Seebeck coefficient for the Hubbard model

Sayantan Roy[1]

Collaborators

Willdauany C. de Freitas Silva[2], Maykon V. Araujo[2], Abhisek Samanta[1], Natanael de C.Costa[2], Nandini Trivedi[1], and Thereza Paiva[2]

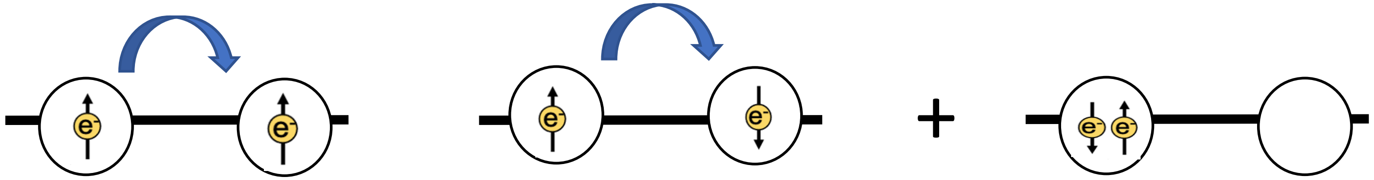
[1] Ohio State University, [2] UFRJ Brazil

Outline

- Hubbard Model, Seebeck Coefficient, Kelvin formula
- Transport results from DQMC
- Parton Mean field theory
- Summary

Repulsive Fermi Hubbard model

- Hubbard model – parent model for high T_c cuprate superconductors



$$H = \sum_{\langle ij \rangle} (t_{ij}^{\sigma\sigma'} c_{i\sigma}^{\dagger} c_{j\sigma'} + \mathrm{h.c}) - \mu \sum_{i\sigma} n_{i\sigma} + U \sum_{i} \left(n_{i\uparrow} - \frac{1}{2}\right)\left(n_{i\downarrow} - \frac{1}{2}\right)$$

Symmetries

- Particle hole transformation on a bipartite lattice

$$\hat{c}_{i\sigma} \rightarrow (-1)^{i} \hat{b}_{i\sigma}^{\dagger} \longrightarrow n(\mu) = 2 - n(-\mu)$$

- SU(2) Invariance: $\left(n_{i\uparrow} - \frac{1}{2}\right)\left(n_{i\downarrow} - \frac{1}{2}\right) \leftrightarrow -\frac{2}{3}\vec{S}_i \cdot \vec{S}_i + \frac{1}{4} n_i$

Lieb Mattis transformation between +U and –U Hubbard model

(Partial particle hole transformation)

Low energy Hamiltonian

$n = 1:$

$$H_{eff} = \frac{4t^2}{U} \sum_{ij} \vec{S}_i \cdot \vec{S}_j$$

$n \neq 1:$

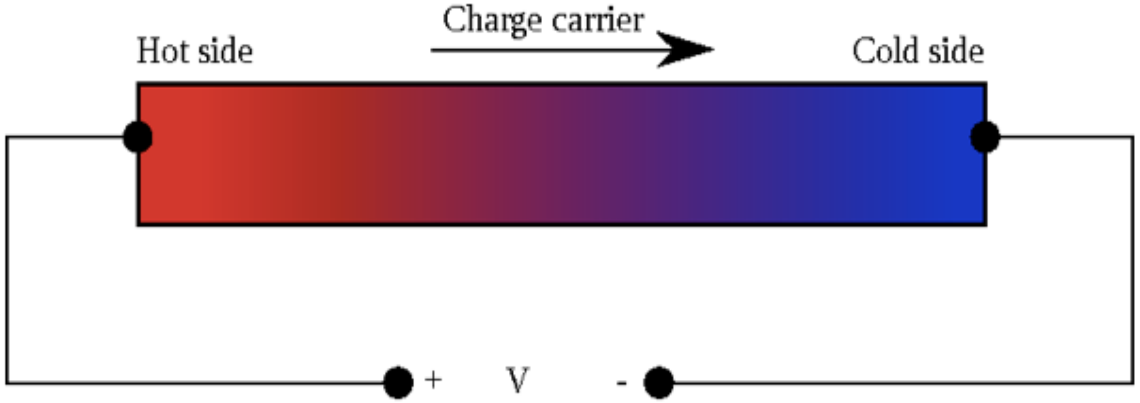
$$H_{eff} = -\sum_{ij} [t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \mathrm{h.c}] + \frac{4t^2}{U} \sum_{ij} [\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j]$$

A. H. MacDonald, S. M. Girvin, and D. Yoshioka, Phys. Rev. B **37**, 9753(1988)

Seebeck coefficient

Development of voltage due to a temperature gradient (open circuit)

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



Transport theory -

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

Kubo formula -

$$S(q_x,\omega) = \frac{1}{T}\frac{\chi_{\hat{\rho}(q_x),\hat{K}(-q_x)}(\omega)}{\chi_{\hat{\rho}(q_x)\hat{\rho}(-q_x)}(\omega)} \xrightarrow{\text{“Slow transport limit”}} S_{\text{Kelvin}} = \lim_{\omega\to 0, q_x\to 0} S_{\text{Kubo}}(q_x,\omega)$$

- Has information about many body DOS, can capture low frequency behavior
- Ignores kinematic factors, involves only thermodynamic quantities

Seebeck coefficient for Hubbard model on square, triangular, honeycomb lattices $\longrightarrow$ Analysis using DQMC+Parton Mean field theory

