Seebeck coefficient in the repulsive Fermi Hubbard model

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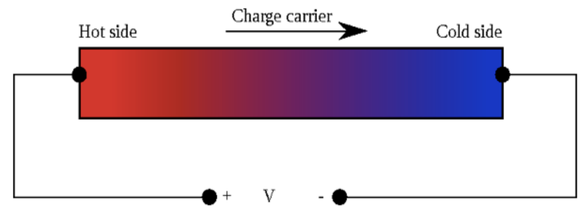
Introduction

Seebeck coefficient:



$$S = -\frac{\Delta V}{\Delta T}$$

Transport coefficients

$$\vec{j} = L^{11}\vec{E} + L^{12}(-\vec{\nabla}T)$$
$$\vec{j}^{q} = L^{21}\vec{E} + L^{22}(-\vec{\nabla}T)$$
$$\rightarrow \quad S = \frac{(L^{12})_{xx}}{(L^{11})_{xx}} = \frac{1}{T}\frac{(L^{21})_{xx}}{(L^{11})_{xx}}$$

Kubo representation: $S(q_x,\omega) = \frac{1}{T}\frac{\chi_{\hat{\rho}(q_x),\hat{K}(-q_x)}(\omega)}{\chi_{\hat{\rho}(q_x)\hat{\rho}(-q_x)}(\omega)}$

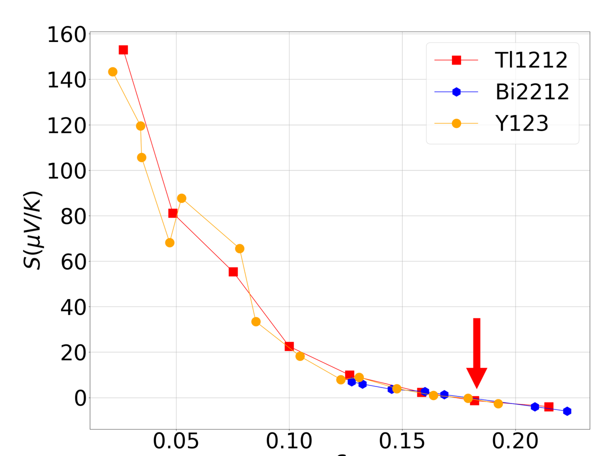
Grand canonical hamiltonian

Charge density

Kelvin formula for thermopower:

$$S_{\text{Kelvin}} = \lim_{q_x\to 0,\omega\to 0} S_{\text{Kubo}}(q_x,\omega) = -\frac{1}{e}\frac{\partial\mu}{\partial T}\Big|_{V,n} = \frac{1}{e}\frac{\partial s}{\partial n}\Big|_{T,V}$$

Seebeck coefficient in the cuprates:



Universal signatures of Seebeck coefficient in cuprates:

- Anomalous sign change at finite doping.
- Divergence near half filling.

Interaction/charge gap driven?

Parent hamiltonian of cuprates – Repulsive Fermi Hubbard model

$$H = -\sum_{\langle i,j\rangle,\sigma}(t_{ij}\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \text{h.c}) - \mu\sum_{i,\sigma}\hat{n}_{i,\sigma} + U\sum_{i,\sigma}(\hat{n}_{i,\uparrow}-\frac{1}{2})(\hat{n}_{i,\downarrow}-\frac{1}{2})$$

nearest neighbor hopping — sets doping — particle hole symmetry

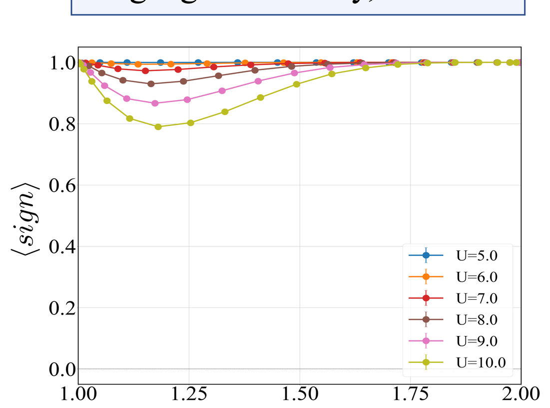
Investigate with Determinantal Quantum Monte Carlo:

- Partition function $Z = \sum_n \langle n|\prod_l e^{-\Delta\tau\hat{K}}e^{-\Delta\tau\hat{V}}|n\rangle$
- Evaluate Z with HS transformation (with $\cosh(\nu) = e^{\frac{U\Delta\tau}{2}}$)

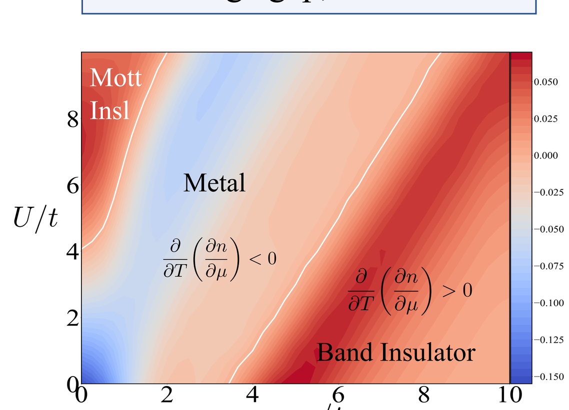
$$e^{-U\Delta\tau(\hat{n}_{i,\uparrow}-\frac{1}{2})(\hat{n}_{i,\downarrow}-\frac{1}{2})} = C\sum_{h_i=\pm 1} e^{\nu h_i(n_{i,\uparrow}-n_{i,\downarrow})}$$

- Transforms Z into: $Z = Tr_{\{h\}}\prod_{\sigma=\uparrow,\downarrow}\text{Det}(I + \prod_l e^{-\Delta\tau K}e^{-\Delta\tau V_l^{\sigma}(\{h\})})$
- Fermion determinants not always > 0. Source of sign problem.

Avg sign vs density, $T/t = 0.5$



Charge gap, $T/t = 0.5$



Transport coefficients in the square lattice

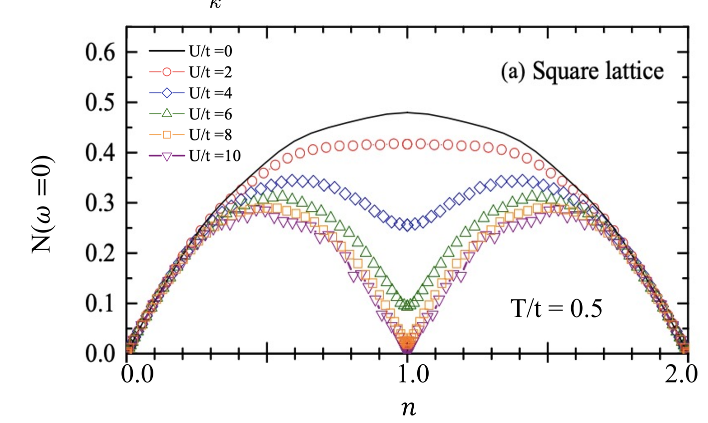
$$G(k,\tau) = \int d\omega \frac{e^{-\omega\tau}}{1+e^{-\beta\omega}}A(k,\omega)$$

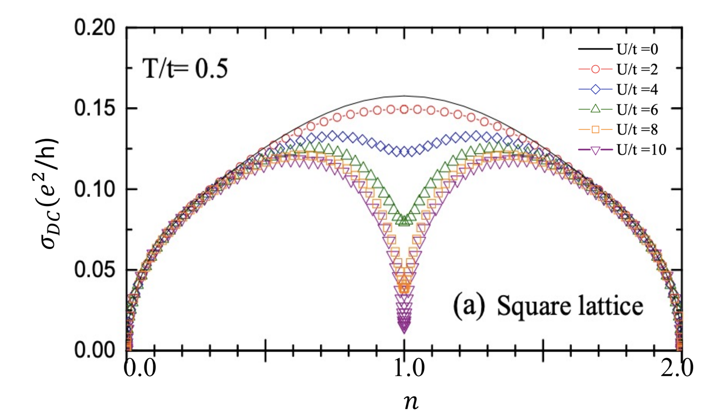
$\beta\Omega >> 1$

$$\rightarrow N(0) = \sum_k A(k,\omega=0) = \frac{\beta}{\pi}(G|i-j|=0,\tau=\beta/2)$$

