# Fermi surface reconstruction in the doped Hubbard model

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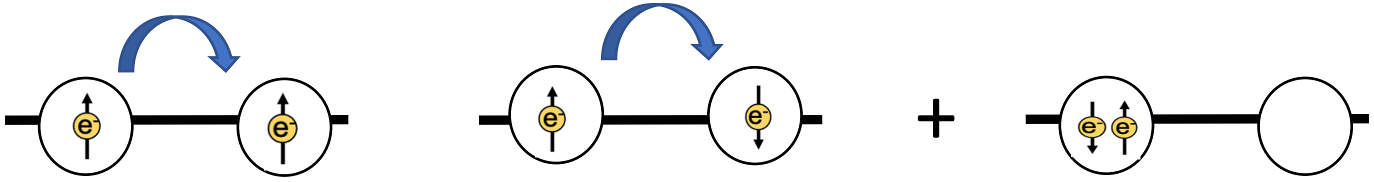
# Outline

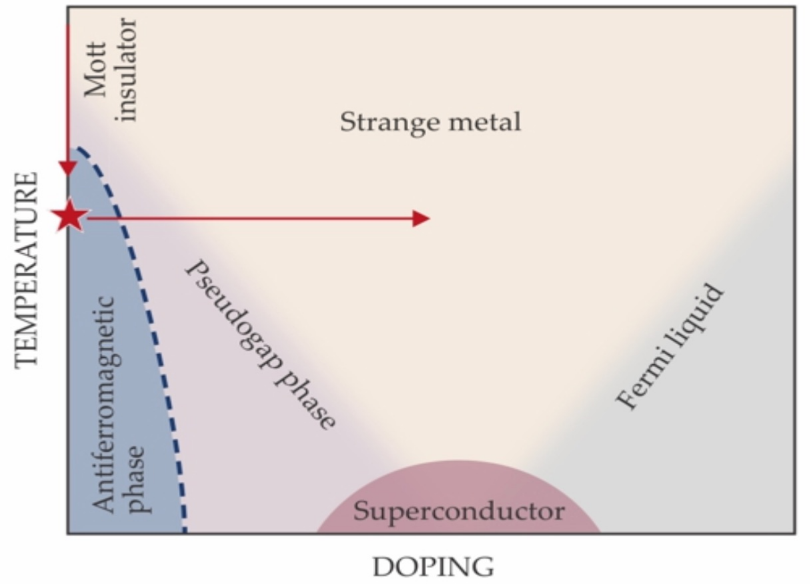
- Hubbard Model, energy scales and Determinant Quantum Monte Carlo
- Fermi surface at finite doping, Luttinger theorem
- Connection with thermopower (temperature and doping dependence)
- Bad metallic phase?

# Repulsive Fermi Hubbard model

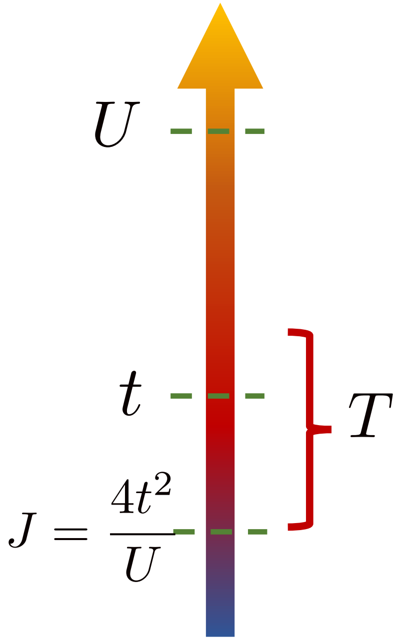
- Hubbard model – parent model for high $T_c$ cuprate superconductors




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




Energy scales




- No spontaneous symmetry breaking.
- Minimal sign problem.

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

$$\xrightarrow[\textbf{MaxEnt}]{}$$

Kramers-Kronig relation: $ReG(k,\omega) = \mathcal{P}\int_{-\infty}^{+\infty} d\omega' \frac{A(k,\omega')}{\omega - \omega'}$

# Operational definition of Fermi surface at finite temperature

Experiment: Momentum distribution curves (MDCs) of ARPES spectra. Look at peaks of $A(k, \omega = 0)$

DQMC: (a) Location of low energy excitations- Single particle spectral functions $A(k, \omega = 0)$

(b) Zeros of Single particle Green's function $ReG(k, \omega = 0) = \mathcal{P} \int_{-\infty}^{\infty} d\omega \frac{A(k, \omega)}{\omega}$ More rigorous!

