Transport in strongly correlated systems

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Lecture 4: Transport at finite and infinite frequency

- Revisiting the Kubo formula
- Sum rules for conductivities
- Infinite frequency calculation of transport coefficients

Transport at finite frequency ω

Transport coefficients have interesting sum rules

Infinite frequency limit is particularly interesting

Infinite frequency calculations can be useful at zero frequency

$$\tilde{\sigma}_{xx}\left(k_x, \omega_c\right) = \frac{1}{\hbar k_x V} \int_{-\infty}^{0} dt \; e^{-i\omega_c t} \left\langle \left[\hat{J}_x(k_x, t=0), \hat{n}(-k_x, t) \right] \right\rangle$$

$$\omega_c = \omega + i0^+$$

$$\begin{aligned} \tilde{\sigma}_{xx}\left(k_x, \omega_c\right) \quad = \quad & -\frac{i}{\hbar \omega_c k_x V} \left(\left\langle \left[\hat{J}_x(k_x), \hat{n}(-k_x) \right] \right\rangle \right) \\ & + \frac{1}{\hbar k_x V} \int_{-\infty}^{0} dt \; e^{-i\omega_c t} \left\langle \left[\hat{J}_x(k_x), \left[\hat{n}(-k_x, t), \hat{H} \right] \right] \right\rangle \end{aligned}$$

$$\hat{A}(k_x) = \hat{A}(k_x, t=0)$$

$$\tilde{\sigma}_{xx}(\omega_c) = \frac{i}{\hbar\omega_c V}\left[\langle\hat{\tau}_{xx}\rangle - i\int_0^\infty dt\; e^{i\omega_c t}\left\langle\left[\hat{J}_x(k_x), \hat{J}_x(0)\right]\right\rangle\right]$$

in the limit $k_x \to 0$

$$\hat{\tau}_{xx} = \frac{d}{dk_x}\left[\hat{J}_x(k_x), \hat{n}(-k_x)\right]\Big|_{k_x\to 0}$$

$$\tilde{\sigma}_{xx}(\omega_c) = \frac{i}{\hbar\omega_c} D_c + \frac{1}{V}\int_0^\infty dt\; e^{i\omega_c t}\int_0^\beta d\beta' \left\langle \hat{J}_x(-t - i\beta')\hat{J}_x(0)\right\rangle$$

$$D_c = \frac{1}{V}\left[\langle\hat{\tau}_{xx}\rangle - \hbar\sum_{n,m}\frac{p_n - p_m}{E_n - E_m}\left|\langle n|\hat{J}_x|m\rangle\right|^2\right]$$

$$p_n = \frac{e^{-\beta E_n}}{Z}$$

Meissner stiffness

$$\sigma_{xx}(\omega) = \pi \bar{D}_c \delta(\hbar\omega) + \frac{\pi}{V} \left(\frac{1 - e^{-\beta\hbar\omega}}{\omega} \right) \sum_{E_n \neq E_m} p_n \left| \langle n | \hat{J}_x | m \rangle \right|^2 \delta \left(E_m - E_n - \hbar\omega \right)$$

$$\sigma_{xx} = \Re e \left[\tilde{\sigma}_{xx} \right]$$

$$\bar{D}_c = \frac{1}{V} \left[\langle \hat{\tau}_{xx} \rangle - \hbar \sum_{E_n \neq E_m} \frac{p_n - p_m}{E_n - E_m} \left| \langle n | \hat{J}_x | m \rangle \right|^2 \right]$$

Charge stiffness or Drude weight

$$D_c = \frac{1}{V} \left[\langle \hat{\tau}_{xx} \rangle - \hbar \sum_{n,m} \frac{p_n - p_m}{E_n - E_m} \left| \langle n | \hat{J}_x | m \rangle \right|^2 \right]$$

$$\bar{D}_c - D_c = \pi \frac{\beta\hbar}{V} \sum_{E_n = E_m} p_n \left| \langle n | \hat{J}_x | m \rangle \right|^2$$

When does

$$\sigma_{xx}(\omega) = \pi \bar{D}_c \delta(\hbar\omega) + \frac{\pi}{V} \left(\frac{1 - e^{-\beta\hbar\omega}}{\omega} \right) \sum_{E_n \neq E_m} p_n \left| \langle n | \hat{J}_x | m \rangle \right|^2 \delta\left(E_m - E_n - \hbar\omega\right)$$

reduce to

$$\sigma_{xx}(\omega) = \frac{\pi\left(1 - e^{-\beta\hbar\omega}\right)}{\omega V} \sum_{n,m} p_n \left| \langle n | \hat{J}_x | m \rangle \right|^2 \delta\left(E_m - E_n - \hbar\omega\right)?$$

(Expression from lecture # 1)

Answer: When $\bar{D}_c = \pi \frac{\beta\hbar}{V} \sum_{E_n = E_m} p_n \left| \langle n | \hat{J}_x | m \rangle \right|^2$

or when the Meissner stiffness $D_c = 0$.