$$\Lambda_{xx}(q,\tau) = \int d\omega\frac{e^{-\omega\tau}}{1-e^{-\beta\omega}}\sigma(q,\omega)$$
$$\Lambda_{xx}(q,\tau) = \langle j_x(q,\tau)j_x(-q,0)\rangle$$

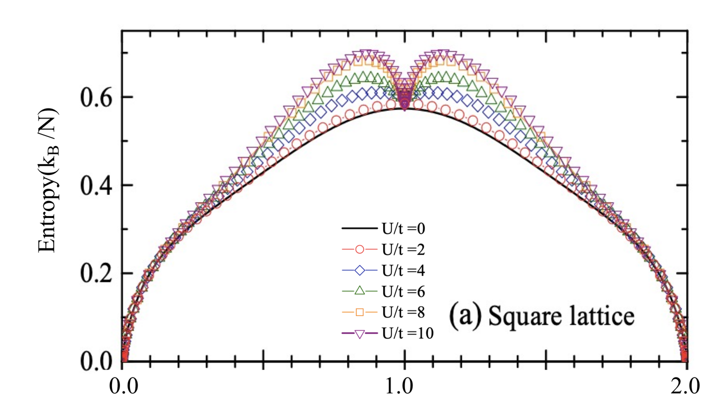
$\beta\Omega >> 1$ $\rightarrow$ $\sigma_{DC} = \frac{\beta^2}{\pi}\Lambda_{xx}(q=0,\tau=\beta/2)$

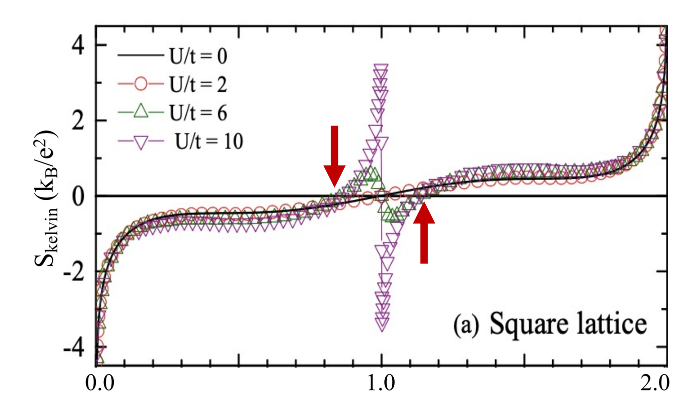




- Vanishing σ_{DC} follows depletion of $N(\omega = 0)$ with large interactions.
- Onset of Mott Insulator at half filling.

Thermodynamic entropy: $s(\mu,T) = \int_{-\infty}^{\mu} d\mu \frac{\partial n}{\partial T}\Big|_{\mu}$ $\rightarrow$ $S_{\text{Kelvin}} = \frac{1}{e}\frac{\partial s}{\partial n}\Big|_{T,V}$