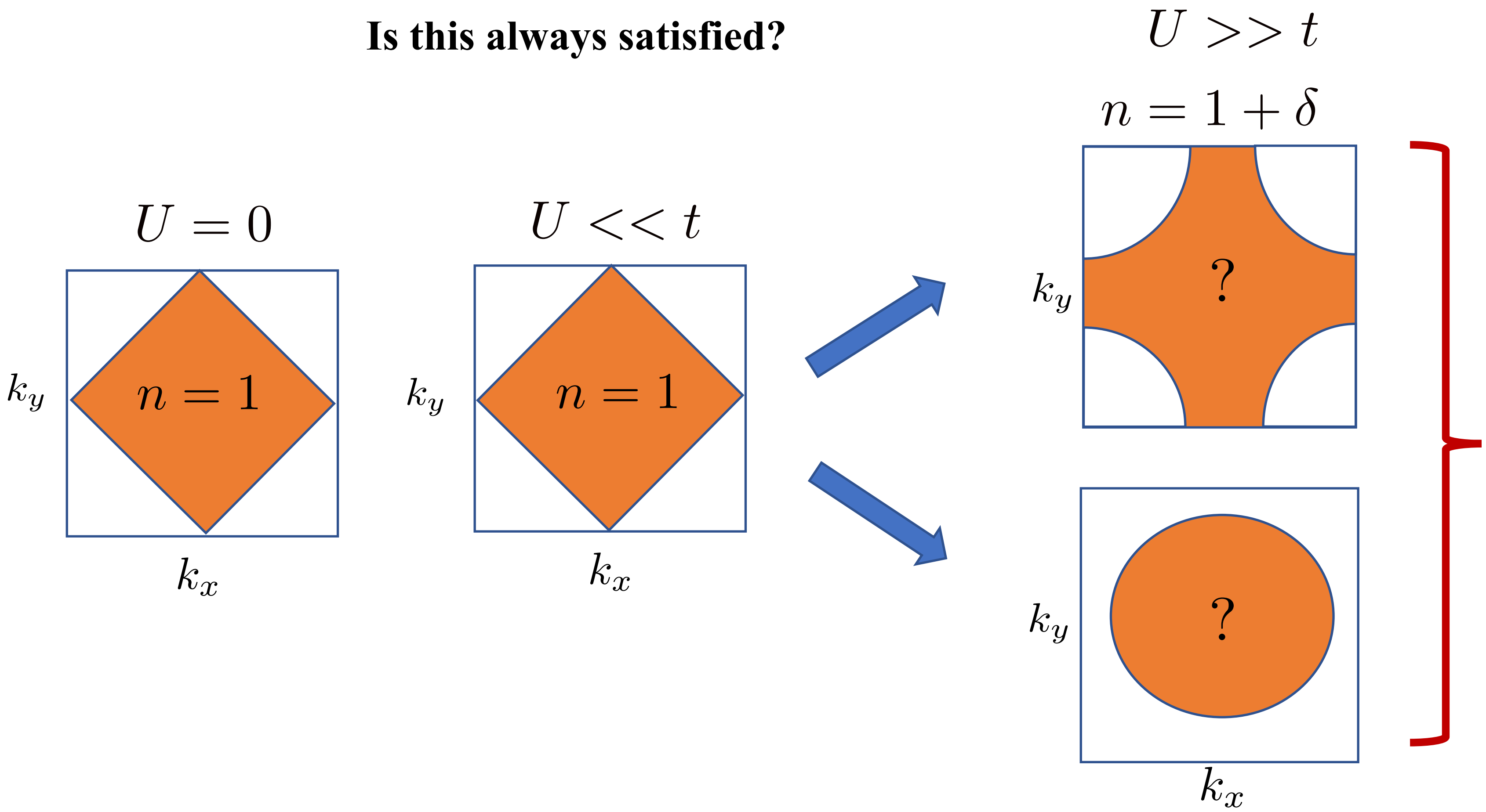
Luttinger's theorem:

$$\underbrace{\frac{1}{V} \langle \sum_k c_k^\dagger c_k \rangle}_{n} = \frac{1}{V} \sum_k \oint \frac{d\omega}{2\pi} \frac{e^{i\omega 0^+}}{i\omega - \epsilon(k) - \Sigma(k, \omega)} = \underbrace{\sum_k \Theta(\mathrm{Re}G(k, \omega = 0))}_{\text{Fermi surface volume}}$$