LDOS and σ_{DC} from DQMC

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

DQMC $\xrightarrow{\text{Maxent}}$ Experiments

$$\boxed{\beta\Omega >> 1}$$

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

N. Trivedi and M. Randeria, Phys. Rev. Lett. **75**, 312(1995)

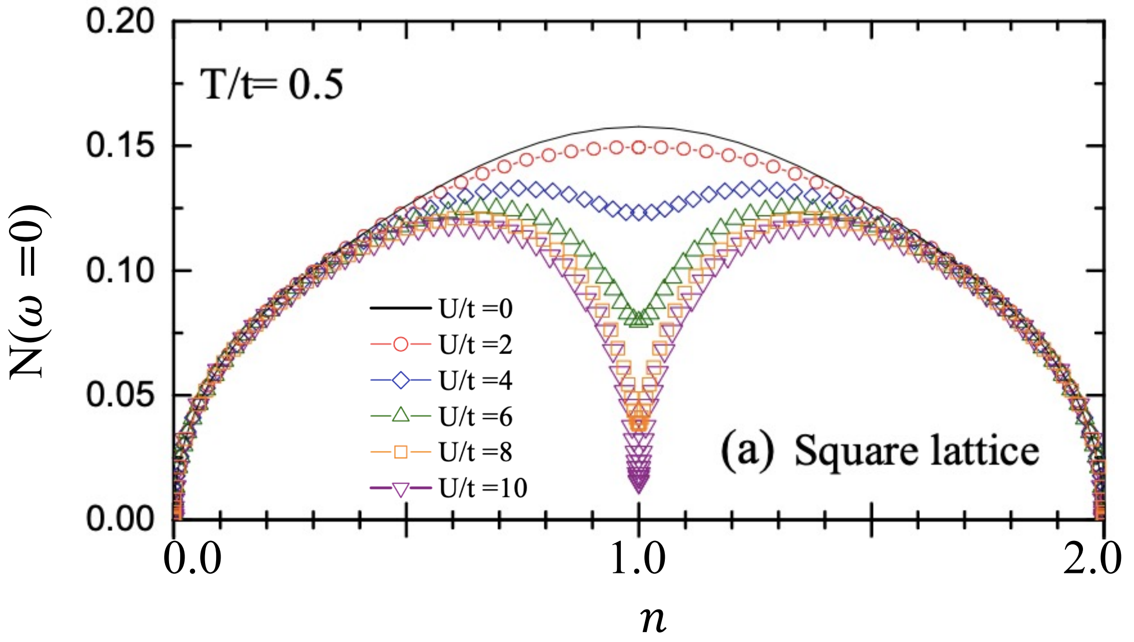
$$\Lambda_{xx}(q,\tau) = \langle j_x(q,\tau) j_x(-q,0)\rangle$$

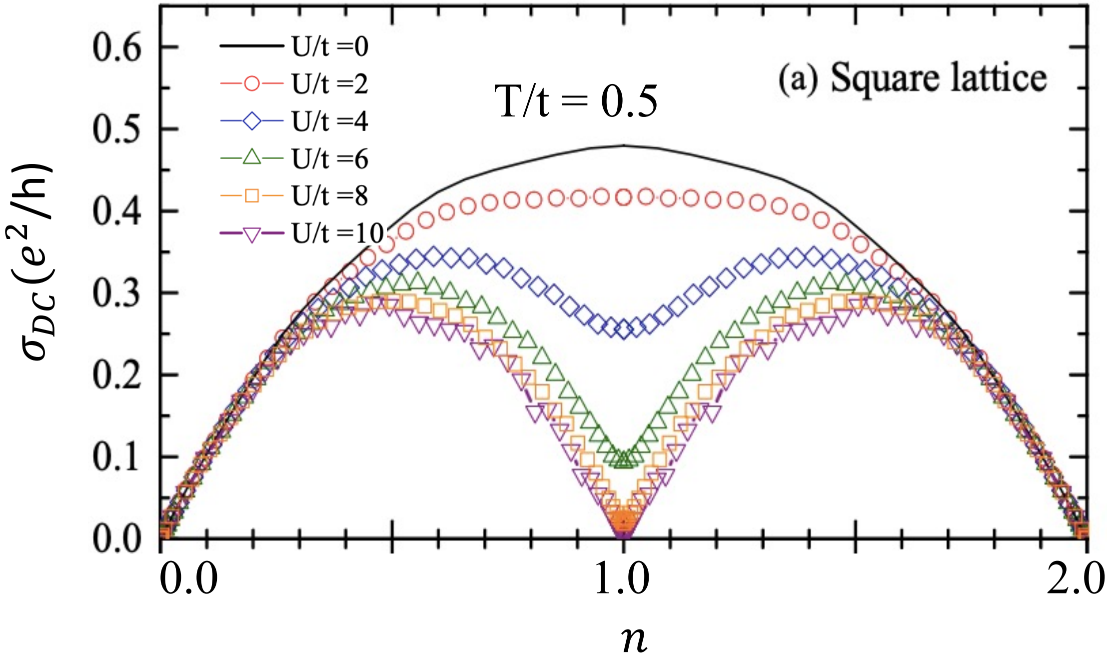
$$\Lambda_{xx}(q,\tau) = \int d\omega \frac{e^{-\omega\tau}}{1-e^{-\beta\omega}} \sigma(q,\omega)$$