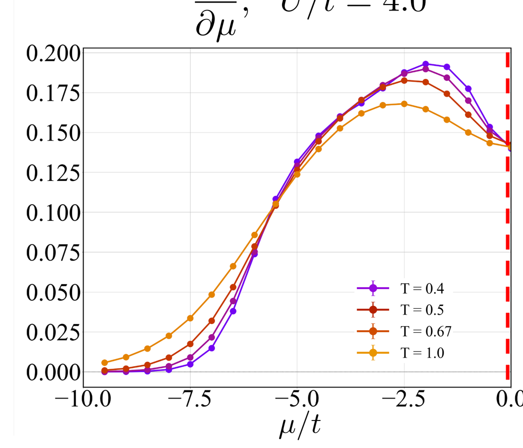


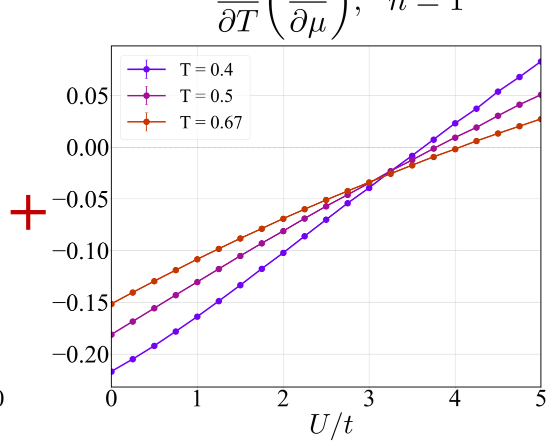
- Divergence near half filling increases with U/t
- Anomalous sign change

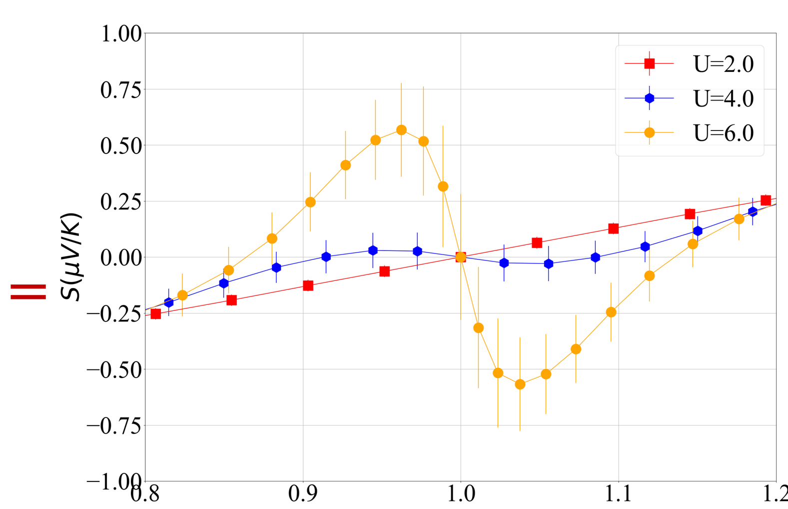
Divergence near half filling due to vanishing of σ_{DC}. What causes the anomalous sign change?

$\rightarrow$ Look at opening of charge gap!

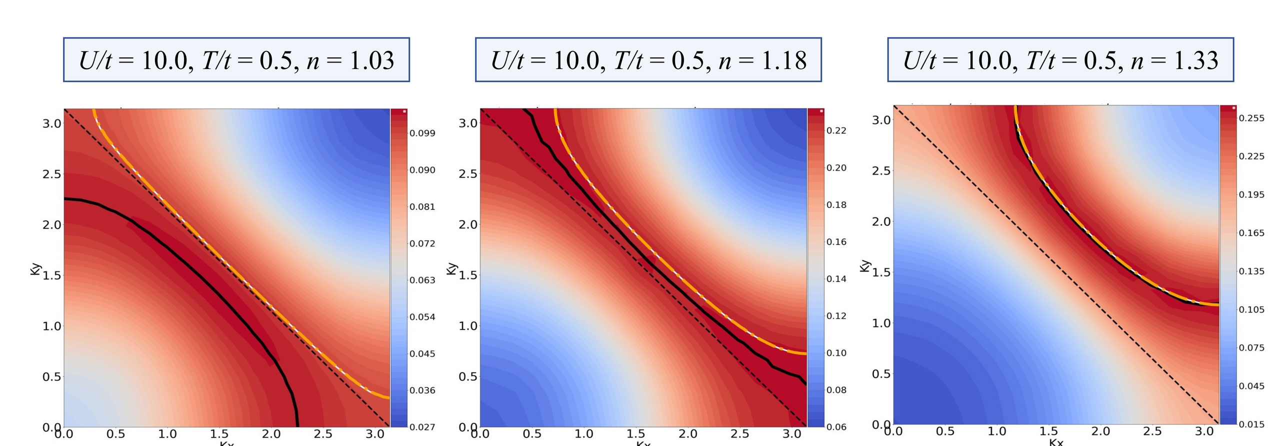
$\frac{\partial n}{\partial \mu}$, $U/t = 4.0$ + $\frac{\partial}{\partial T}\left(\frac{\partial n}{\partial \mu}\right)$, $n = 1$ =





