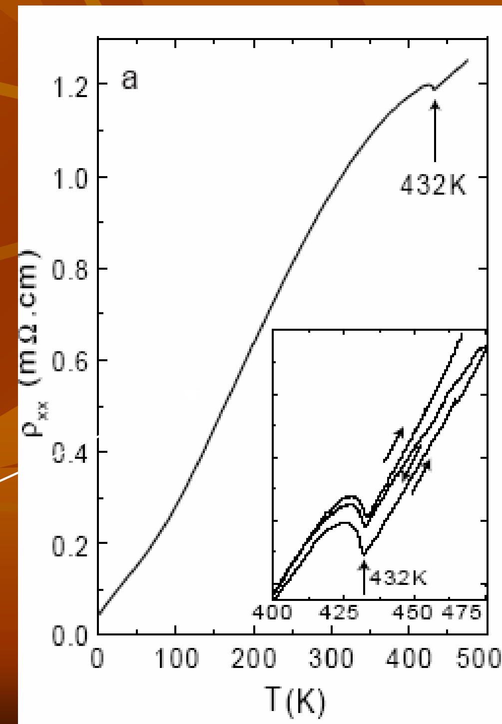
The Hall coefficient R_H of Na_xCoO_2 ($x = 0.68$) behaves anomalously at high temperatures (T) From 200 to 500 K, R_H increases linearly with T to 8 times the expected Drude value, with no sign of saturation. Together with the thermopower Q, the behavior of R_H provides firm evidence for strong correlation. 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 200⁰ to 436⁰ (predicted by theory of triangular lattice transport KS)

STRONG CORRELATIONS & Narrow Bands

T Linear resistivity



Need similar high frequency formulas for S and thermal conductivity.

Requirement::: $L_{ij}(\omega)$

Did not exist, so had lots of fun with Luttinger's formalism of a gravitational field, now made time dependent.

$$K_{tot} = \sum K(r)(1 + \psi(r,t))$$

$$\nabla(\psi(r,T)) \sim \nabla T(r,t)/T$$

	i=1	i=2
	Charge	Energy
$\mathcal{I}_i$	$\hat{J}_x(q_x)$	$\hat{J}^Q_x(q_x)$
$\mathcal{U}_i$	$\rho(-q_x)$	$K(-q_x)$
$\mathcal{Y}_i$	$E^x_q = iq_x\phi_q$	$iq_x\psi_q.$

(1)

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

$$\langle\mathcal{T}_{ij}\rangle = -\lim_{q_x\to 0}\langle[\mathcal{I}_i, \mathcal{U}_j]\rangle\frac{1}{q_x}. \tag{2}$$

Stress tensor	Thermal operator	Thermoelectric operator
$\mathcal{T}_{11}$	$\mathcal{T}_{22}$	$\mathcal{T}_{12} = \mathcal{T}_{21}$
τ^{xx}	Θ^{xx}	Φ^{xx}
$-\frac{d}{dq_x}\left[\hat{J}_x(q_x), \rho(-q_x)\right]_{q_x\to 0}$	$-\frac{d}{dq_x}\left[\hat{J}^Q_x(q_x), K(-q_x)\right]_{q_x\to 0}$	$-\frac{d}{dq_x}\left[\hat{J}_x(q_x), K(-q_x)\right]_{q_x\to 0}$
		(1)

We thus see that a knowledge of the three operators gives us a interesting starting point for correlated matter:

$$
\begin{aligned}
\text{High Freq Thermopower} \quad & S^* = \frac{\langle \Phi^{xx} \rangle}{T \langle \tau^{xx} \rangle} \\
\text{High Freq Lorentz Number} \quad & \mathbf{L}^* = \frac{\langle \Theta^{xx} \rangle}{T^2 \langle \tau^{xx} \rangle} - (S^*)^2 \\
\text{High Freq Figure of Merit} \quad & \mathbf{Z}^* T = \frac{\langle \Phi^{xx} \rangle^2}{\langle \Theta^{xx} \rangle \langle \tau^{xx} \rangle - \langle \Phi^{xx} \rangle^2}.
\end{aligned}
\tag{1}
$$

$$
\kappa_{zc}(\omega) = \frac{1}{T} \left[L_{22}(\omega) - \frac{L_{12}(\omega)^2}{L_{11}(\omega)} \right],
$$

This leads to interesting sum rules a là the f-sum rule for conductivity.

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

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

F sum rule

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

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.

Thermo power operator for Hubbard model

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

This object can be expressed completely in Fourier space as

$$\Phi^{xx} = q_e\sum_{\vec{p}}\frac{\partial}{\partial p_x}\left\{v_p^x(\varepsilon_{\vec{p}}-\mu)\right\}c^\dagger_{\vec{p},\sigma}c_{\vec{p},\sigma} + \frac{q_eU}{2\mathcal{L}}\sum_{\vec{l},\vec{p},\vec{q},\sigma,\sigma'}\frac{\partial^2}{\partial l_x^2}\left\{\varepsilon_{\vec{l}}+\varepsilon_{\vec{l}+\vec{q}}\right\}c^\dagger_{\vec{l}+\vec{q},\sigma}c_{\vec{l},\sigma}c^\dagger_{\vec{p}-\vec{q},\bar{\sigma}'}c_{\vec{p},\bar{\sigma}'}.$$

$$\tau^{xx} = \frac{q_e^2}{\hbar}\sum\eta_x^2\,t(\vec{\eta})\,c^\dagger_{\vec{r}+\vec{\eta},\sigma}c_{\vec{r},\sigma} \quad \text{or}$$

$$= \frac{q_e^2}{\hbar}\sum_{\vec{k}}\frac{d^2\varepsilon_{\vec{k}}}{dk_x^2}c^\dagger_{\vec{k},\sigma}c_{\vec{k},\sigma}$$

$$
\Theta^{xx} = \sum_{p,\sigma} \frac{\partial}{\partial p_x} \left\{ v^x_{\vec{p}} (\varepsilon_{\vec{p}} - \mu)^2 \right\} \; c^\dagger_{\vec{p},\sigma} c_{\vec{p},\sigma} + \frac{U^2}{4} \sum_{\eta,\sigma} t(\vec{\eta}) \eta_x^2 (n_{\vec{r},\bar{\sigma}} + n_{\vec{r}+\vec{\eta},\bar{\sigma}})^2 c^\dagger_{\vec{r}+\vec{\eta},\sigma} c_{\vec{r},\sigma}
$$