$$\boxed{\beta\Omega >> 1}$$

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

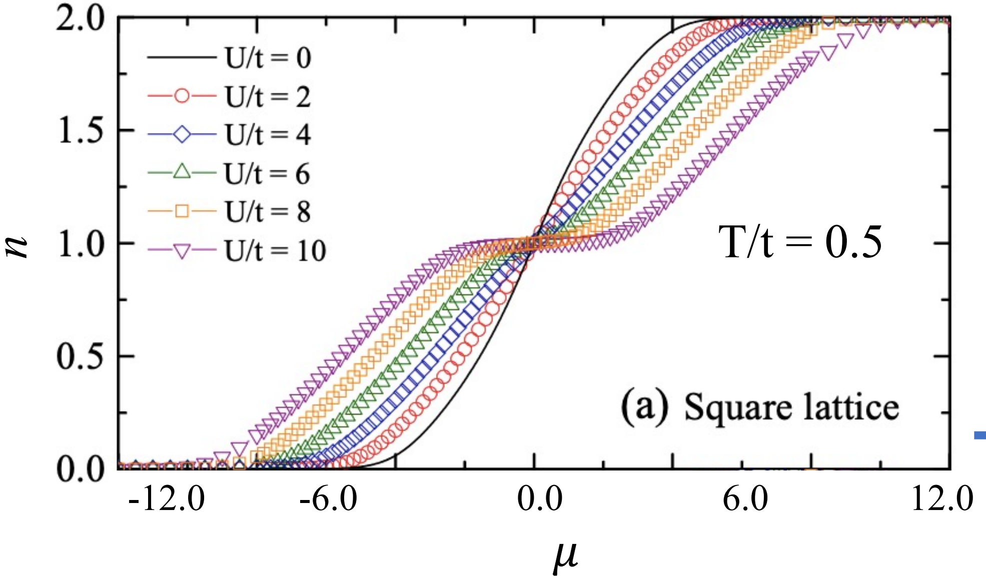
N. Trivedi, R.T. Scalettar, and M. Randeria, Phys. Rev. B **54**, R3756(R) (1996)

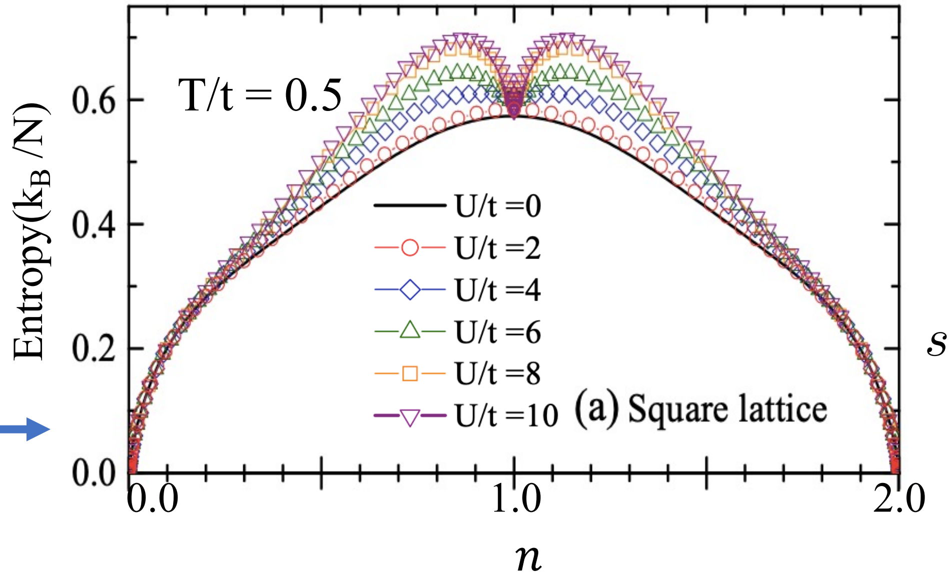




S_{Kelvin} from DQMC

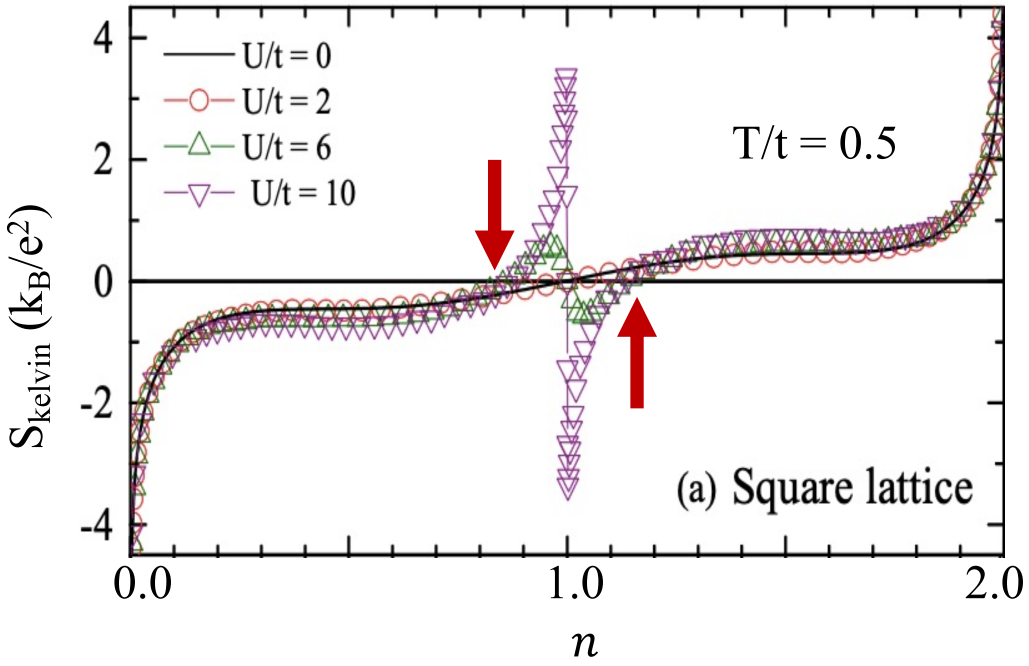
Equation of state $n(\mu)$





Entropy

$$s(\mu, T) = \int_{-\infty}^{\mu} d\mu \frac{\partial n}{\partial T}\bigg|_{\mu}$$



Kelvin formula

$$S_{\text{Kelvin}} = \frac{1}{e}\frac{\partial s}{\partial n}\bigg|_{T,V}$$

- Large divergence of S_{kelvin} at half filling.

$$S = \frac{(L^{12})_{xx}}{(L^{11})_{xx}} = \frac{1}{T}\frac{(L^{21})_{xx}}{(L^{11})_{xx}} \rightarrow 0 \text{ at } n = 0!!$$

- Sign change of Seebeck coefficient near half filling at large U.