# Luttinger theorem

**Number density = Volume defined by locus of low energy excitations**

**Is this always satisfied?**

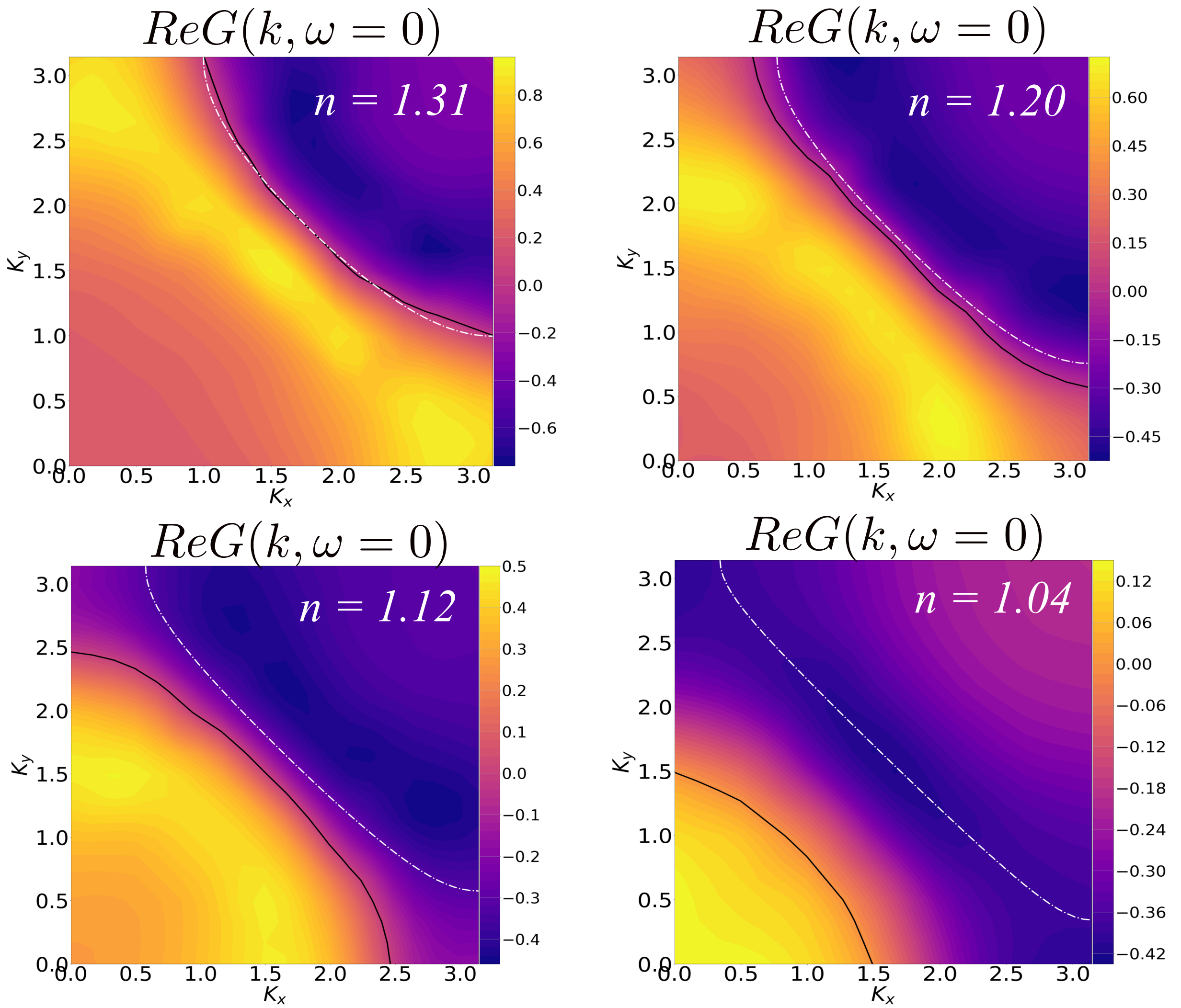


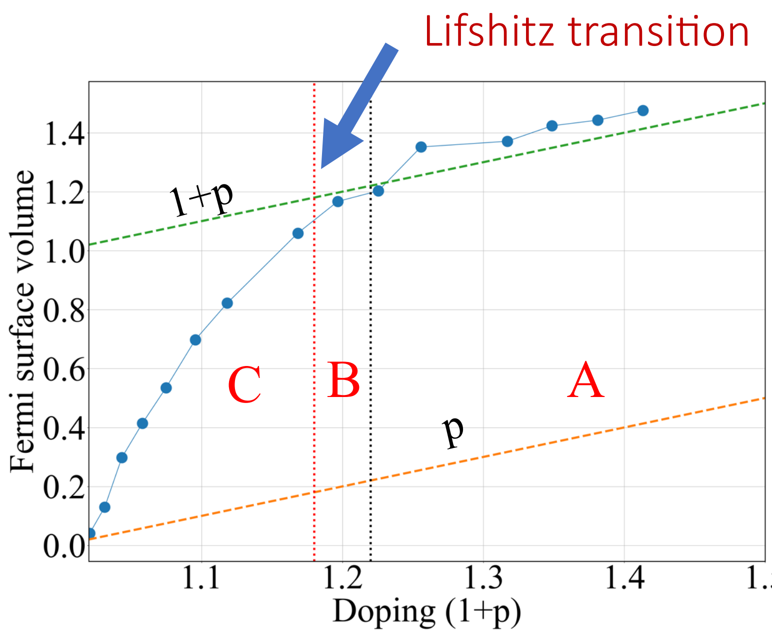

- Fate of Luttinger theorem temperature and doping?
- Low energy Density of states?
- Thermoelectric transport?

# Fermi surface with large interaction (U=10t, T/t = 0.5)

Look at contours of $ReG(k,\omega=0) = \mathcal{P}\int_{-\infty}^{\infty} d\omega \frac{A(k,\omega)}{\omega}$ (black lines)

Non interacting Fermi surface: $\varepsilon_K - \mu(n,T) = 0$ (white lines)