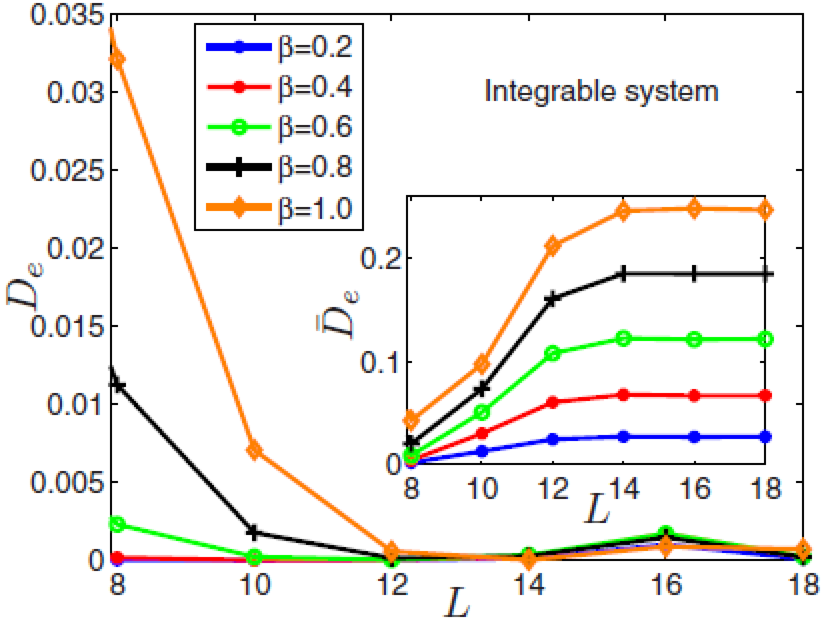
The usual Kubo formula works fine except for systems with broken gauge symmtery.

$$D_c = \frac{\hbar e^2}{m}\rho_s,\ \rho_s = \left.\frac{\partial^2 F(\phi)}{\partial \phi^2}\right|_{\phi\to 0},\ \text{Superfluid stiffness}$$

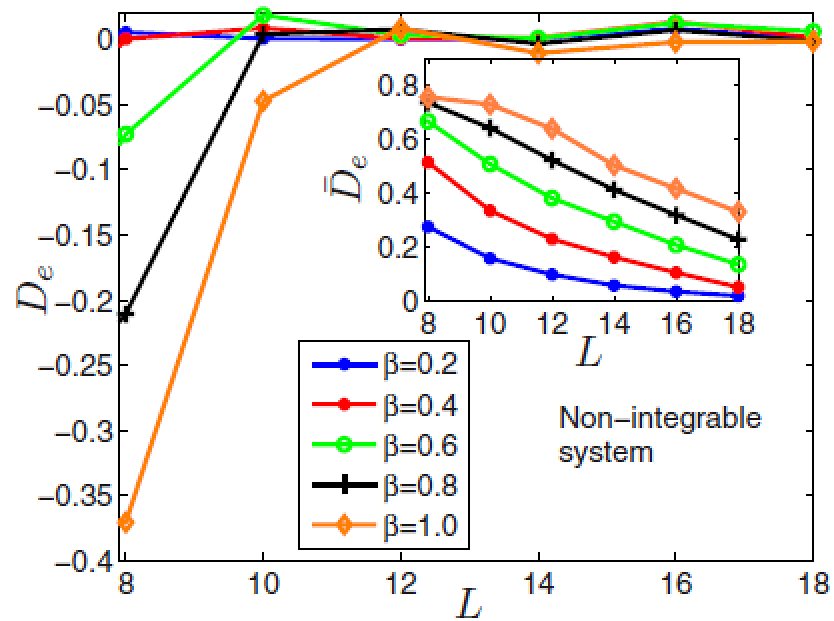
If $D_c \neq 0$, infinite conductivity at $\omega = 0$ but not necessarily a superconductor since D_c can be zero.

At finite temperature this is a very special situation and can occur for integrable systems

Exact diagonalization on 1D lattices



spinless fermions with only nearest neighbour hopping and nearest neighbour interactions



next nearest neighbour hopping breaks integrability

[S. Mukerjee and B. S. Shastry, *Phys. Rev. B* **77** 245131 (2008)]

Optical sum rule

$$\int_0^\infty \sigma_{xx}(\omega) d\omega = \frac{\pi}{2\hbar V} \langle \hat{\tau}_{xx} \rangle$$

What is $\hat{\tau}_{xx}$?

For $\hat{H} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + V\left(\{n_{i\sigma}\}\right)$

$$\hat{\tau}_{xx} = \frac{e^2}{\hbar} \sum_{\mathbf{k}\sigma} \frac{d^2 \epsilon_{\mathbf{k}}}{dk_x^2} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$$

With only nearest neighbour interactions $\hat{\tau}_{xx}$ is the KE operator

In general

$$\tilde{L}^{\alpha\beta}_{xx}(\omega_c) = \frac{i}{\hbar\omega_c} D^{\alpha\beta} + \frac{1}{V}\int_0^\infty dt\; e^{i\omega_c t}\int_0^\beta d\beta' \left\langle \hat{J}^\beta_x(-t-i\beta')\hat{J}^\alpha_x(0)\right\rangle$$

$$D^{\alpha\beta} = \frac{1}{V}\left[\left\langle \hat{W}^{\alpha\beta}_{xx}\right\rangle - \hbar\sum_{n,m}\frac{p_n - p_m}{E_n - E_m}\langle n|\hat{J}^\alpha_x|m\rangle\langle m|\hat{J}^\beta_x|n\rangle\right]$$

$$\hat{W}^{\alpha\beta}_{xx} = \frac{d}{dk_x}\left[\hat{J}^\alpha_x(k_x), \hat{\rho}^\beta(-k_x)\right]\Big|_{k_x\to 0}$$

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

	Charge	Heat
Current	$\hat{\mathbf{J}}$	$\hat{\mathbf{J}}^Q$
Operator ($\hat{\rho}$)	$\hat{n}$	$\hat{H} - \mu\hat{n}$

$$\hat{K} = \hat{H} - \mu\hat{n}$$

$$\hat{\Phi}_{xx} = \frac{d}{dk_x}\left[\hat{J}_x(k_x), \hat{K}(-k_x)\right]\bigg|_{k_x \to 0}$$

$$\hat{\Theta}_{xx} = \frac{d}{dk_x}\left[\hat{J}^Q_x(k_x), \hat{K}(-k_x)\right]\bigg|_{k_x \to 0}$$

$$\boxed{\int_0^\infty Q_{xx}(\omega)d\omega = \frac{\pi}{2T\hbar V}\left\langle \hat{\Theta}_{xx} \right\rangle}$$