→ Possible FS reconstruction?

Parton Mean field theory

Write electron operators in terms of doublons, holons, spinons

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

→ 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) $\hat{c}^\dagger_{i\sigma}\hat{c}_{i\sigma} = \hat{d}^\dagger_i \hat{d}_i + \hat{f}^\dagger_{i\sigma}\hat{f}_{i\sigma}$

Projected low energy Hamiltonian – *t-J* model

Order parameters:

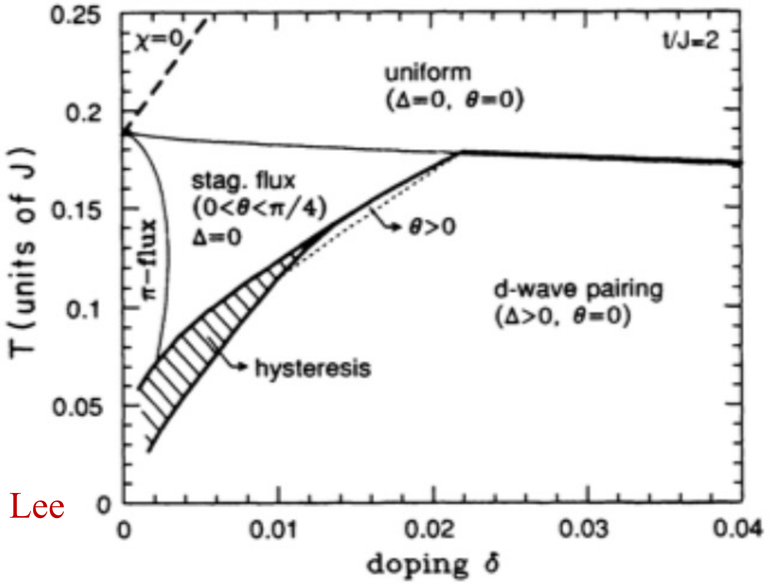
Densities: $n_d = \frac{1}{\Omega}\sum_k \langle \hat{d}^\dagger_k \hat{d}_k\rangle, \quad n_h = \frac{1}{\Omega}\sum_k \langle \hat{h}^\dagger_k \hat{h}_k\rangle, \quad n_f = \frac{1}{2}\frac{1}{\Omega}\sum_k\sum_\sigma \langle \hat{f}^\dagger_{k\sigma}\hat{f}_{k\sigma}\rangle$

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

Mean field Hamiltonian decouples into bosonic and fermionic sectors

$$H^B_{MF} = \sum_k \Phi^\dagger_k H^B(k)\Phi_k, \qquad \Phi^T_k = [\hat{d}^\dagger_k \quad \hat{h}^\dagger_k]$$

$$H^F_{MF} = \sum_k \Psi^\dagger_k H^F(k)\Psi_k, \quad \Psi^T_k = [\hat{f}^\dagger_{k\uparrow} \quad \hat{f}^\dagger_{k\downarrow}]$$



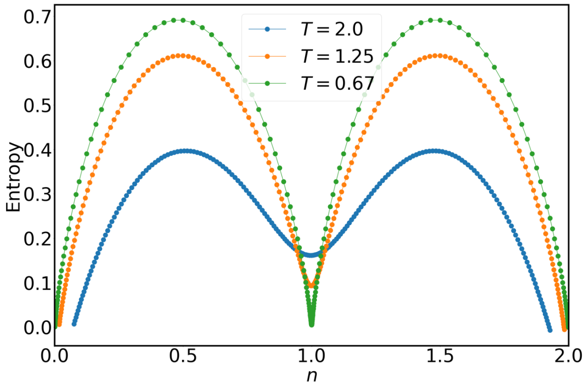
Menke U. Ubbens and Patrick A. Lee
Phys. Rev. B **46**, 8434 (1992)

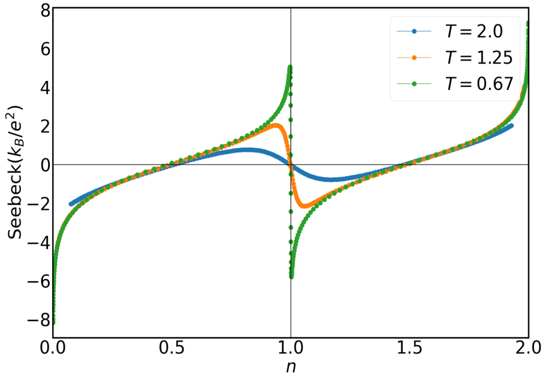
Seebeck coefficient from MFT

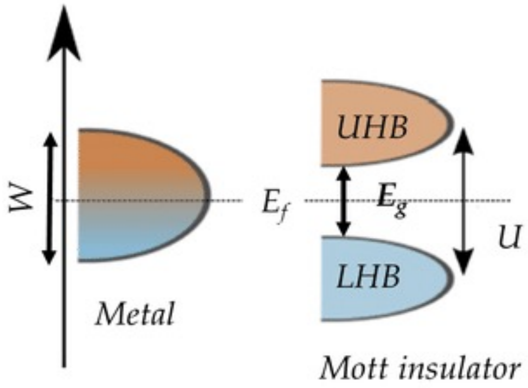
Solution with densities

$$H_{MF} = U\sum_i \hat{d}_i^\dagger \hat{d}_i - \mu \sum_{i\sigma}[\hat{d}_i^\dagger \hat{d}_i + \hat{f}_{i\sigma}^\dagger \hat{f}_{i\sigma}] + g.c$$