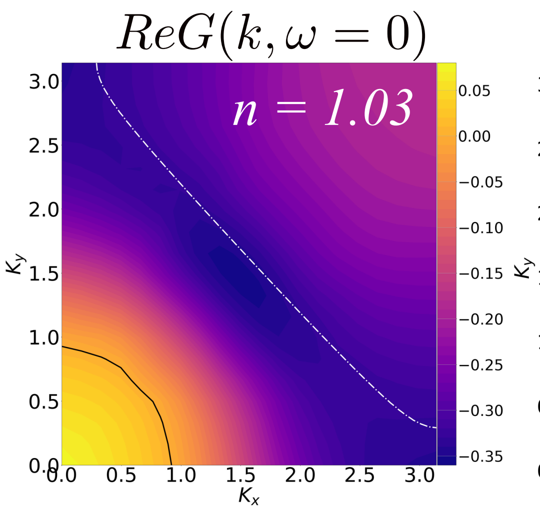

Results on a 12x12 lattice

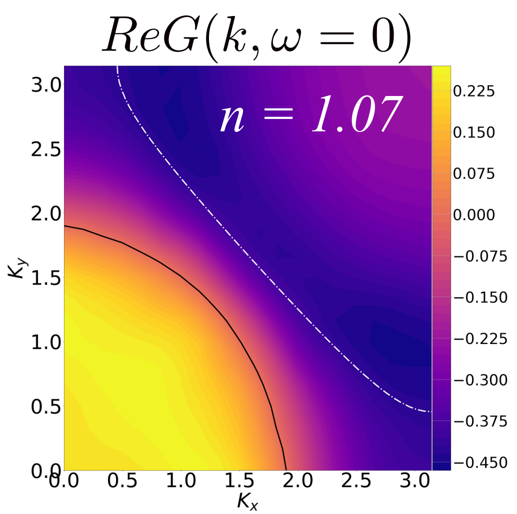
- Region A – Luttinger volume conserved; excitations are electron like like.
- Region B – Luttinger volume violated; excitations are electron like.
- Region C – Luttinger volume violated; excitations are hole like.