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

$\hat{\tau}_{xx}$, $\hat{\Phi}_{xx}$ and $\hat{\Theta}_{xx}$ are useful operators

$$\tilde{\sigma}_{xx}\left(\omega_c\right) = \frac{i}{\hbar\omega_c V}\left[\langle\hat{\tau}_{xx}\rangle + \frac{1}{\omega_c^2}\left\langle\left[\left[\hat{J}_x, \hat{H}\right], \hat{H}\right]\right\rangle + O\left(\frac{1}{\omega_c^4}\right)\right]$$

As $\omega \rightarrow \infty$

$$\tilde{\sigma}_{xx}\left(\omega_c\right) \sim \frac{i}{\hbar\omega_c V}\langle\hat{\tau}_{xx}\rangle$$

Similarly

$$\tilde{\alpha}_{xx}\left(\omega_c\right) \sim \frac{i}{\hbar T\omega_c V}\langle\hat{\Phi}_{xx}\rangle$$

$$\tilde{Q}_{xx}\left(\omega_c\right) \sim \frac{i}{\hbar T\omega_c V}\langle\hat{\Theta}_{xx}\rangle$$

$$S(\omega_c) = \alpha_{xx}(\omega_c)/\sigma_{xx}(\omega_c)$$

$$S(\omega_c) = \frac{\left\langle \hat{\Phi}_{xx} \right\rangle}{T \langle \hat{\tau}_{xx} \rangle} = S^* \qquad \text{as } \omega \to \infty$$

$$L(\omega_c) = \kappa(\omega_c)/T\sigma(\omega_c)$$

$$L(\omega_c) = \frac{1}{T^2} \left(\frac{\left\langle \hat{\Theta}_{xx} \right\rangle}{\langle \hat{\tau}_{xx} \rangle} - \frac{\left\langle \hat{\Phi}_{xx} \right\rangle^2}{\langle \hat{\tau}_{xx} \rangle^2} \right) = L^* \qquad \text{as } \omega \to \infty$$

$$Z^* T = \left(S^*\right)^2 / L^*$$

For certain models

$$S^* = S(\omega = 0),\ L^* = L(\omega = 0) \text{ and } Z^*T = Z(\omega = 0)T$$

The zero frequency values require calculations of the appropriate conductivities

This can be quite difficult for strongly correlated systems

The infinite frequency values require calculating $\langle \hat{\tau}_{xx} \rangle$, $\left\langle \hat{\Phi}_{xx} \right\rangle$ and $\left\langle \hat{\Theta}_{xx} \right\rangle$ which can be more straightforward analytically and numerically

Inspiration: simple Drude model

Any diagonal conductivity $A_{xx}(\omega) \sim \frac{1}{\omega + i/\tau}$

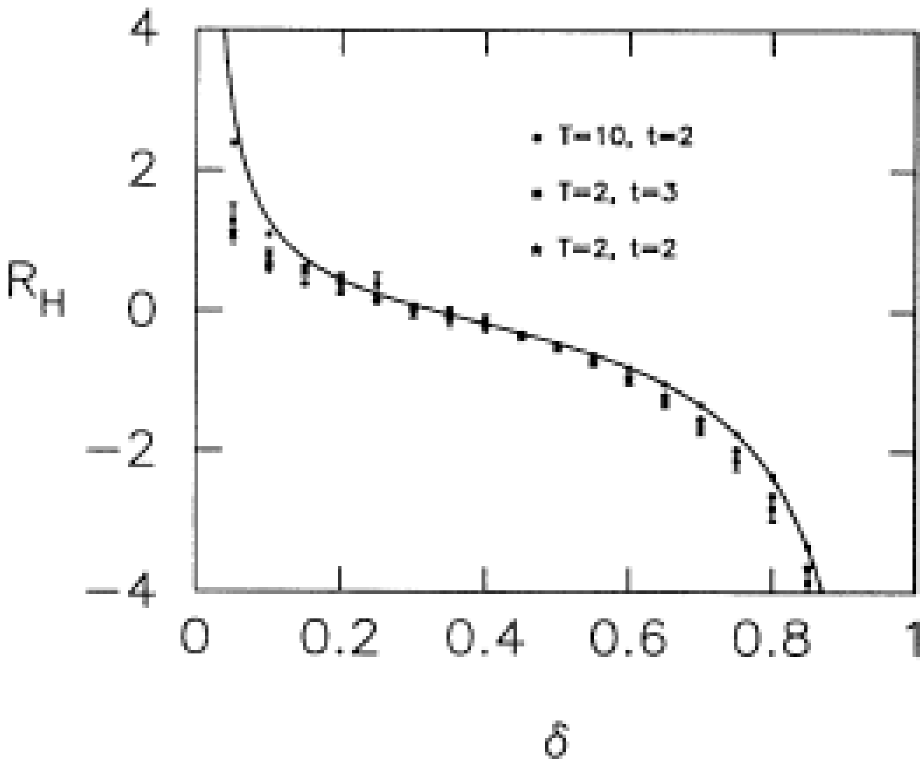
Models where infinite and zero frequency ratios are different: ones with energy dependent scattering rates

$\hat{\tau}_{xx}$, $\hat{\Phi}_{xx}$ and $\hat{\Theta}_{xx}$ can be computed for several models

- Electron gas
- Hubbard model
- Disordered electron systems
- Anharmonic lattice