Opening of Mott Gap ⇒ Divergence of Seebeck coefficient

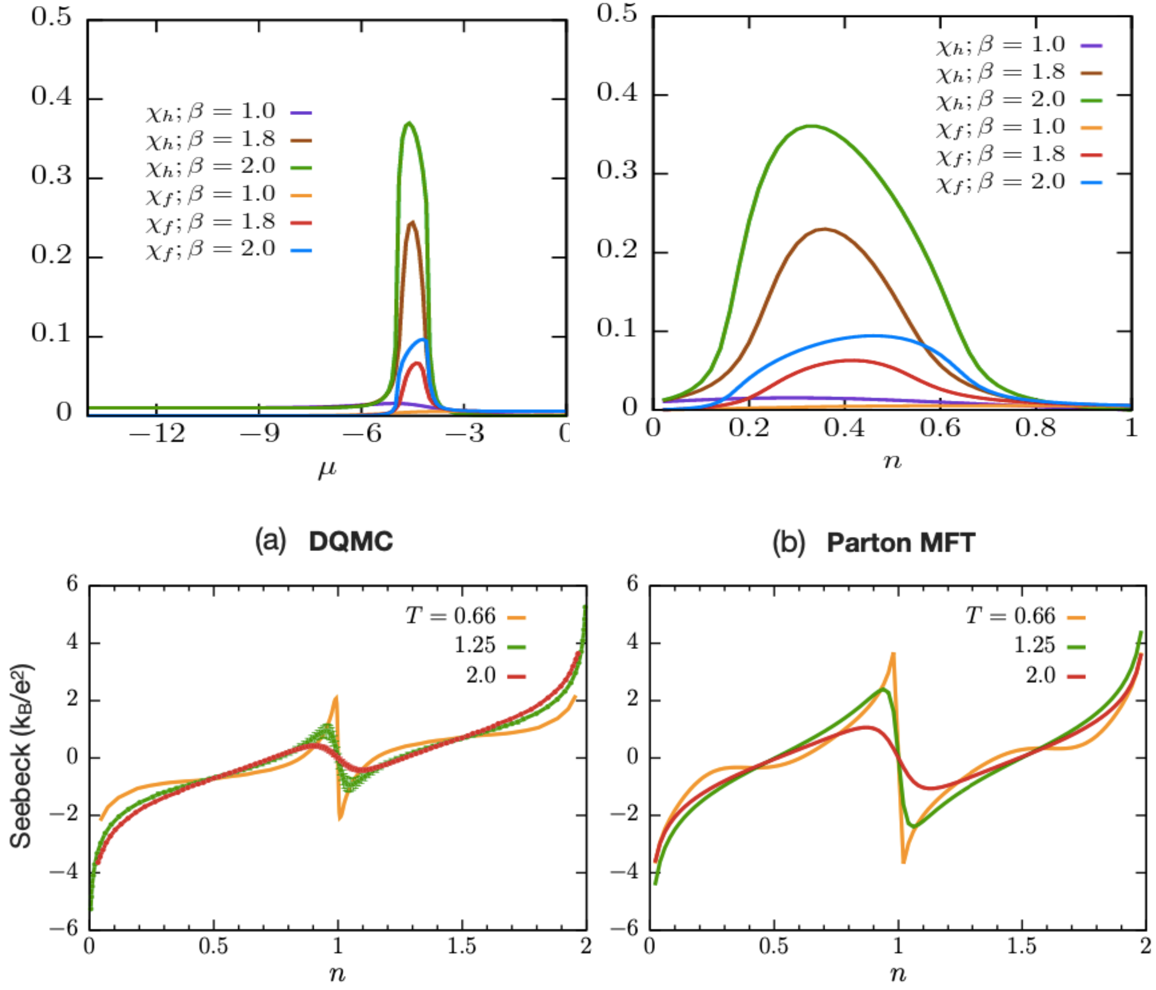






Filling of Hubbard band determines type of carriers, sign of Seebeck coefficient

Solution with densities + gauge fields



Parton MFT is able to capture qualitative features in Seebeck!

Summary

- Kelvin formula for Seebeck coefficient can capture many body effects in the low frequency regime.

- DQMC results show enhancement in Seebeck coefficient near half filling. Divergence due to Mott gap opening up.

- Nontrivial sign change signalling change in carrier type. Possible fermi surface reconstruction?

- S_{kelvin} captures particle hole asymmetry in spectrum. Different behavior of thermopower for bipartite lattices (square and honeycomb) and non bipartite lattice(triangle).

- Parton mean field theory qualitatively reproduces S_{Kelvin} from DQMC.