# Effect of temperature on Luttinger breaking phase

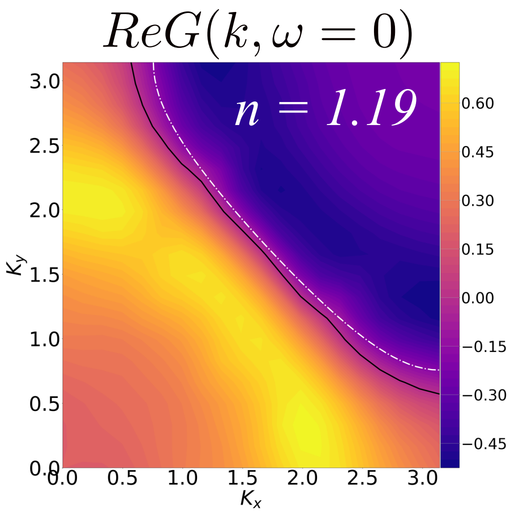
U/t = 10, T/t = 0.5

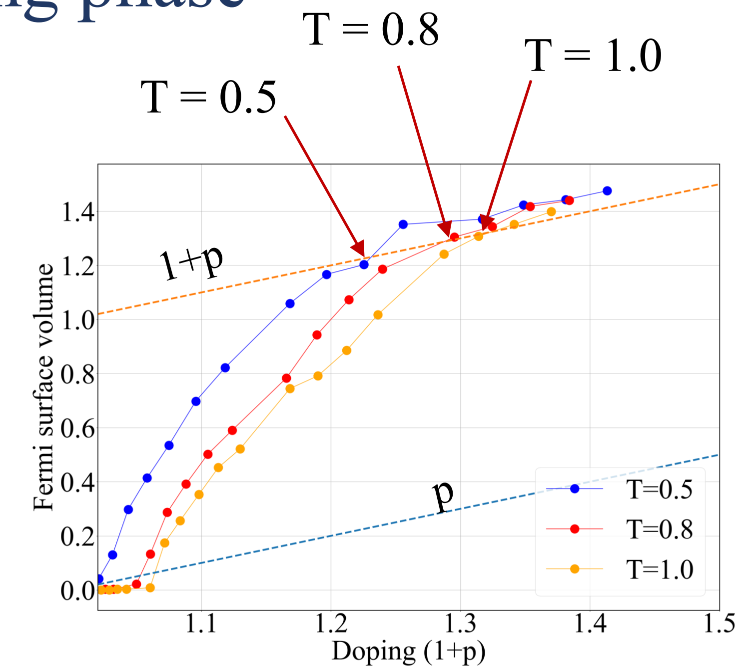
Luttinger Volume violated



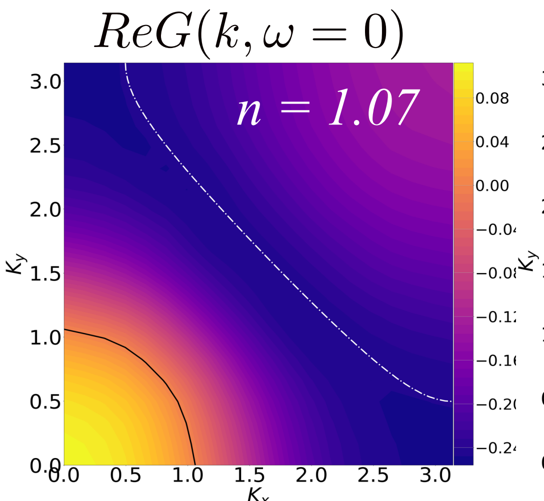

Luttinger Volume preserved

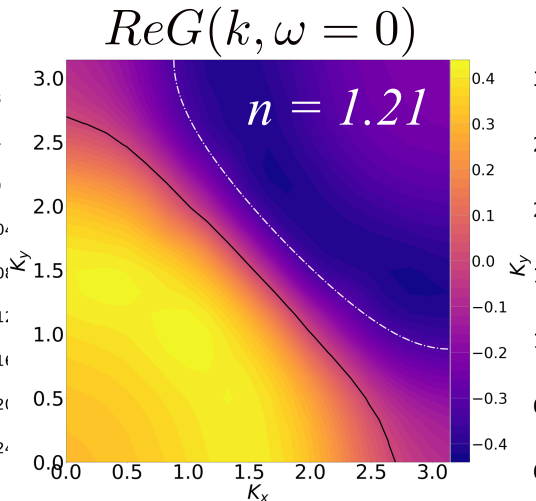


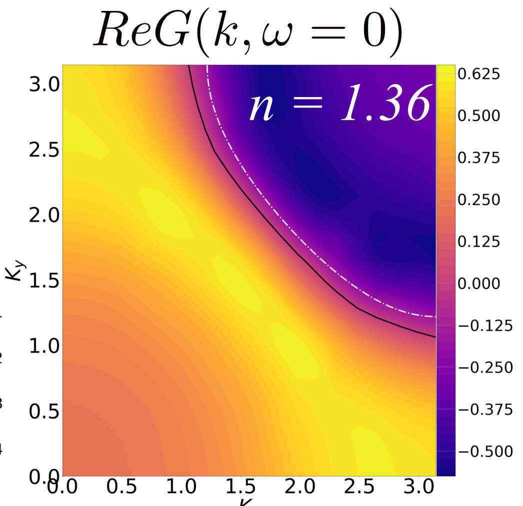

U/t = 10, T/t = 1.0

Luttinger Volume violated




Luttinger Volume preserved

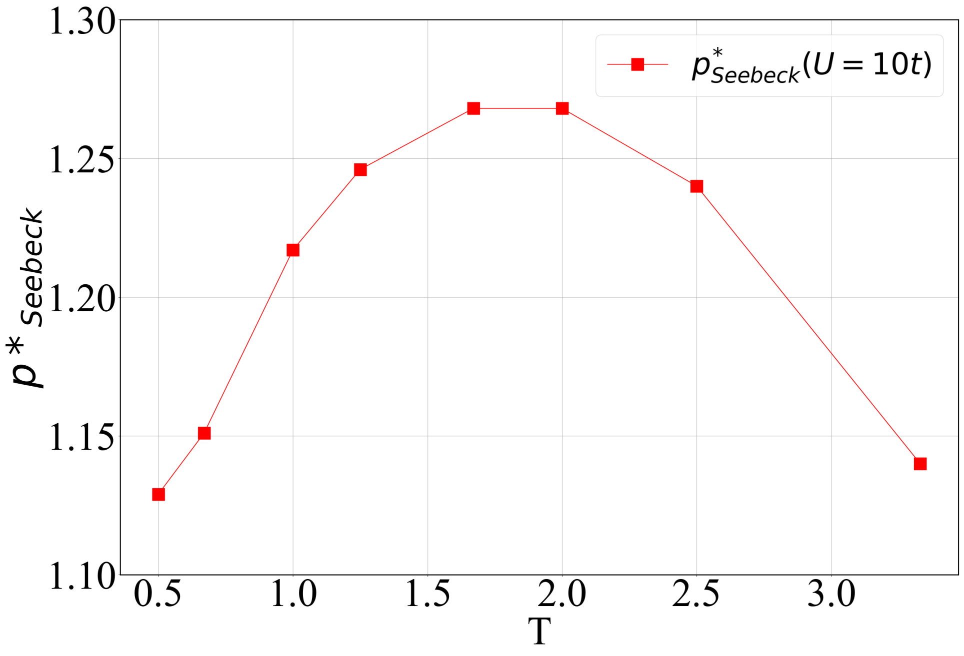



- Doping at which Luttinger count is recovered increases with increasing temperature!
- Possible connection to transport coefficients?