First applied to the calculation of Hall constant

(Hall resistance also frequency independent in Drude theory)



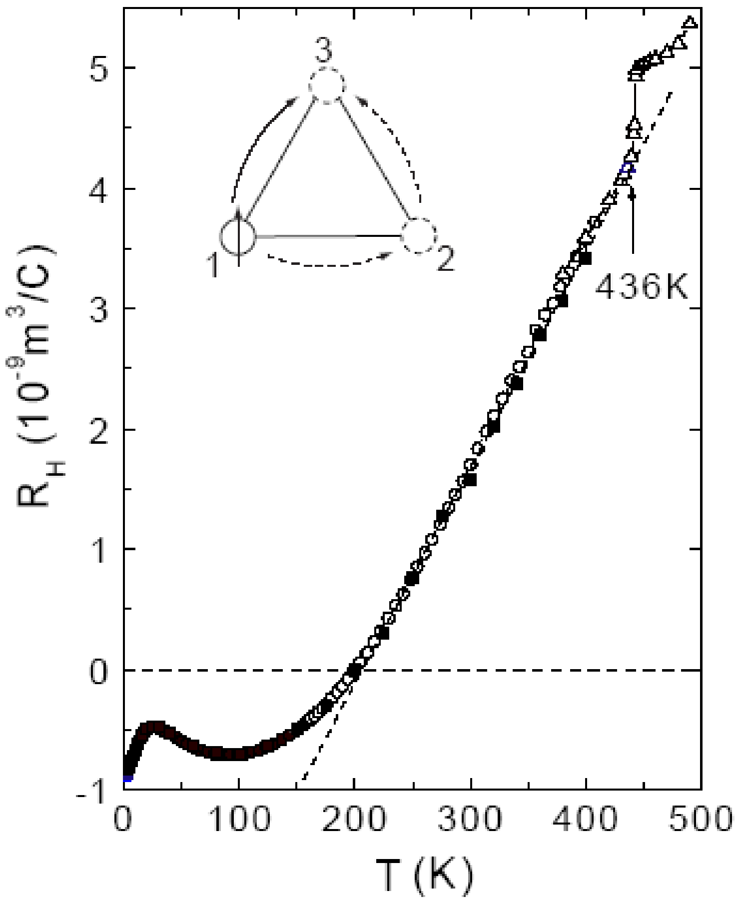
Hall constant changes sign at $\delta \sim 0.3$

Seen in LSCO data

[H. Takagi *et. al*, *Phys. Rev. B* **40** 2254 (1989)]

[B. S. Shastry, B. I. Shraiman and R. R. Singh, *Phys. Rev. Lett.* **70** 2004 (1993)]

Another prediction: Linear in T Hall resistance on a triangular lattice



Na_xCoO_2

N. P. Ong's group (2003)

[Y. Wang *et. al*, cond-mat/0305455 (2003)]

For the free electron gas

$$\langle \hat{\tau}_{xx} \rangle = \frac{2e^2}{V} \sum_{\mathbf{p}} n_{\mathbf{p}} \frac{d}{dp_x} v_x(\mathbf{p})$$

$$\langle \hat{\Phi}_{xx} \rangle = \frac{2e}{V} \sum_{\mathbf{p}} n_{\mathbf{p}} \frac{d}{dp_x} \left[v_x(\mathbf{p}) \left(\epsilon_{\mathbf{p}} - \mu \right) \right]$$

$$\langle \hat{\Theta}_{xx} \rangle = \frac{2}{V} \sum_{\mathbf{p}} n_{\mathbf{p}} \frac{d}{dp_x} \left[v_x(\mathbf{p}) \left(\epsilon_{\mathbf{p}} - \mu \right)^2 \right]$$

For $T \to 0$

$$S^* = \frac{\pi^2 k_B^2 T}{3e^2} \; \frac{d}{d\epsilon} \log \left[\rho(\epsilon) \left\langle v_x(\epsilon)^2 \right\rangle\right]\Big|_{\epsilon=\epsilon_F}$$

Regular Mott formula

$$L^* = \frac{\pi^2 k_B^2}{3e^2}$$

Wiedemann-Franz law

Agrees with zero frequency values

Hubbard model

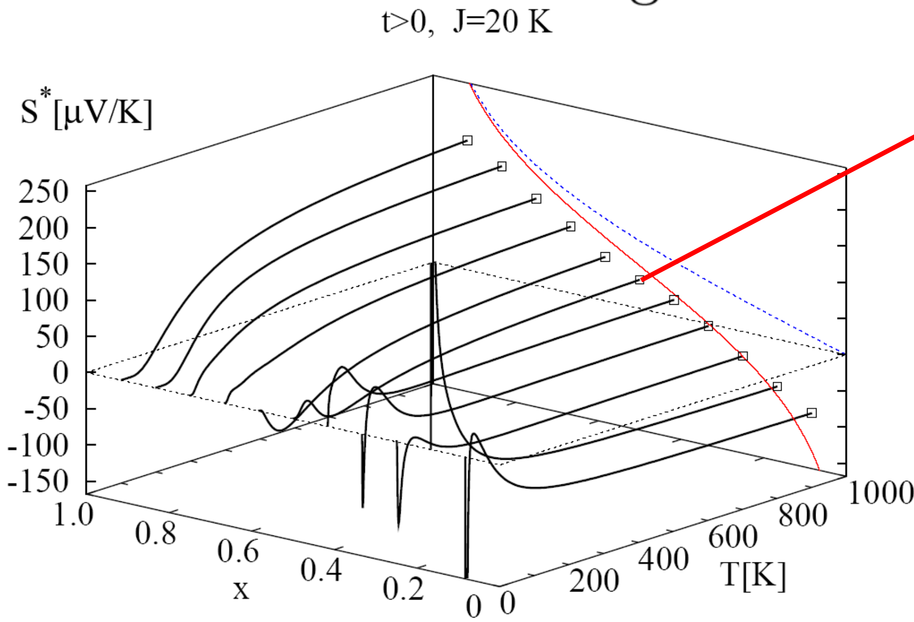
$$\hat{H} = \sum_{\mathbf{p}\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