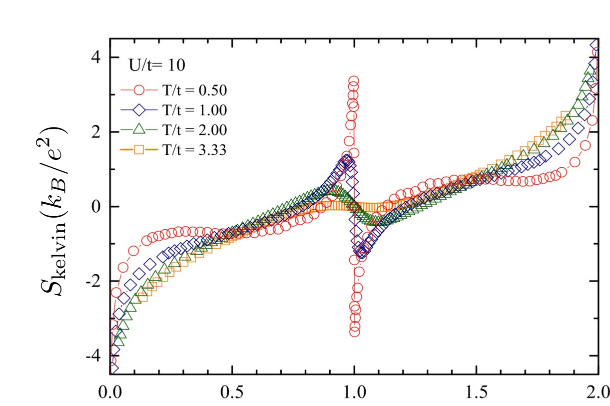


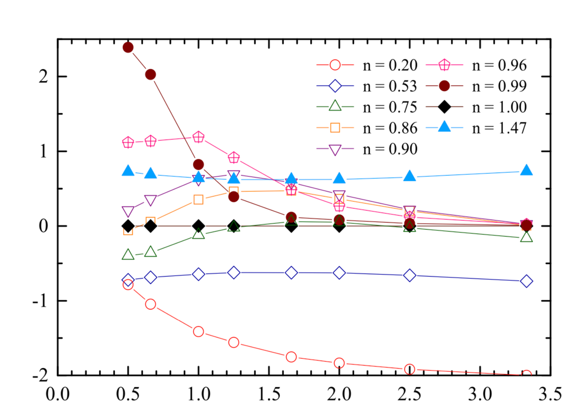
- Sign of Seebeck coefficient -> information about type of carriers.
- Anomalous sign change of Seebeck coefficient accompanies violation of Luttinger theorem.
- High temperature – No spontaneous symmetry breaking.



Temperature dependence of Seebeck coefficient:

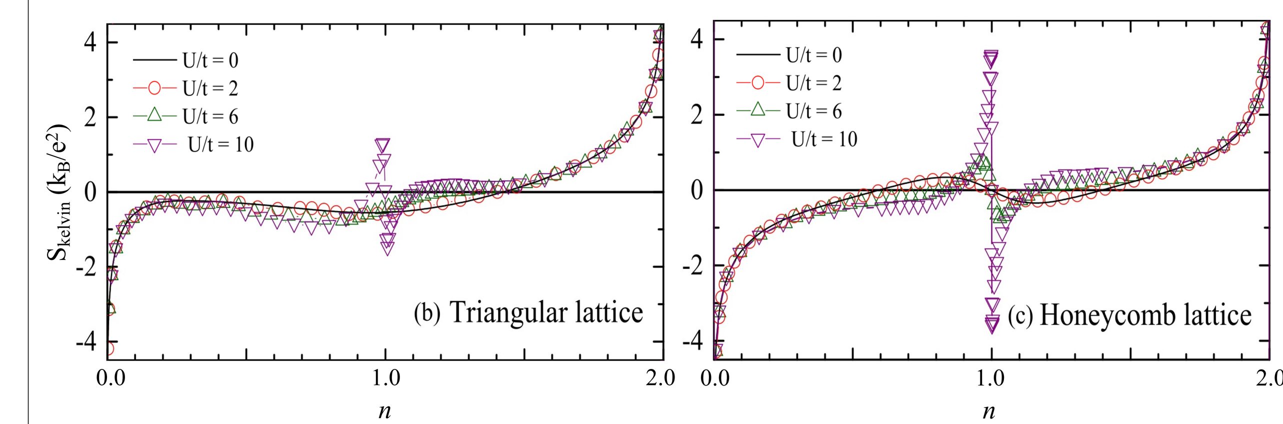
- Seebeck coefficient returns to free particle limit as $T/t \rightarrow O(U/t)$
- In the anomalous region ($0.75<n<1$), peaks in Seebeck coefficient are closer to lower temperatures for doping levels closer to half filling.