$$
-\mu U \sum_{\vec{\eta},\sigma} t(\vec{\eta}) \eta_x^2 (n_{\vec{r},\bar{\sigma}} + n_{\vec{r}+\vec{\eta},\bar{\sigma}}) c^\dagger_{\vec{r}+\vec{\eta},\sigma} c_{\vec{r},\sigma}
$$

$$
-\frac{U}{8} \sum_{\vec{\eta},\vec{\eta}',\sigma} t(\vec{\eta}) t(\vec{\eta}') (\eta_x + \eta'_x)^2 \left\{ 3 n_{\vec{r},\bar{\sigma}} + n_{\vec{r}+\vec{\eta},\bar{\sigma}} + n_{\vec{r}+\vec{\eta}',\bar{\sigma}} + 3 n_{\vec{r}+\vec{\eta}+\vec{\eta}',\bar{\sigma}} \right\} c^\dagger_{\vec{r}+\vec{\eta}+\vec{\eta}',\sigma} c_{\vec{r},\sigma}
$$

$$
+\frac{U}{4} \sum_{\vec{\eta},\vec{\eta}',\sigma} t(\vec{\eta}) t(\vec{\eta}') (\eta_x + \eta'_x) \eta'_x c^\dagger_{\vec{r}+\vec{\eta},\sigma} c_{\vec{r},\sigma} \left\{ c^\dagger_{\vec{r}+\vec{\eta},\bar{\sigma}} c_{\vec{r}+\vec{\eta}+\vec{\eta}',\bar{\sigma}} + c^\dagger_{\vec{r}-\vec{\eta}',\bar{\sigma}} c_{\vec{r},\bar{\sigma}} - h.c. \right\} . \quad (1)
$$

Unpublished- For Hubbard model
using “Ward type identity” can
show a simpler result for \Phi.

$$
\langle \Phi^{xx} \rangle = \frac{q_e}{c} k_B T \; \sum_{m,\sigma,\vec{k}} G_\sigma(k, i\omega_m) \left[\frac{d}{dk_x} \; (v^x_k(\varepsilon_k - \mu)) \; + \frac{d^2 \varepsilon_k}{dk_x^2} \; \Sigma_\sigma(k, i\omega_m) \right]
$$

New Formalism:*

- Novel way for computing thermopower of isolated system (absolute Thermopower)
- Leads to correct Onsager formula (a la Kubo)
- Leads to other insights and other useful formulae
- Settles the Kelvin- Onsager debate.
  - Kelvin derived reciprocity between Peltier and Seebeck Coefficient using only thermodynamics,
  - Onsager insisted that Dynamics is needed to establish reciprocity.
  - According to Wannier’s book on Statistical Physics “Opinions are divided on whether Kelvin’s derivation is fundamentally correct or not”.

*[1] Shastry, Phys. Rev. B 73, 085117 (2006)

*[2] Shastry, 43rd Karpacz (Poland) Winter School proceedings (2007)

Use Luttinger's technique

Turn on spatially inhomogeneous time dependent potential adiabatically from remote past.

$$H_1 = \sum_j H(r_j)\psi(r_j)\exp{(\eta - i\omega)t}$$

$$H_1 \sim \sum_j \frac{H(r_j)}{c^2} V_{gravity}(r_j)$$

Dark sphere!

System of Length L, open at the two surfaces 1 and 2

T_1	**Sample along x axis**	**T_2**

Choose linear gravitational potential $\psi(r_j) = \frac{x}{L}\psi_0$.

Fundamental theorem of Luttinger: Gravitational pot ~ temperature. More precisely: in a suitable limit

$$\nabla\psi(r) \to \frac{\nabla T(r)}{T}$$

1. Compute the induced change in particle density profile:
2. Particles run away from hot end to cold end, hence pileup a charge imbalance i.e. a dipole moment :
3. Linear response theory gives the dipole moment amplitude:

$$
\begin{aligned}
P_{Thermal} &= \sum_r \langle xn(r) \rangle \exp i\omega t \\
&= q_e^2 \frac{T_2 - T_1}{T} \chi_{[\sum xn(r), \sum x(H(r) - \mu n(r)]}(\omega)
\end{aligned}
$$

Susceptibility of two measurables A, B is written as

$$\chi_{[A,B]}(\omega)$$

Identical calculation with electrostatic potential gives:

$$P_{Elec} = q_e(\phi_2 - \phi_1)\chi_{[\sum xn(r), \sum xn(r)]}(\omega)$$

Hence: the thermo-power is obtained by asking for the ratio of forces that produce the same dipole moment! (balance condition)

$$
\begin{aligned}
S &= \frac{\phi_1 - \phi_2}{T_1 - T_2} \\
&= \frac{q_e}{T} \frac{\chi_{[\sum xn(r), \sum x(H(r) - \mu n(r)]}(\omega)}{\chi_{[\sum xn(r), \sum xn(r)]}(\omega)}
\end{aligned}
$$

What about Kelvin-Onsager?

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

Large box then static limit

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

Static limit then large box

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

Large box then frequency larger than characteristic w's

For a weakly interacting diffusive metal, we can compute all three S's. Here is the result:

Density Of States

Velocity averaged over FS

Energy dependent relaxation time.

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

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

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

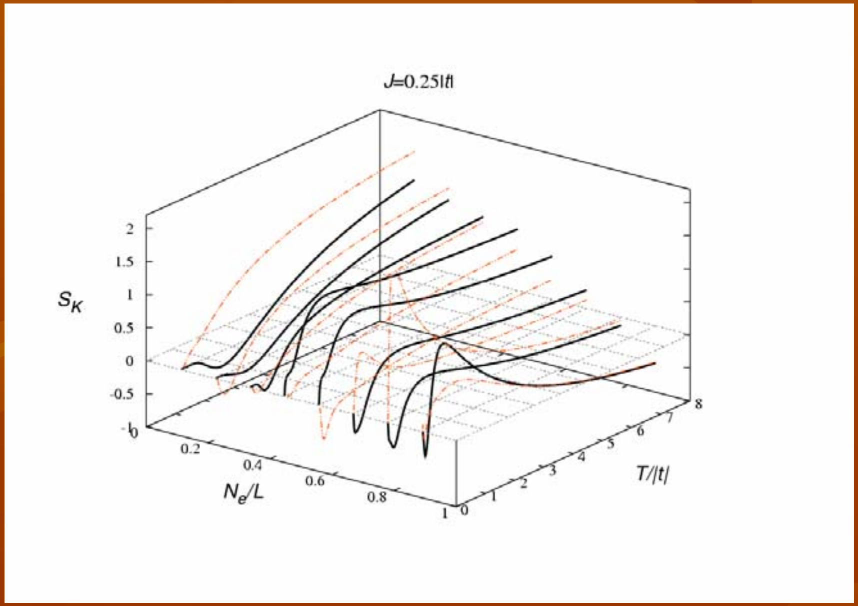
$$S^* = T\frac{\pi^2 k_B^2}{3q_e}\frac{d}{d\varepsilon}\ln[\rho(\varepsilon)\langle(v^x)^2\rangle_\varepsilon]_{\varepsilon\to\mu} \text{ High frequency formula}$$