$$\hat{\tau}_{xx} = \frac{e^2}{\hbar} \sum_{\mathbf{k}\sigma} \frac{d^2 \epsilon_{\mathbf{k}}}{dk_x^2} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$$

$$\begin{aligned} \hat{\Phi}_{xx} &= \frac{e}{\hbar} \sum_{\mathbf{k}\sigma} \frac{\partial}{\partial k_x} \left[v_x(\mathbf{k}) \left(\epsilon_{\mathbf{k}} - \mu \right) \right] c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \\ &+ \frac{eU}{2V\hbar^2} \sum_{\mathbf{k},\kappa,\mathbf{q},\sigma,\sigma'} \frac{\partial^2}{\partial k_x^2} \left\{ \epsilon_{\mathbf{k}} + \epsilon_{\mathbf{k}+\mathbf{q}} \right\} c^{\dagger}_{\kappa+\mathbf{q}\sigma} c_{\kappa\sigma} c^{\dagger}_{\mathbf{k}-\mathbf{q}\sigma'} c_{\mathbf{k}\sigma'} \end{aligned}$$

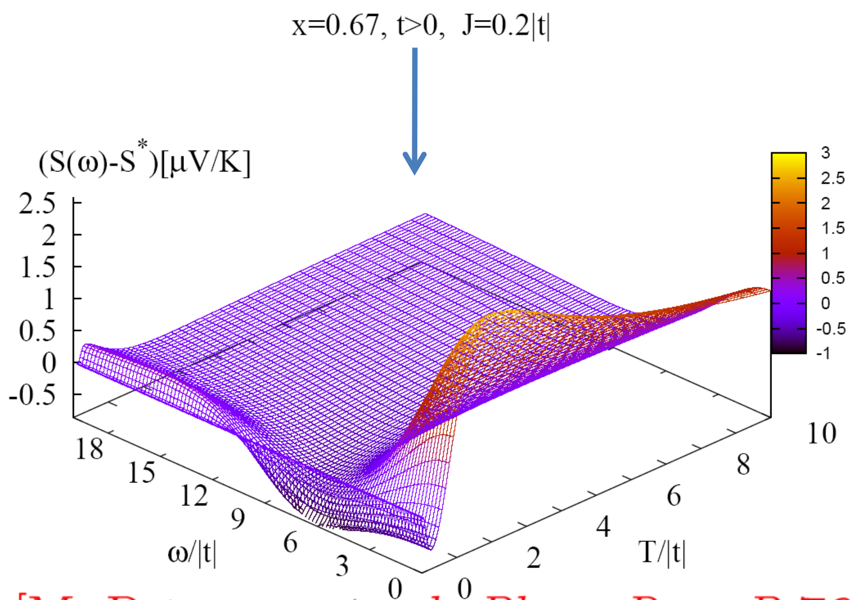
$\hat{\Theta}_{xx}$ fairly complicated looking