Effect of lattice geometry on Seebeck coefficient

Seebeck coefficient with and without particle hole symmetry:



- Triangular lattice has asymmetric DOS; no sign change of Seebeck coefficient in the hole doped side.
- Honeycomb lattice shows sign change at finite doping, at U/t = 0, due to valence and conduction bands.

Parton Mean field theory

Effective low energy hamiltonian – *t-J* model: $H_{eff} = -t\sum_{\langle ij\rangle,\sigma}\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + J\sum_{\langle ij\rangle}[\vec{S}^{i}\cdot\vec{S}^{j} - \frac{1}{4}n_i n_j]$

Write electron operators in terms of doublons, holons, spinons:

$$\hat{c}^{\dagger}_{i\sigma} = \hat{f}^{\dagger}_{i\sigma}\hat{h}_i + \sigma\hat{f}_{i\bar{\sigma}}\hat{d}^{\dagger}_i$$
$$\hat{c}_{i\sigma} = \hat{h}^{\dagger}_i\hat{f}_{i\sigma} + \sigma\hat{d}_i\hat{f}^{\dagger}_{i\bar{\sigma}}$$

$\rightarrow$ Subject to constraints

(1) $\hat{d}^{\dagger}_i\hat{d}_i + \hat{h}^{\dagger}_i\hat{h}_i + \sum_{\sigma}\hat{f}^{\dagger}_{i,\sigma}\hat{f}_{i\sigma} = 1$

(2) $\hat{c}^{\dagger}_{i\sigma}\hat{c}_{i\sigma} = \hat{d}^{\dagger}_i\hat{d}_i + \hat{f}^{\dagger}_{i\sigma}\hat{f}_{i\sigma}$

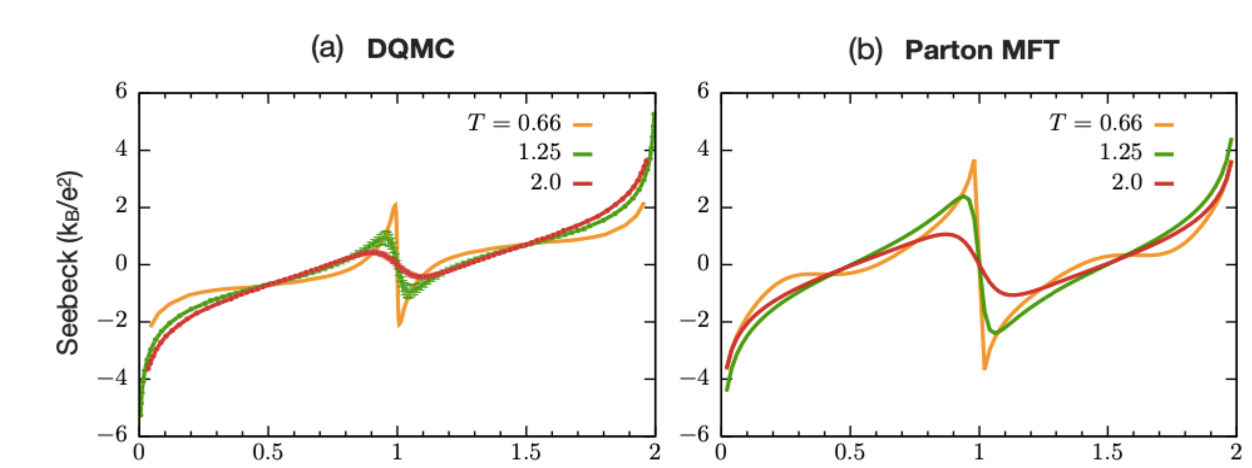
$[\hat{d}_i,\hat{d}^{\dagger}_j] = \delta_{ij}$, $[\hat{h}_i,\hat{h}^{\dagger}_j] = \delta_{ij}$ $\longrightarrow$ Carry charge, but no spin