Theorem:

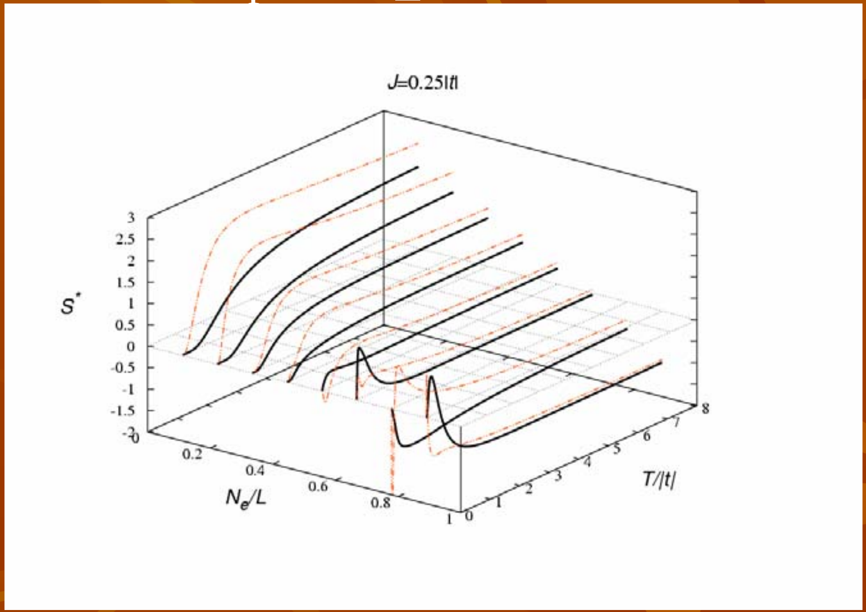
Kelvin inspired formula is the best possible thermodynamic approximation to Onsager Kubo transport formula

Some results: M Peterson SS 2008 Unpublished

Unflipped-NCO



Flipped- Fiduciary hole doped CO_2



And now for some results:

Triangular lattice t-J exact diagonalization (full spectrum)

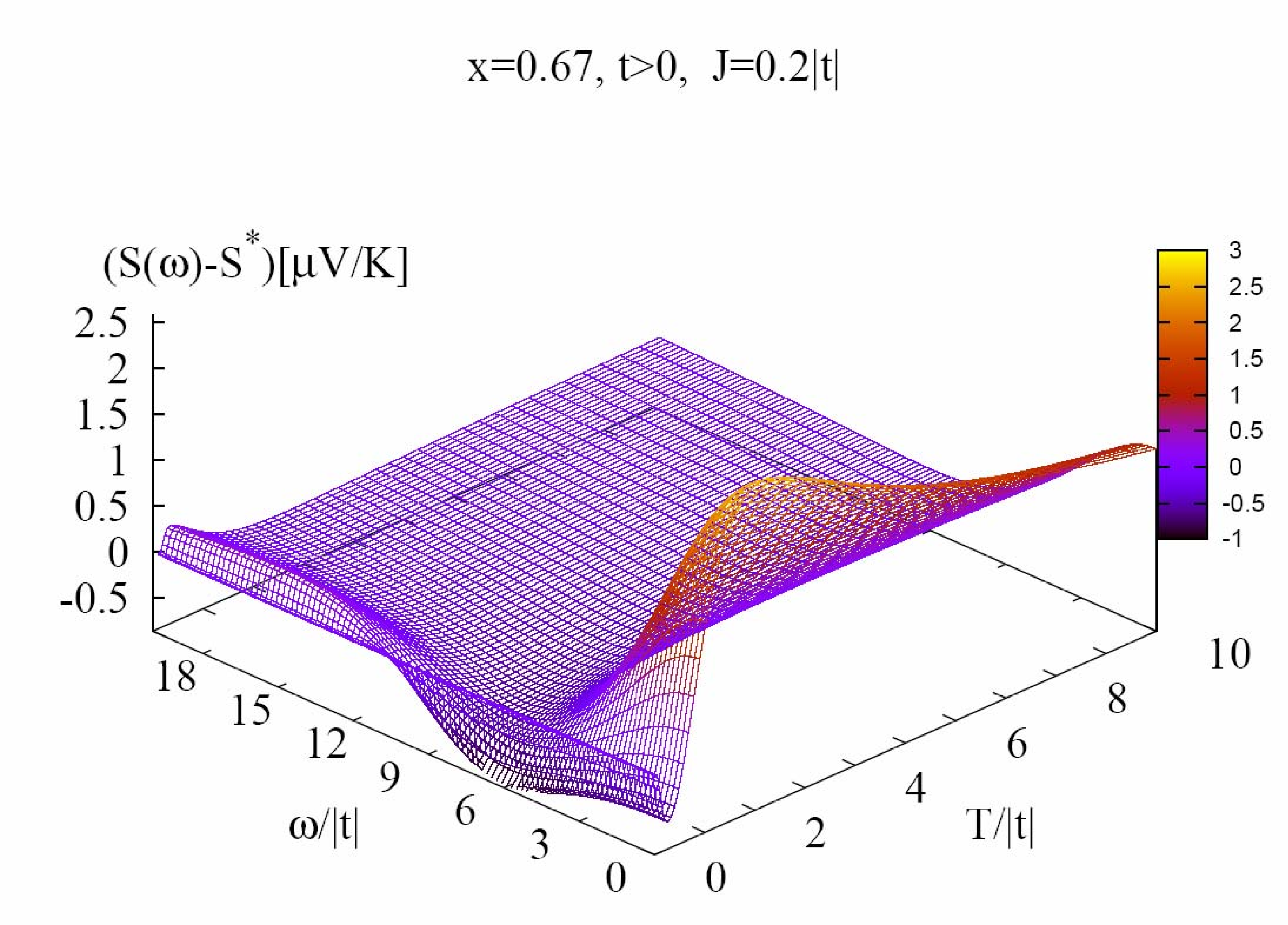
Collaboration and hard work by:-

J Haerter, M. Peterson, S. Mukerjee (UC Berkeley)

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

A numerical benchmark: Max deviation 3% anywhere !!