Numerical exact diagonalization for Na_xCoO_2



Heikes limit

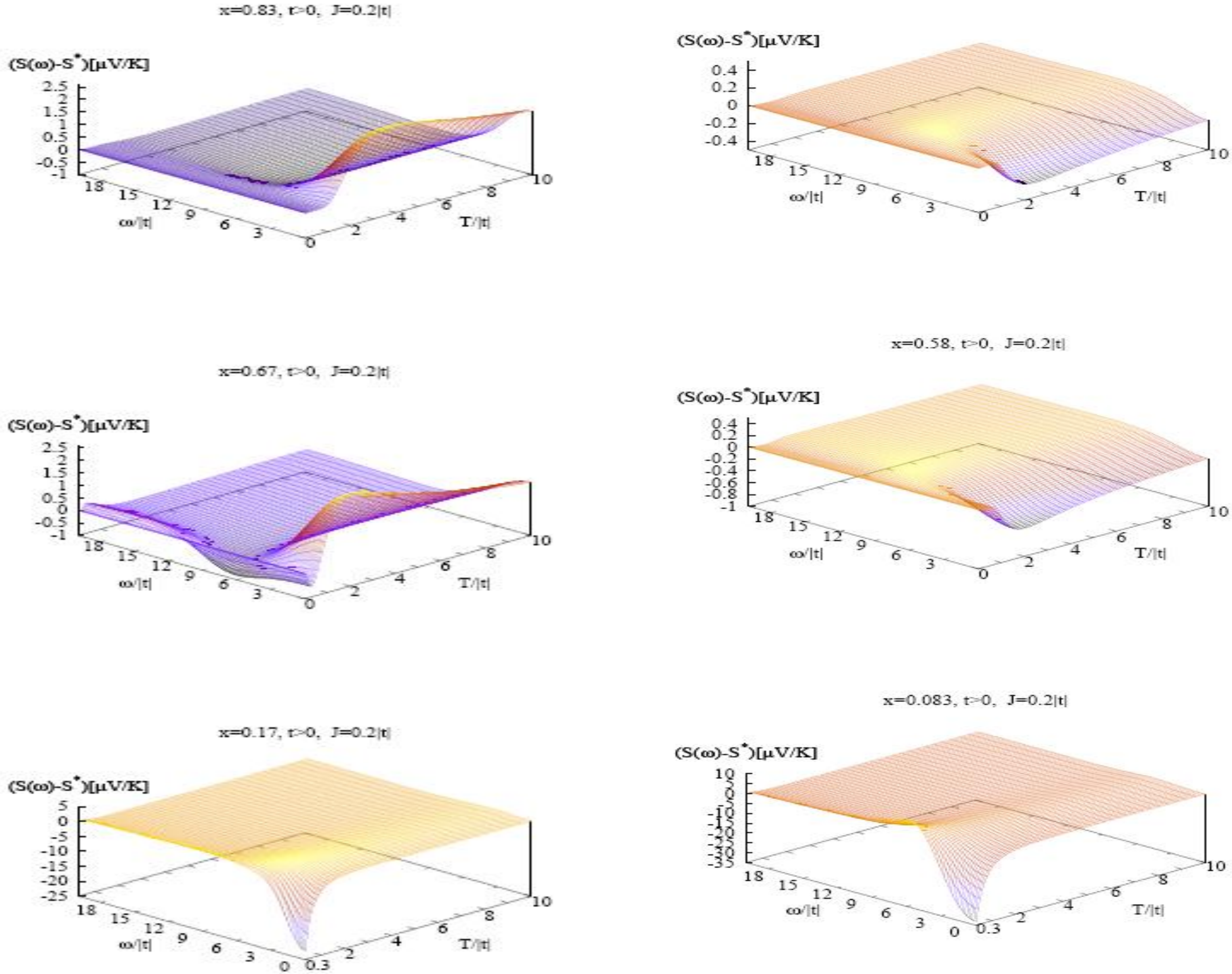
$$J = \frac{4t^2}{U}$$



Max. deviation 3 %

[M. Peterson *et. al.* *Phys. Rev. B* **76** 165118 (2007)]

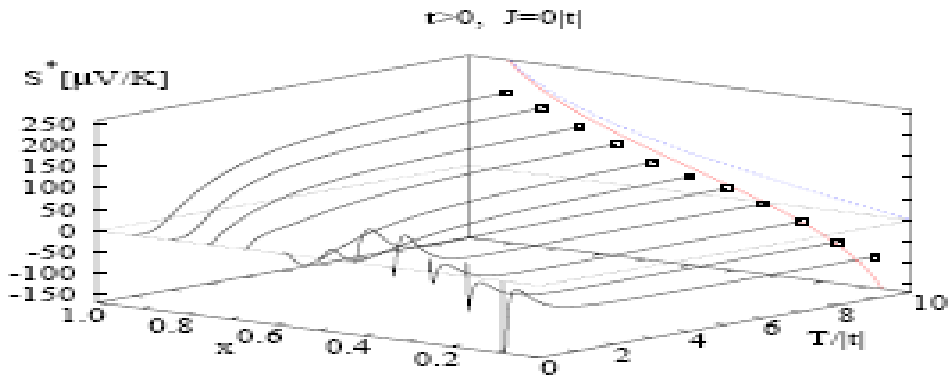
2D *t-J* model

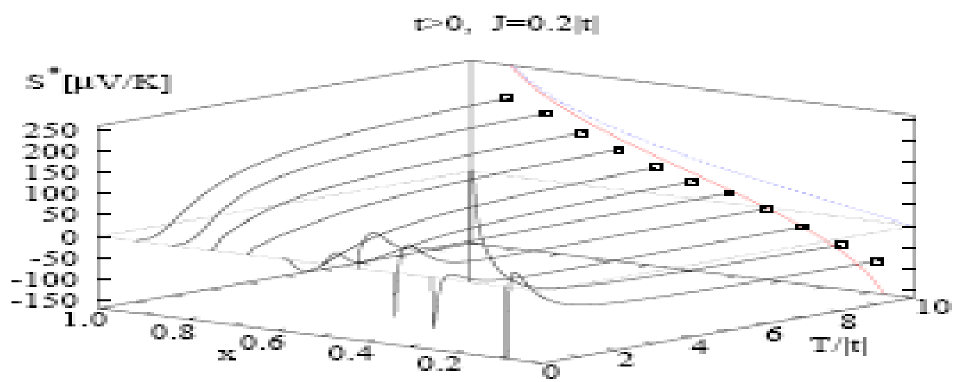


Max variation about 5%

[M. Peterson *et. al.* *Phys. Rev. B* **76** 165118 (2007)]