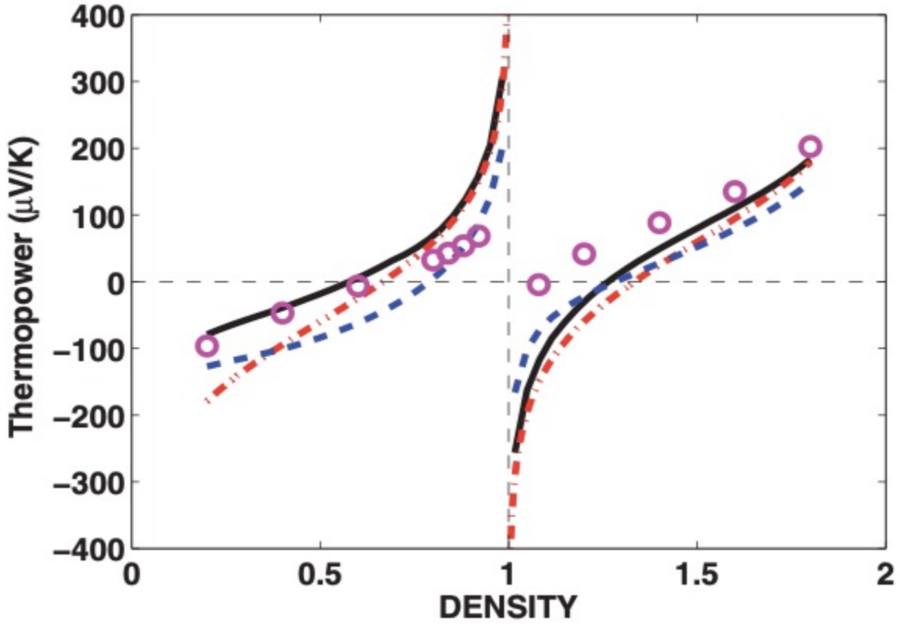
Backup slides

Kelvin formula for Seebeck coefficient

"Slow" transport limit of Kubo formula: $$S_{\text{Kelvin}} = \lim_{\omega \to 0, q_x \to 0} S_{\text{Kubo}}(q_x, \omega)$$

Switching to Lehmann representation, $$S_{\text{Kelvin}} = \frac{1}{q_e T} \frac{\left[\frac{d}{d\mu} \langle H \rangle - \mu \frac{d}{d\mu} \langle N \rangle \right]}{\frac{d}{d\mu} \langle N \rangle}$$

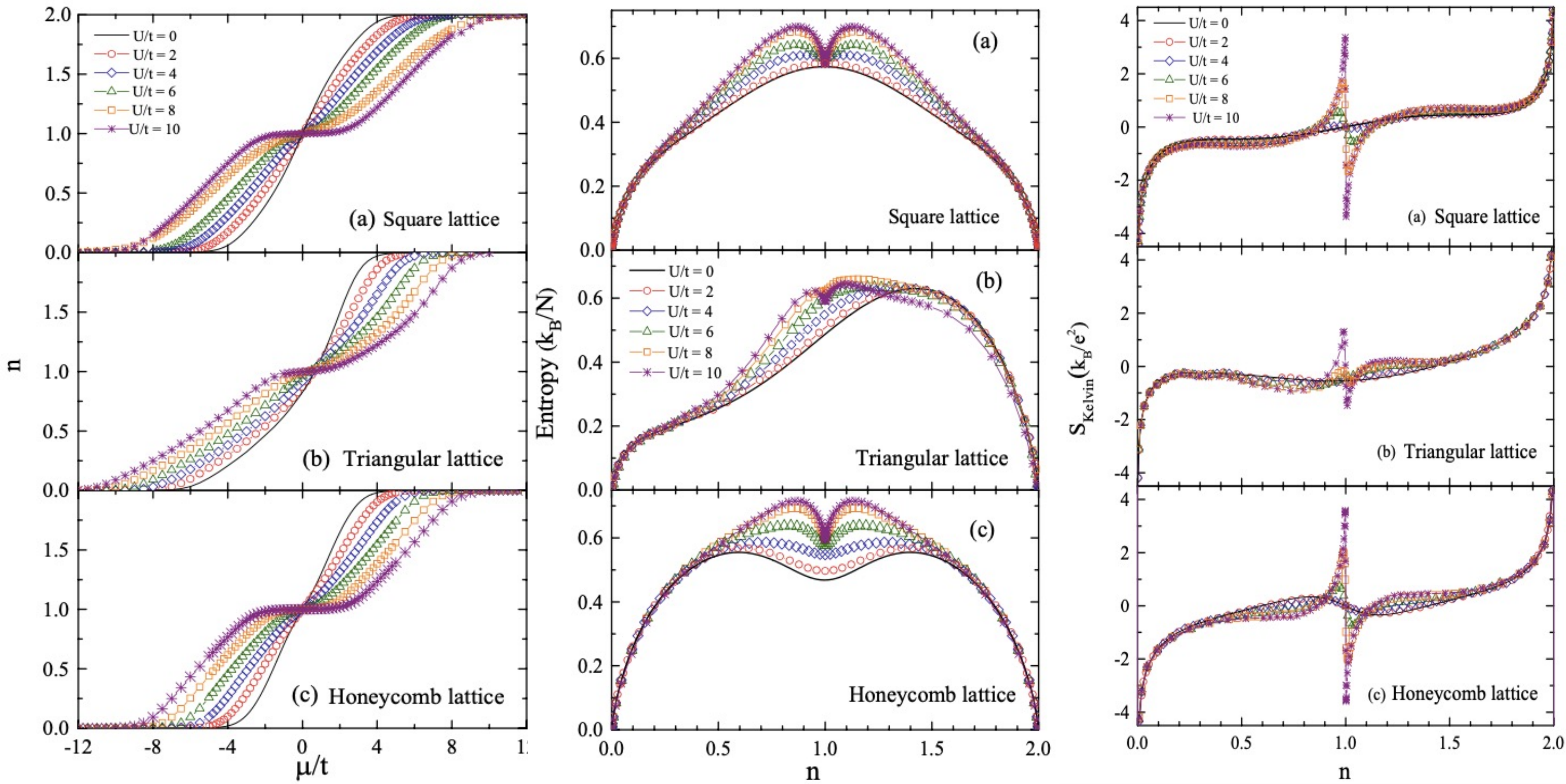
Using Maxwell's relation, $$S_{\text{Kelvin}} = -\frac{1}{e} \frac{\partial \mu}{\partial T} \bigg|_{V,n} = \frac{1}{e} \frac{\partial s}{\partial n} \bigg|_{T,V}$$