As good as exact!



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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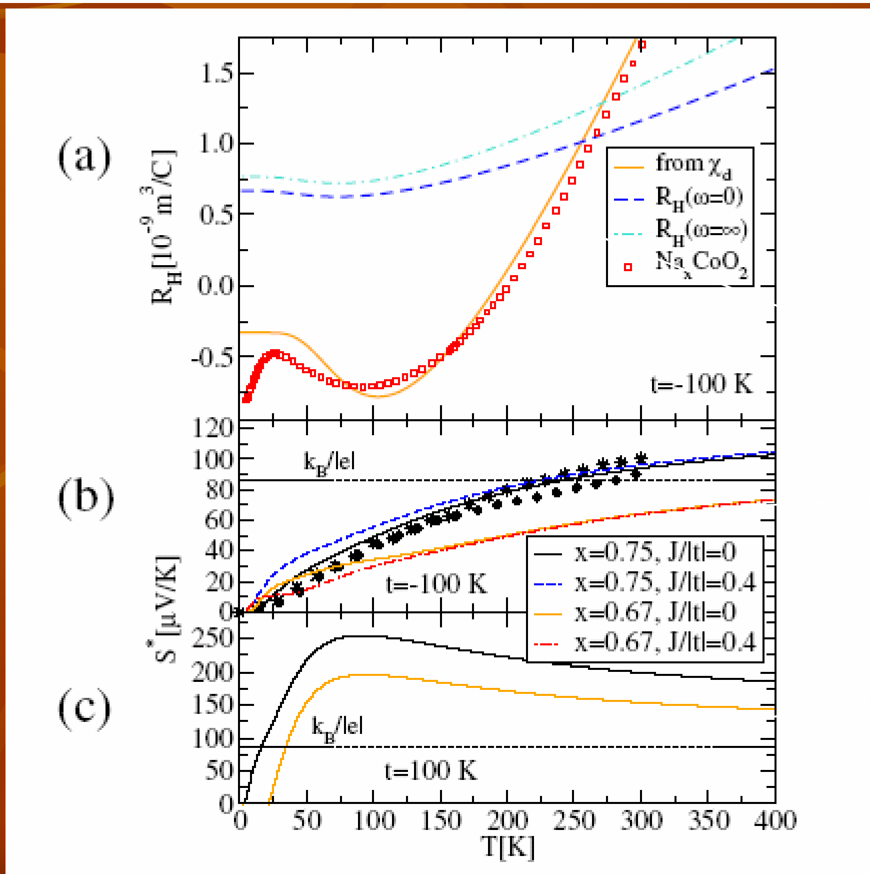
(Received 21 July 2006; published 28 November 2006)



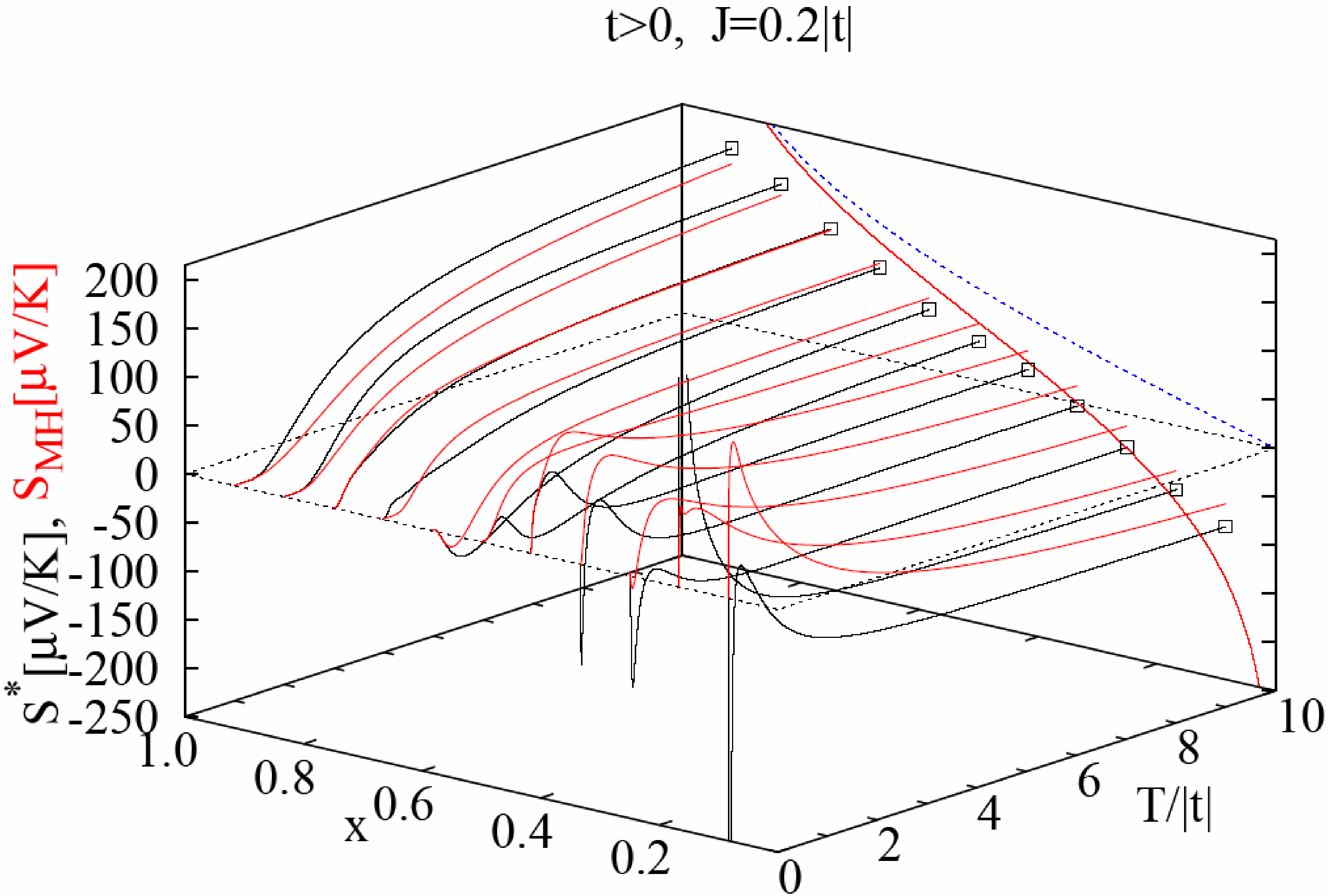
T linear Hall constant for triangular lattice predicted in 1993 by Shastry Shraiman Singh! Quantitative agreement hard to get with scale of "t"

Comparision with data on absolute scale!