2D *t-J* model

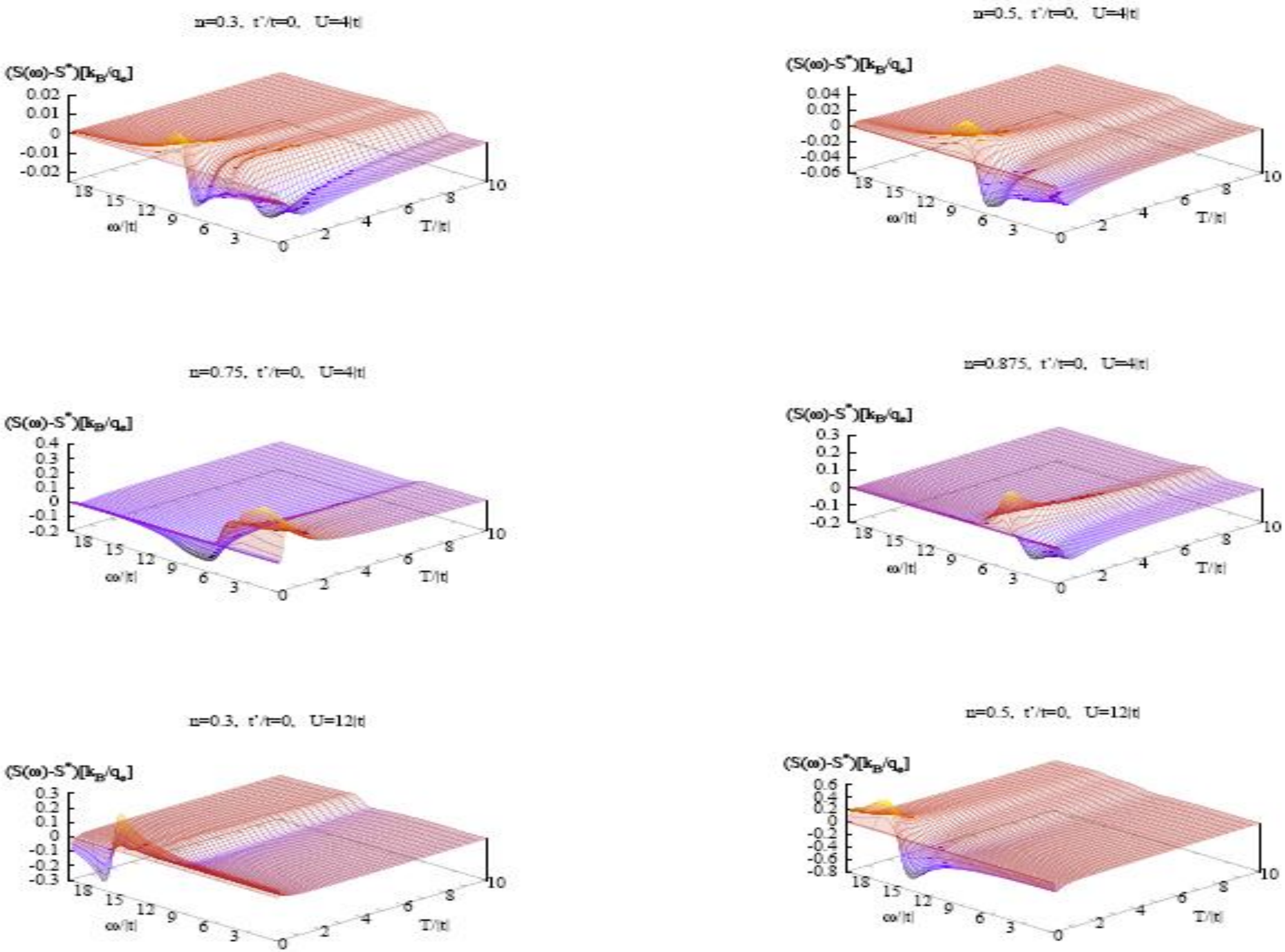




Works fairly well except for $T \ll |t|$

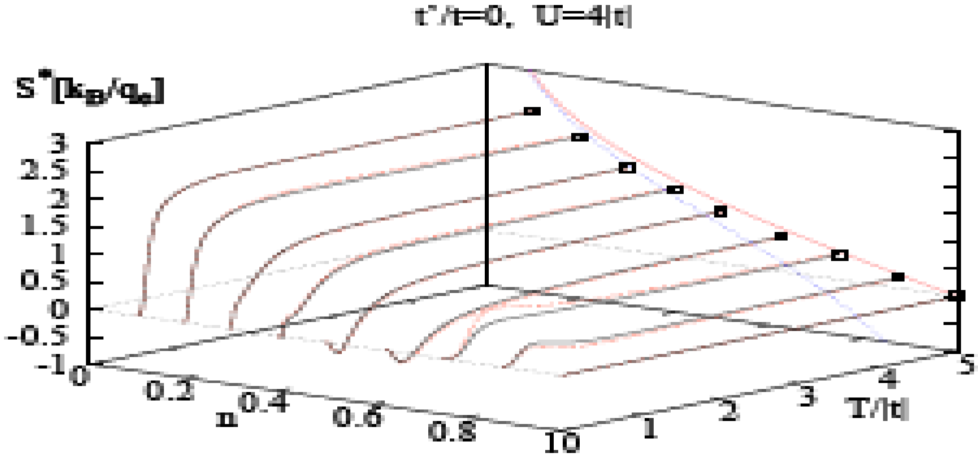
[M. Peterson *et. al. Phys. Rev. B* **76** 165118 (2008)]

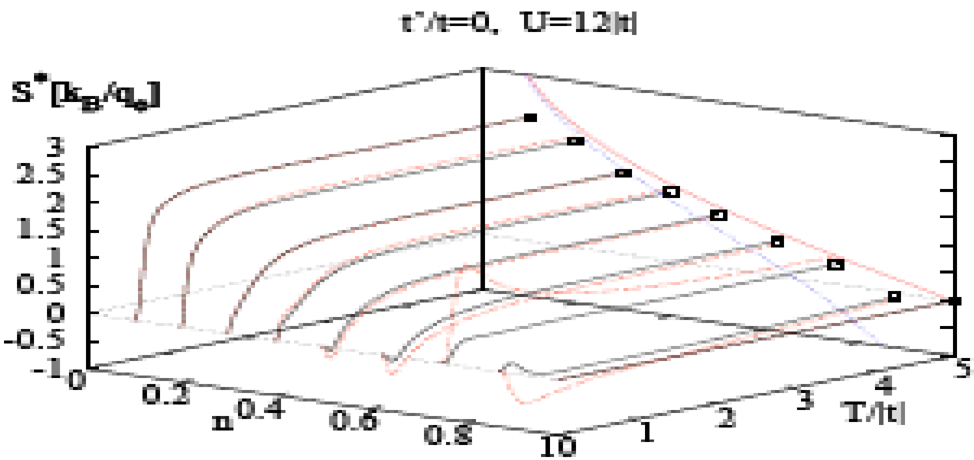
1D Hubbard model



Max variation about 5%   [M. Peterson *et. al. Phys. Rev. B* **76** 125110 (2007)]