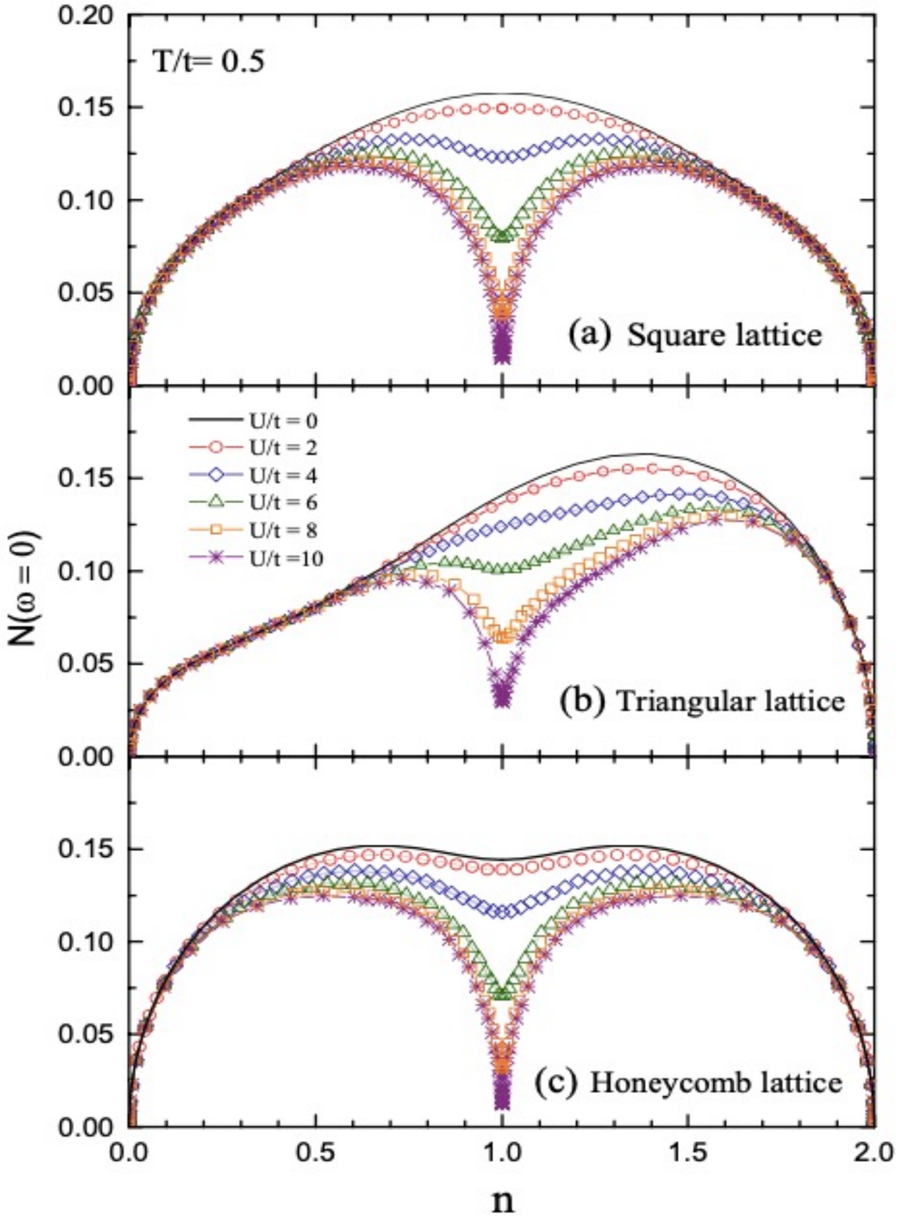
Louis-François Arsenault, B. Sriram Shastry, Patrick Sémon, and A.-M. S. Tremblay
Phys. Rev. B **87**, 035126 (2013)

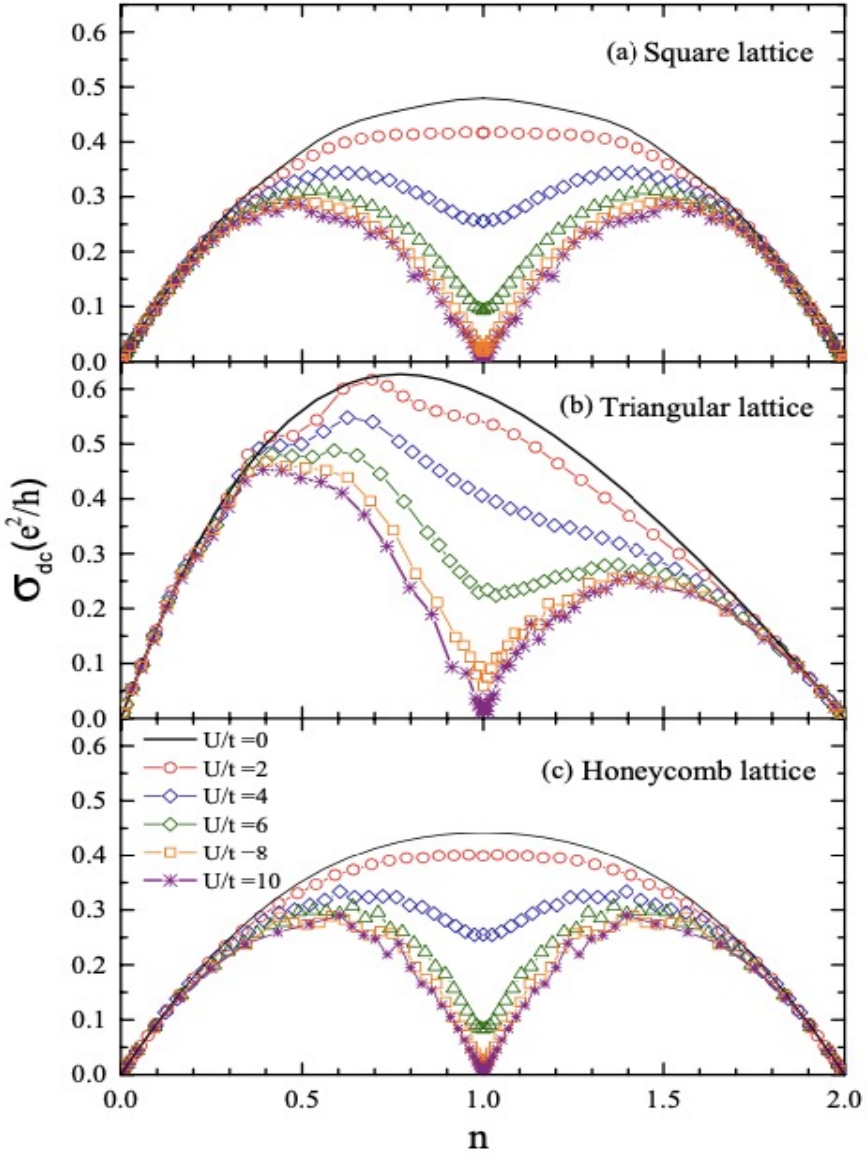
Black – Kubo, Blue dashed – Kelvin formula, Red dashed – Mott Heikes, Magenta circles – High frequency Seebeck