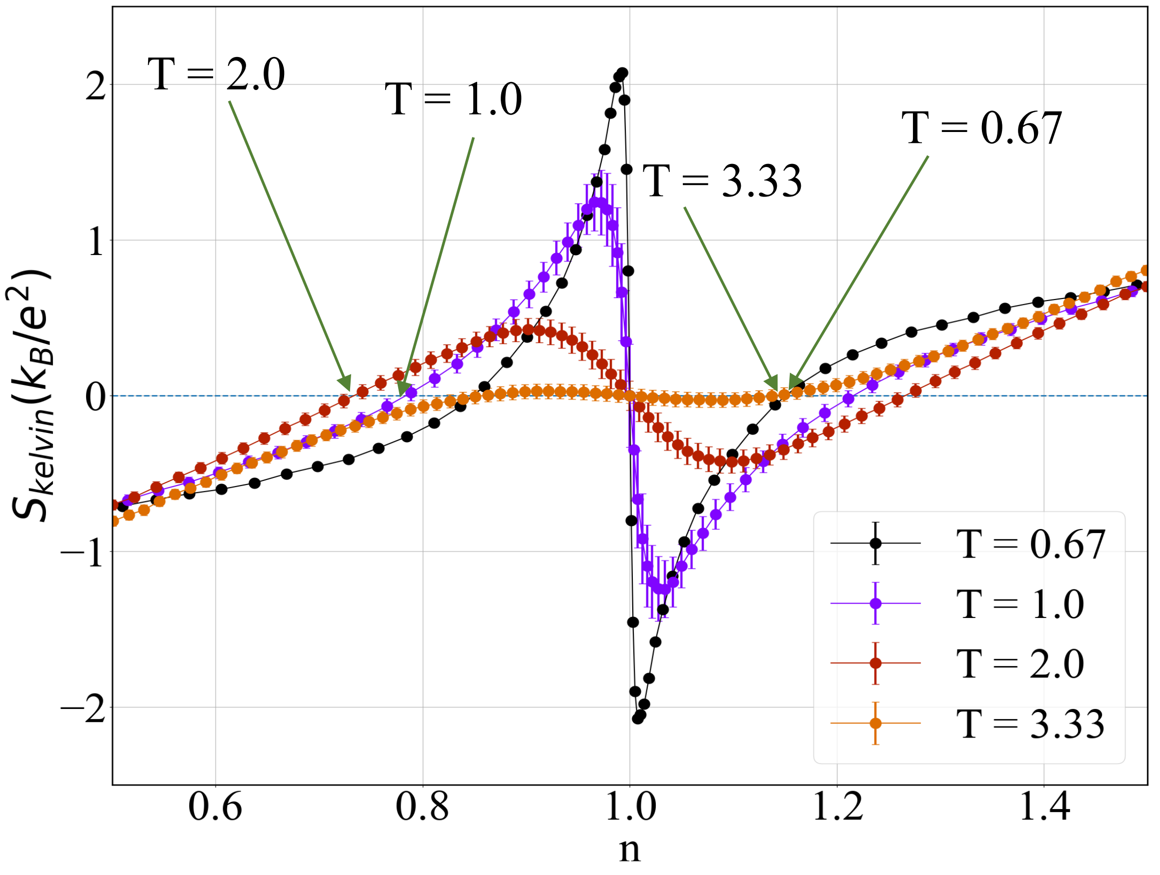
# Seebeck coefficient for doped Hubbard model

$$\mathbf{j} = \mathbf{L}_{11}\mathbf{E} + \mathbf{L}_{12}\left(-\nabla T/T\right)$$
$$\mathbf{j_Q} = \mathbf{L}_{21}\mathbf{E} + \mathbf{L}_{22}\left(-\nabla T/T\right)$$
$$\Rightarrow S = \frac{\mathbf{L}_{12}}{T\mathbf{L}_{11}}$$

$$S_{kelvin} = \frac{1}{q}\frac{\partial \mu}{\partial T}\bigg|_n = \frac{1}{q}\frac{\partial s}{\partial n}\bigg|_T$$



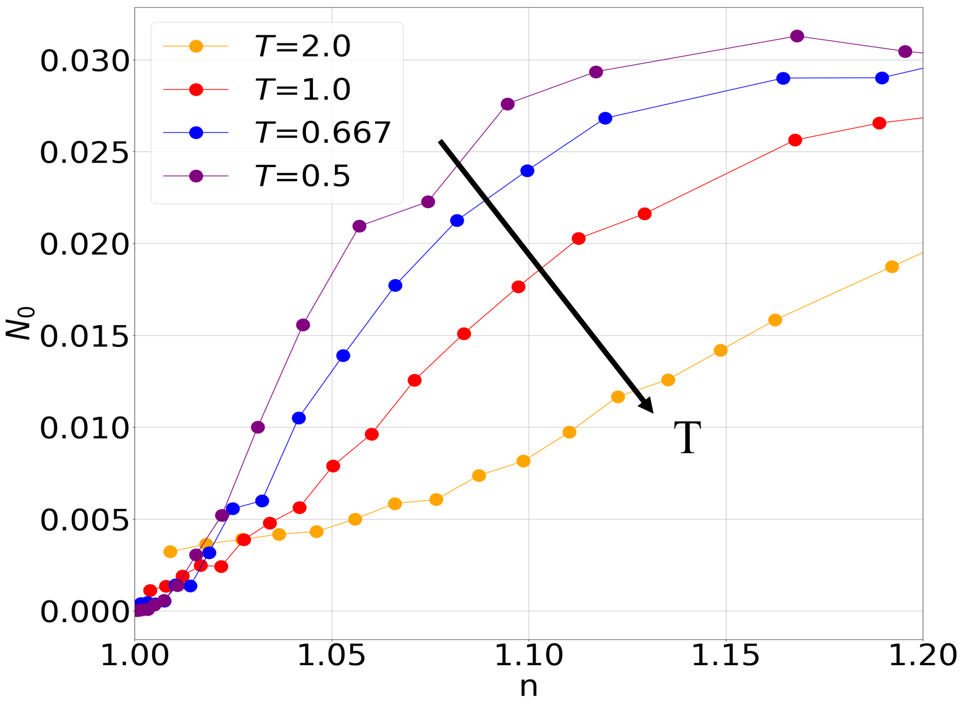

Seebeck coefficient: U/t = 10



# Low Energy DOS and DC conductivity

Look at Integrated low energy spectral weight

$$N_0 = \frac{1}{2\delta\Omega}\int_{-\delta\Omega}^{\delta\Omega} d\omega N(\omega)$$