1D Hubbard model





[M. Peterson *et. al. Phys. Rev. B* **76** 125110 (2007)]

For the $U \to \infty$ case ($t - J$ model) at high temperature

$$S^* = -\frac{\mu}{eT} + \frac{e\Delta}{T \langle \hat{\tau}_{xx} \rangle}$$

first correction to the Heikes formula

$$\Delta = -\frac{1}{2} \sum_{\vec{\eta},\vec{\eta}',\vec{r}} (\eta_x + \eta'_x)^2 \, t(\vec{\eta}) t(\vec{\eta}') Y_{\sigma,\sigma'}(\vec{r} + \vec{\eta}) \left\langle c^{\dagger}_{\vec{r}+\vec{\eta}+\vec{\eta}'\sigma} c_{\vec{r}\sigma} \right\rangle$$

$t(\vec{\eta})$ hopping matrix element to a site $\vec{\eta}$ away

$$Y_{\sigma,\sigma'}(\vec{r}) = \delta_{\sigma\sigma'} \left(1 - n_{\vec{r}\sigma}\right) + \left(1 - \delta_{\sigma\sigma'}\right) P_G c^{\dagger}_{\vec{r}\sigma} c_{\vec{r}\sigma'} P_G$$

On a triangular lattice

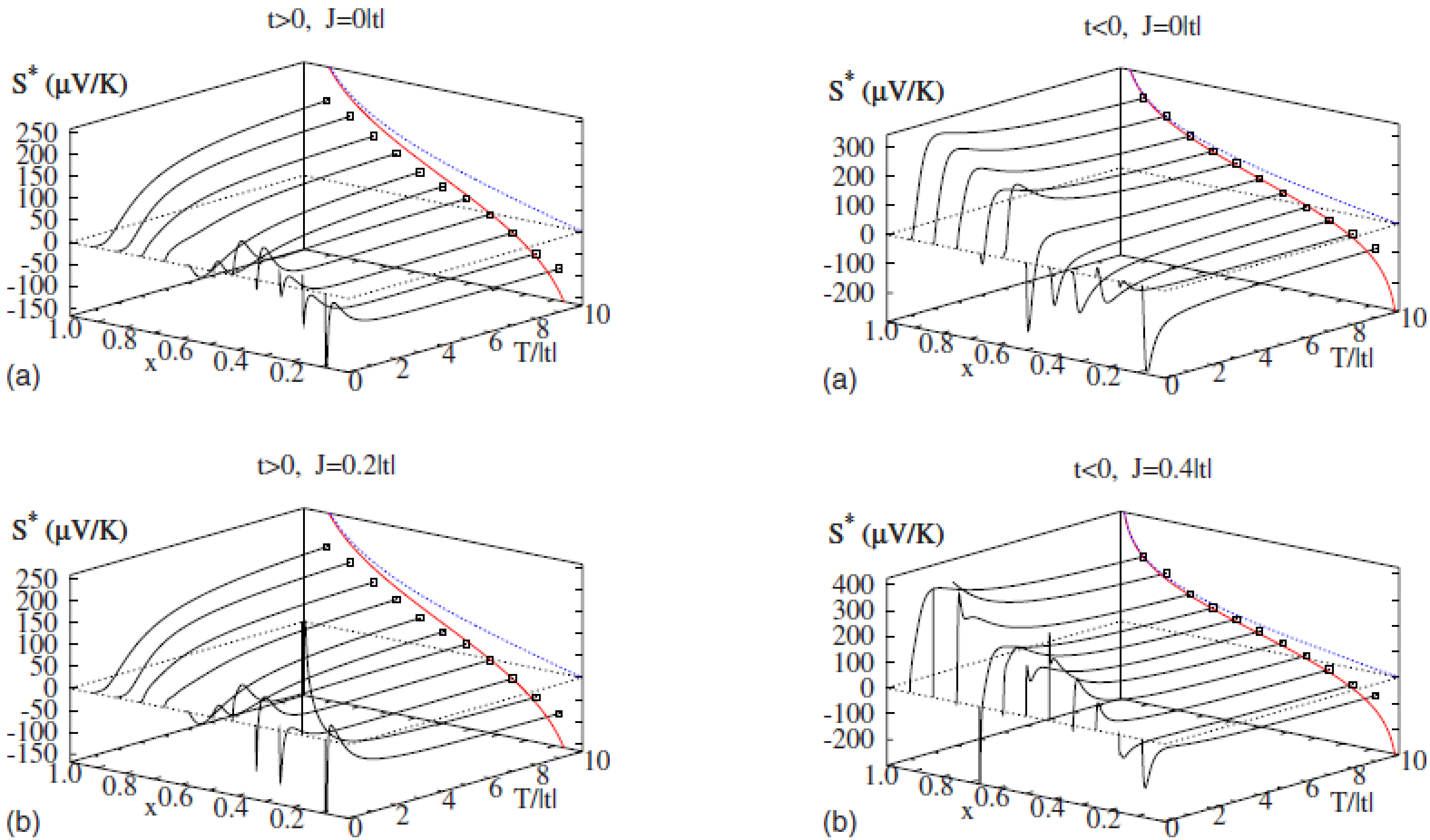
$$S^* = \frac{k_B}{e}\left\{\log\left[\frac{2(1-n)}{n}\right] - \beta t\frac{2-n}{4}\right\}$$

$$S^*(n) = -S^*(2-n) \text{ for } n > 1$$

Thermopower can be enhanced by a t of the right sign

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

$t - J$ model on a triangular lattice



[M. Peterson *et. al. Phys. Rev. B* **76** 165118 (2007)]