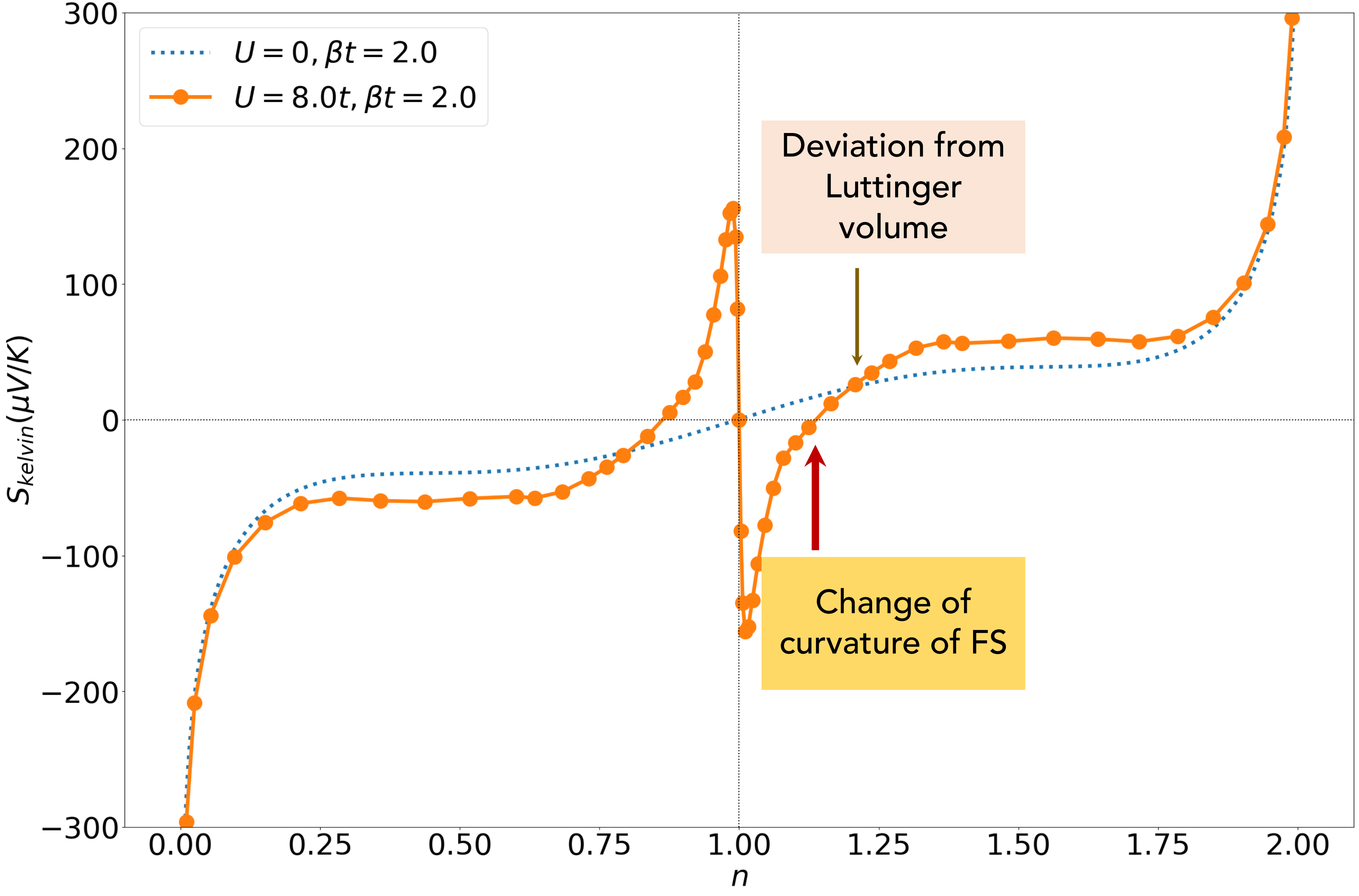
S_{Kelvin} from DQMC



LDOS and σ_{DC} from DQMC







$U = 0, \beta t = 2.0$
$U = 8.0t, \beta t = 2.0$
Deviation from Luttinger volume
Change of curvature of FS
$S_{kelvin}(\mu V/K)$
n
300
200
100
0
−100
−200
−300
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75
2.00

$T = 0.5t$

"Fermi surface" at finite temperatures

U = 0

$\epsilon_k = \mu$ (white)

peak $G_0(\mathbf{k}, \tau = \frac{\beta}{2})$ (orange)

U = 10t

$G(\mathbf{k}, \tau = \frac{\beta}{2})$ peak (black)