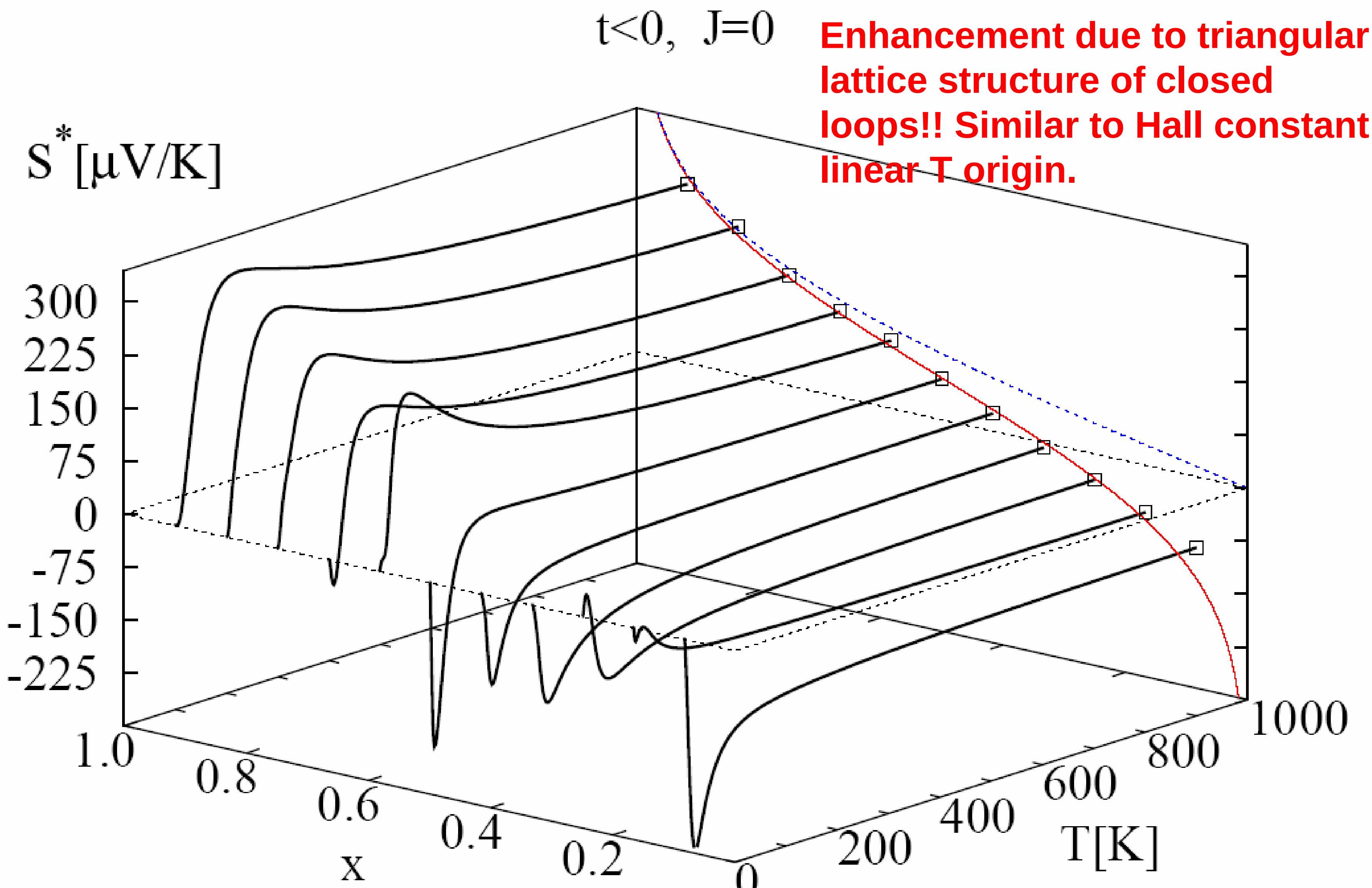
Prediction for t>0 material

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

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



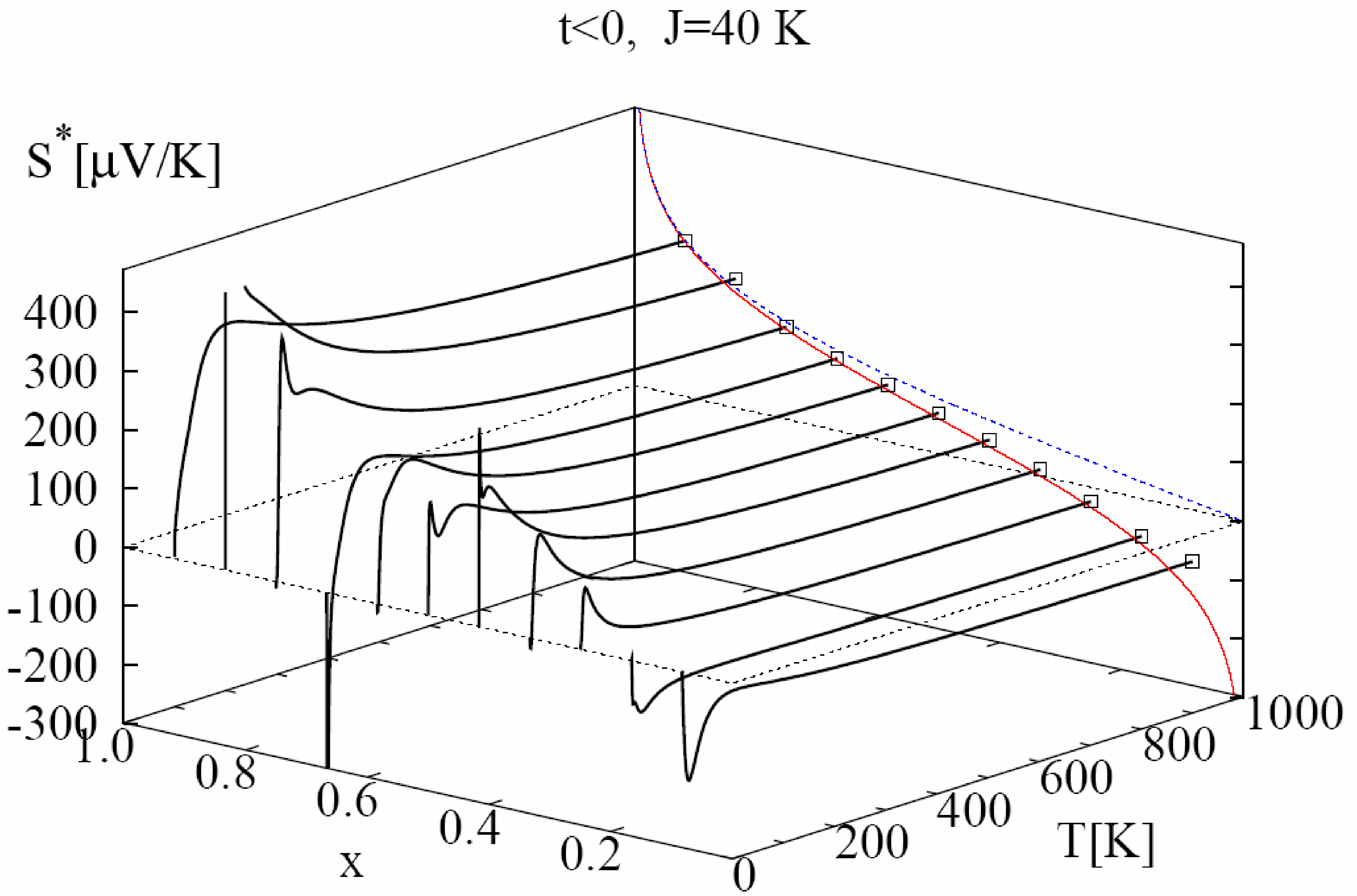
Predicted result for t<0 i.e. fiducary hole doped CoO_2 planes. Notice