$\{\hat{f}_{i\sigma},\hat{f}^{\dagger}_{j\sigma'}\} = \delta_{ij}\delta_{\sigma\sigma'}$ $\longrightarrow$ Carry spin, but no charge

$$H^{B}_{MF} = \sum_k \Phi^{\dagger}_k H^{B}(k)\Phi_k, \quad \Phi^{T}_k = [\hat{d}^{\dagger}_k \;\; \hat{h}^{\dagger}_k]$$
$$H^{F}_{MF} = \sum_k \Psi^{\dagger}_k H^{F}(k)\Psi_k, \quad \Psi^{T}_k = [\hat{f}^{\dagger}_{k\uparrow} \;\; \hat{f}^{\dagger}_{k\downarrow}]$$

Densities: $n_d = \frac{1}{\Omega}\sum_k\langle\hat{d}^{\dagger}_k\hat{d}_k\rangle$, $n_h = \frac{1}{\Omega}\sum_k\langle\hat{h}^{\dagger}_k\hat{h}_k\rangle$, $n_f = \frac{1}{2}\frac{1}{\Omega}\sum_k\sum_\sigma\langle\hat{f}^{\dagger}_{k\sigma}\hat{f}_{k\sigma}\rangle$

Hopping: $\chi_d = \frac{1}{z\Omega}\sum_k\gamma(k)\langle\hat{d}^{\dagger}_k\hat{d}_k\rangle$, $\chi_h = \frac{1}{z\Omega}\sum_k\gamma(k)\langle\hat{h}^{\dagger}_k\hat{h}_k\rangle$, $\chi_f = \frac{1}{2}\frac{1}{z\Omega}\sum_k\sum_\sigma\gamma(k)\langle\hat{f}^{\dagger}_{k\sigma}\hat{f}_{k\sigma}\rangle$



Conclusion

- **Anomalous doping dependent sign change in the Seebeck coefficient is controlled by opening of the charge gap.**
- **Lattice geometry strongly influences the doping dependence of Seebeck coefficient.**
- **Sign change of Seebeck coefficient also signals change of carrier type. Associated with Fermi surface reconstruction.**

Acknowledgment and References

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1) **W. C. de Freitas Silva, M. V. Araujo, S. Roy, A. Samanta, N. de C. Costa, N. Trivedi, T. Paiva, "Effects of strong electronic interactions on the thermopower properties of the repulsive Hubbard model" Phys. Rev. B 108, 075101 (2023)**
2) 2) S. D. Obertelli, J. R. Cooper, J. L. Tallon, "Systematics in the thermoelectric power of high-T_c oxides " Phys. Rev. B VOLUME 46, NUMBER 22 (1992)
3) 3) J. R. Cooper, B. Alavi, L-W. Zhou, W. P. Beyermann, and G. Griiner , "Thermoelectric power of some high-T_c oxides " Phys. Rev. B VOLUME 46, NUMBER 22 (1992)
4) 4) M. R. Peterson, B. S. Shastry, "Kelvin formula for thermopower" Phys. Rev. B **82**, 195105 (2010)
5) 5) N. Trivedi, M. Randeria, "Deviations from Fermi-Liquid Behavior above Tc in 2D Short Coherence Length Superconductors", Phys. Rev. Lett. **75**, 312 (1995)