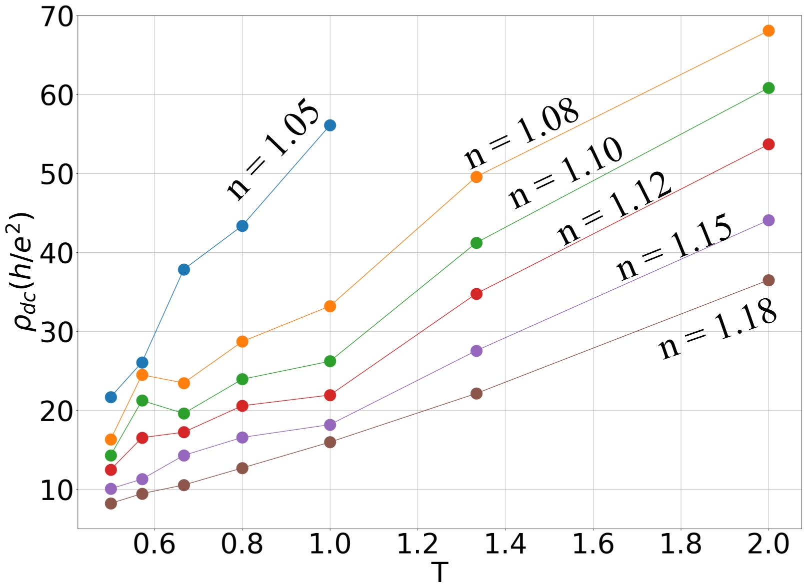

- $N_0$ decreases with increasing T.

No pseudo-gap phase present in the doping window where Luttinger volume violation is observed.

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

Obtain conductivity from: $\Lambda_{xx}(0,\omega) = \int d\omega \frac{e^{-\omega\tau}}{1-e^{-\beta\omega}}\sigma(0,\omega)$

**MaxEnt**




$\rho_{DC}$ increases without saturating!

In the doping window where Luttinger theorem is violated, bad metallic behavior is observed. A pseudogap is not necessarily observed.

# Summary

- At intermediate temperatures, doped Hubbard model violates Luttinger's theorem in a finite doping window near half filling.
- Anomalous Luttinger breaking phase proliferates with temperature. Doping at which Luttinger count is recovered shows non monotonicity with increasing T.
- Luttinger breaking phase T linear DC resistivity, possible bad metallic phase. No pseudogap behavior observed in this phase.

References: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2. ***Topological Approach to Luttinger's Theorem and the Fermi Surface of a Kondo Lattice,*** Masaki Oshikawa, **Phys. Rev. Lett. 84, 3370**
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4. ***Pseudogap and Fermi-Surface Topology in the Two-Dimensional Hubbard Model**,* Wei Wu, Mathias S. Scheurer, Shubhayu Chatterjee, Subir Sachdev, Antoine Georges, and Michel Ferrero **Phys. Rev. X 8, 021048**
5. ***DC Hall coefficient of the strongly correlated Hubbard model**,* Wen O.Wang, Jixun K. Ding, Brian Moritz, Edwin W. Huang and Thomas P Devereaux, **npj Quantum Materials volume 5, Article number: 51 (2020)**
6. ***Change of carrier density at the pseudogap critical point of a cuprate superconductor**,* S. Badoux, W Tabis, F. Laliberte, G. Grissonnanche, B. Vignolle, D. Vignolles, J. Beard, D. A. Bonn, W.N. Hardy, R. Liang, N. Doiron-Leyraud, Louis Taillefer, Cyril Proust, Nature volume 531, pages 210-214 (2016)