much larger scale of S* arising from transport part (not Mott Heikes part!!).



Enhancement due to triangular lattice structure of closed loops!! Similar to Hall constant linear T origin.

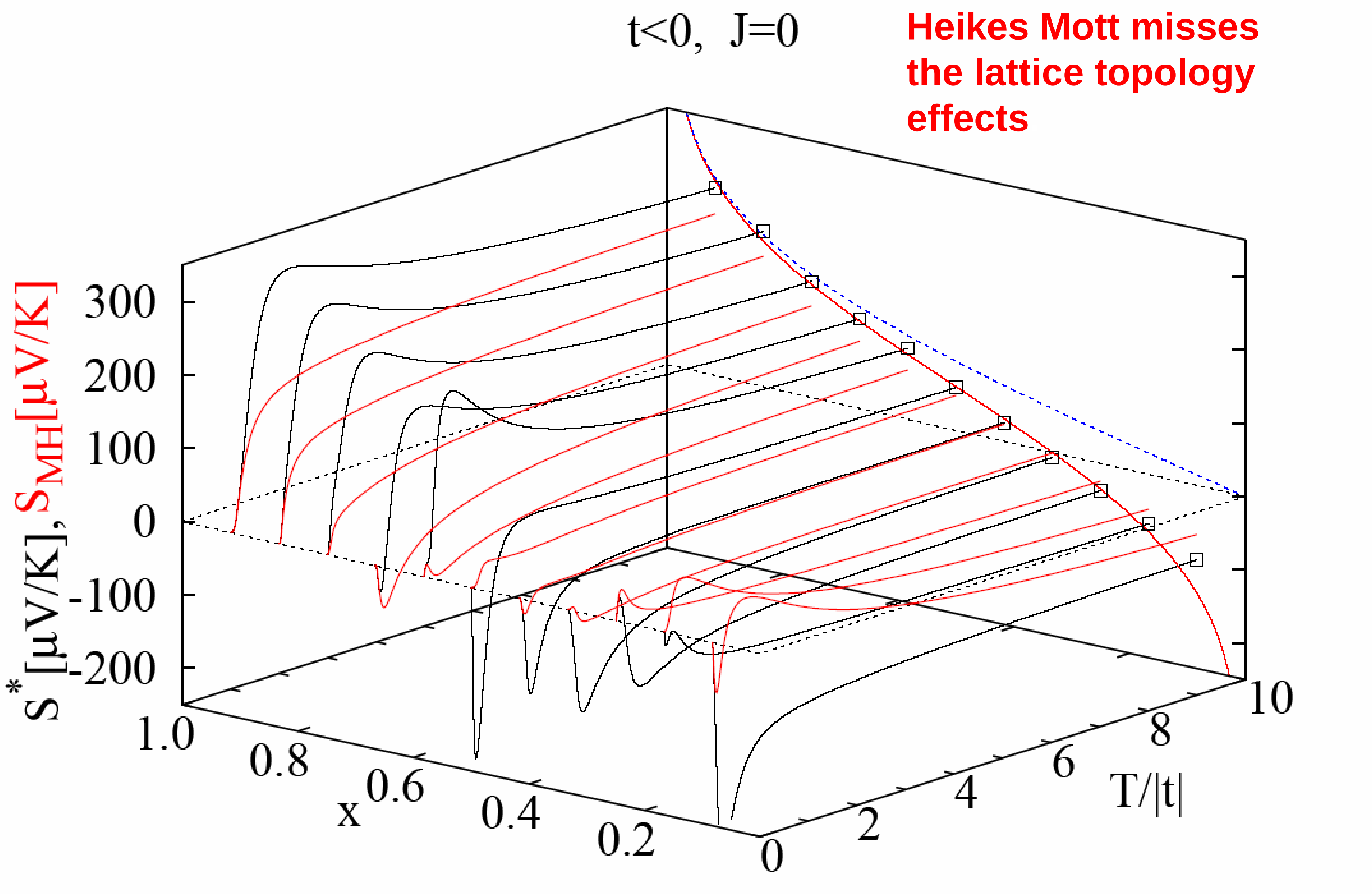
Predicted result for t<0 i.e. fiducary hole doped CoO_2 planes.

Different J higher S.



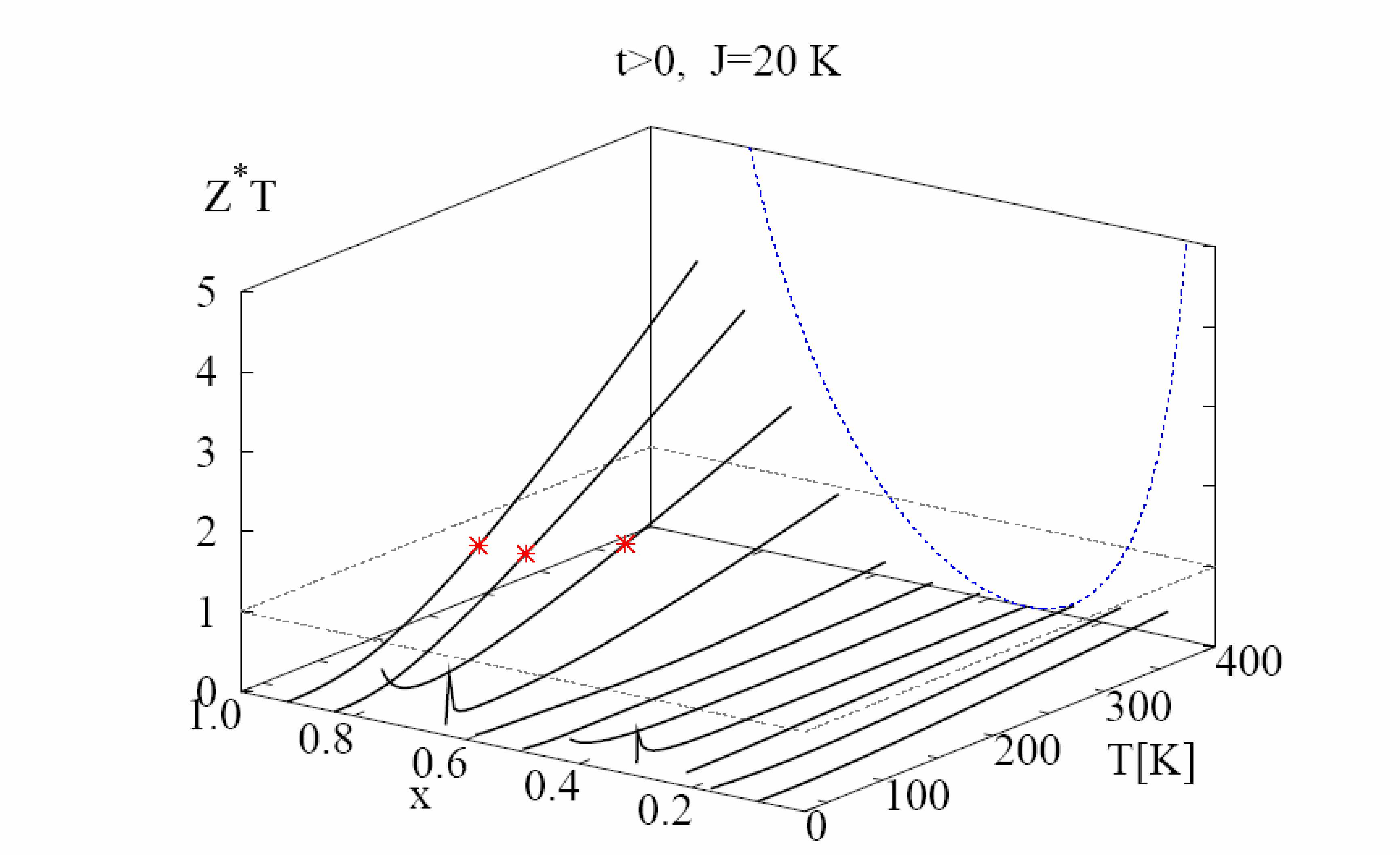
Predictions of S* and the Heikes Mott formula (red) for fiducary hole doped CoO2.

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.

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

and

$$\left[\frac{1}{\tau}+\frac{d}{dt}\right]\langle \hat{J}_x(\vec{r},t)\rangle = -\frac{c_2}{\tau}\nabla\langle K(\vec{r}t)\rangle - \frac{D_c}{\tau}\nabla\langle\rho(\vec{r}t)\rangle - \left\{\frac{\langle\tau^{xx}\rangle_0}{\Omega}\nabla\phi(\vec{r}t)+\frac{\langle\Phi^{xx}\rangle_0}{\Omega}\nabla\psi(\vec{r}t)\right\} \quad (2)$$

Hydrodynamics of energy and charge transport in a band model:

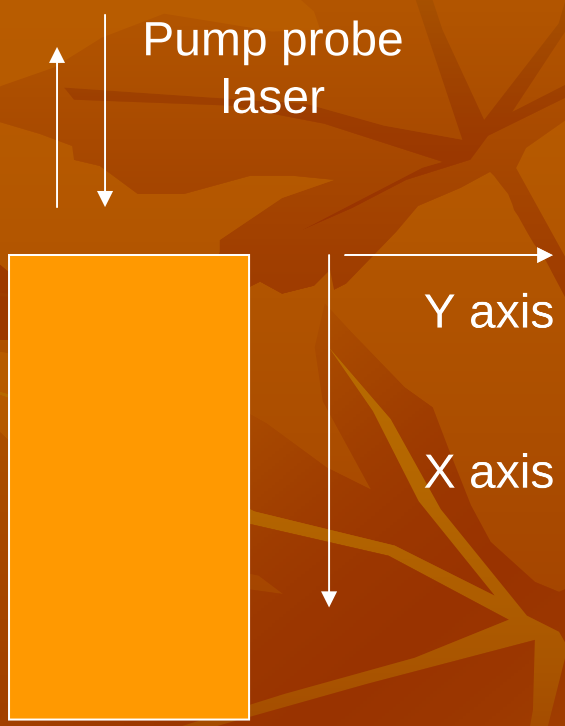
This involves the fundamental operators in a crucial way:

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

Hydrodynamics of energy and charge transport in a band model:

This involves the fundamental operators in a crucial way:

$$\left\{\frac{\partial}{\partial t}+\frac{1}{\tau_c}\right\}\delta J(r)=\frac{1}{\Omega}\langle\tau^{xx}\rangle\left[\frac{1}{q_e^2}\frac{\partial\mu}{\partial n}(-\nabla\rho)-\nabla\phi(r)\right]+\frac{1}{\Omega}\langle\Phi^{xx}\rangle\left[\frac{1}{C(T)}(-\nabla K(r))-\nabla\Psi\right]$$

$$\left\{\frac{\partial}{\partial t}+\frac{1}{\tau_E}\right\}\delta J^Q(r)=\frac{1}{\Omega}\langle\Phi^{xx}\rangle\left[\frac{1}{q_e^2}\frac{\partial\mu}{\partial n}(-\nabla\rho)-\nabla\phi(r)\right]+\frac{1}{\Omega}\langle\Theta^{xx}\rangle\left[\frac{1}{C(T)}(-\nabla K(r))-\nabla\Psi\right]$$

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

Einstein diffusion term of charge

Energy diffusion term

$$\frac{\partial K(r)}{\partial t}+\nabla J^Q(r)=p_{ext}(r)$$

Continuity

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.

Some results from the coupled charge –energy (entropy) hydrodynamics:

$$\mathrm{N}_2 = \frac{1}{A}\frac{\partial \delta K_q}{\partial P_0} \qquad \delta J_x^Q = L_{22}(iq\psi_q) + L_{21}(iq\phi_q) + M_2\frac{P_0}{L}$$

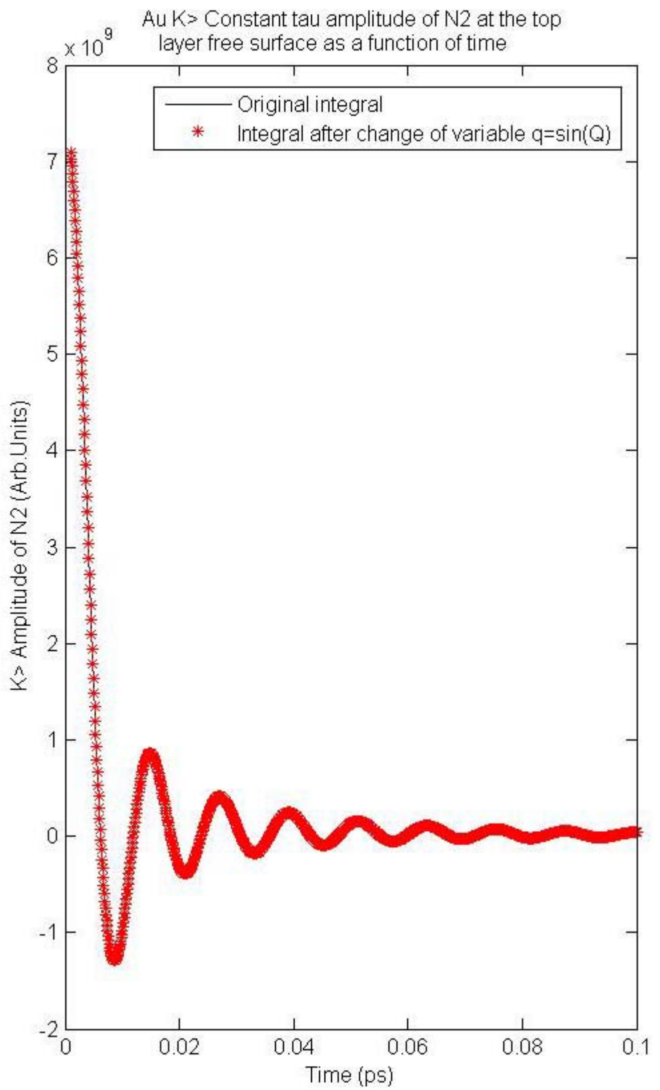
$$\Delta = (1 - i\omega\tau + i\frac{D_Q q^2}{\omega})(1 - i\omega\tau + i\frac{D_c q^2}{\omega}) + \xi D_c D_Q \frac{q^4}{\omega^2},$$

$$\xi = \frac{\langle \Phi^{xx}\rangle_0^2}{\langle \Theta^{xx}\rangle_0 \langle \tau^{xx}\rangle_0} = \frac{Z^*T}{Z^*T+1}$$

$$\mathrm{L}_{22} = \frac{1}{\Delta}\frac{\tau\langle\Theta^{xx}\rangle_0}{\Omega}\left[1 - i\omega\tau + i(1-\xi)\ D_c\ \frac{q^2}{\omega}\right]$$

$$\mathrm{M}_2 = -\frac{1}{\Delta}\ D_Q\ \frac{q}{\omega}\left[1 - i\omega\tau + i(1-\xi)\ D_c\ \frac{q^2}{\omega}\right].$$

$$\mathrm{N}_2 = \frac{i}{\omega} - \frac{q}{\omega}M_2$$



$$\begin{cases} \delta K(t,0) = \delta K^{<}(t,0) + \delta K^{>}(t,0) \\ \delta K^{<}(t,0) = \sqrt{\dfrac{2}{\pi}} P_0 \displaystyle\int_0^{q_0} e^{-\frac{t}{2\tau_q}} \left\{ ch\left[\dfrac{R_q t}{2\tau_q}\right] + \dfrac{sh\left[\dfrac{R_q t}{2\tau_q}\right]}{R_q} \right\} dq \\ \delta K^{>}(t,0) = \sqrt{\dfrac{2}{\pi}} P_0 \displaystyle\int_{q_0}^{q_m} e^{-\frac{t}{2\tau_q}} \left\{ \cos\left[\dfrac{\overline{R}_q t}{2\tau_q}\right] + \dfrac{\sin\left[\dfrac{\overline{R}_q t}{2\tau_q}\right]}{\overline{R}_q} \right\} dq \\ q_m = \dfrac{\pi}{a};\ q_0 = \dfrac{1}{2\sqrt{D_Q \tau_0}};\ R_q = \sqrt{1 - 4 D_Q \tau_0 q^2};\ \text{and } \overline{R}_q = \sqrt{4 D_Q \tau_0 q^2 - 1} \end{cases}$$

Conclusions

- New insights into thermal transport and thermoelectric effects- predictions for new material design.
- Novel framework with new objects
- Simple minded hydrodynamics gives a usef picture of the transport phenomena, as an alternative to usual transport Boltzmann eqns.