# Backup slides

# Onset of Luttinger breaking phase

Black solid line

$$\Theta[\mathrm{Re}G(k,0)]$$

White dashed line

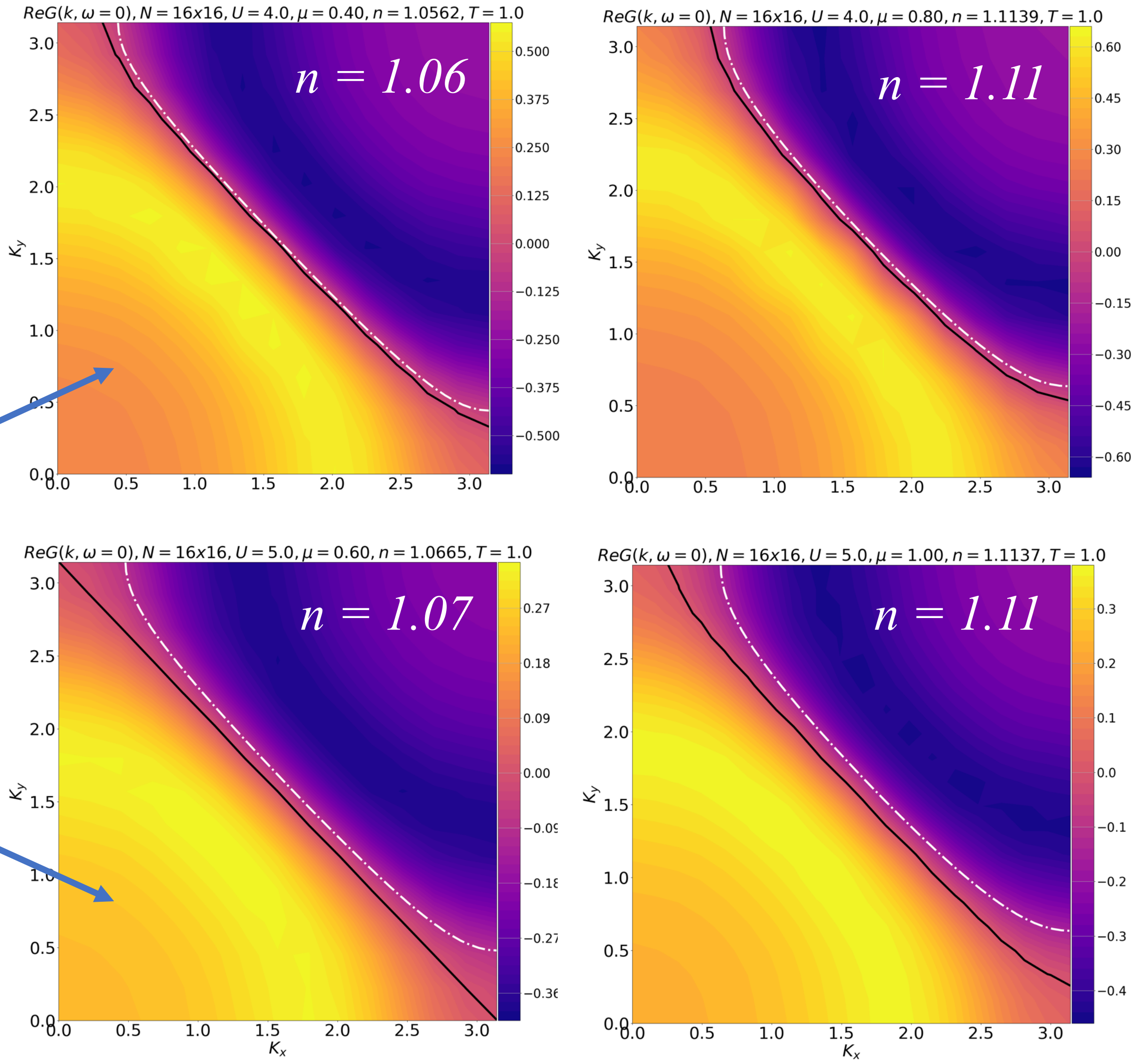
$$\varepsilon_k - \mu(n,T) = 0$$

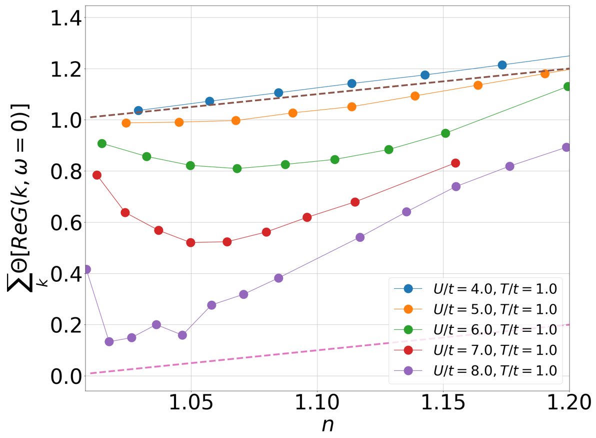
U/t = 4, T/t = 1.0

Luttinger volume preserved !

U/t = 5, T/t = 1.0

Luttinger volume violated !



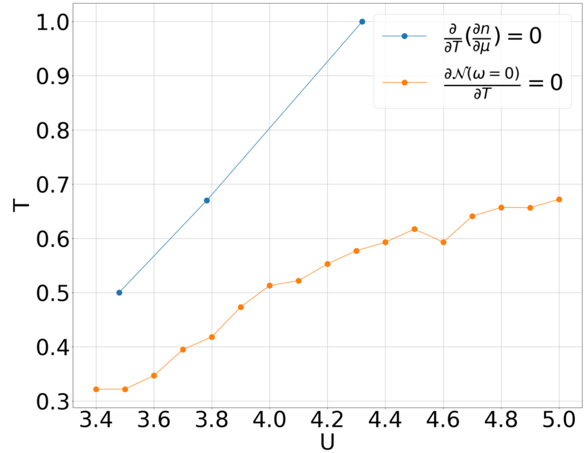




Many body (thermodynamic) gap:

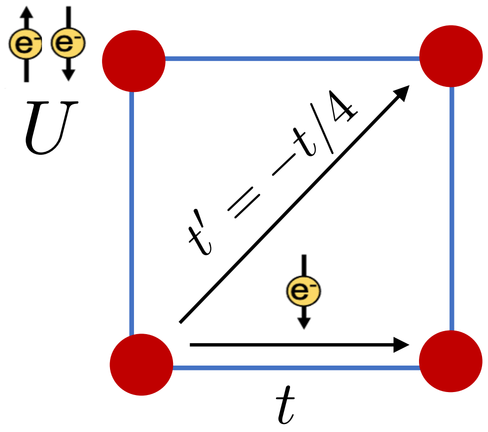
$$\frac{\partial}{\partial T}\left(\frac{\partial n}{\partial \mu}\right) = 0$$

Single particle gap:

$$\frac{\partial \mathcal{N}(0)}{\partial T} = 0$$

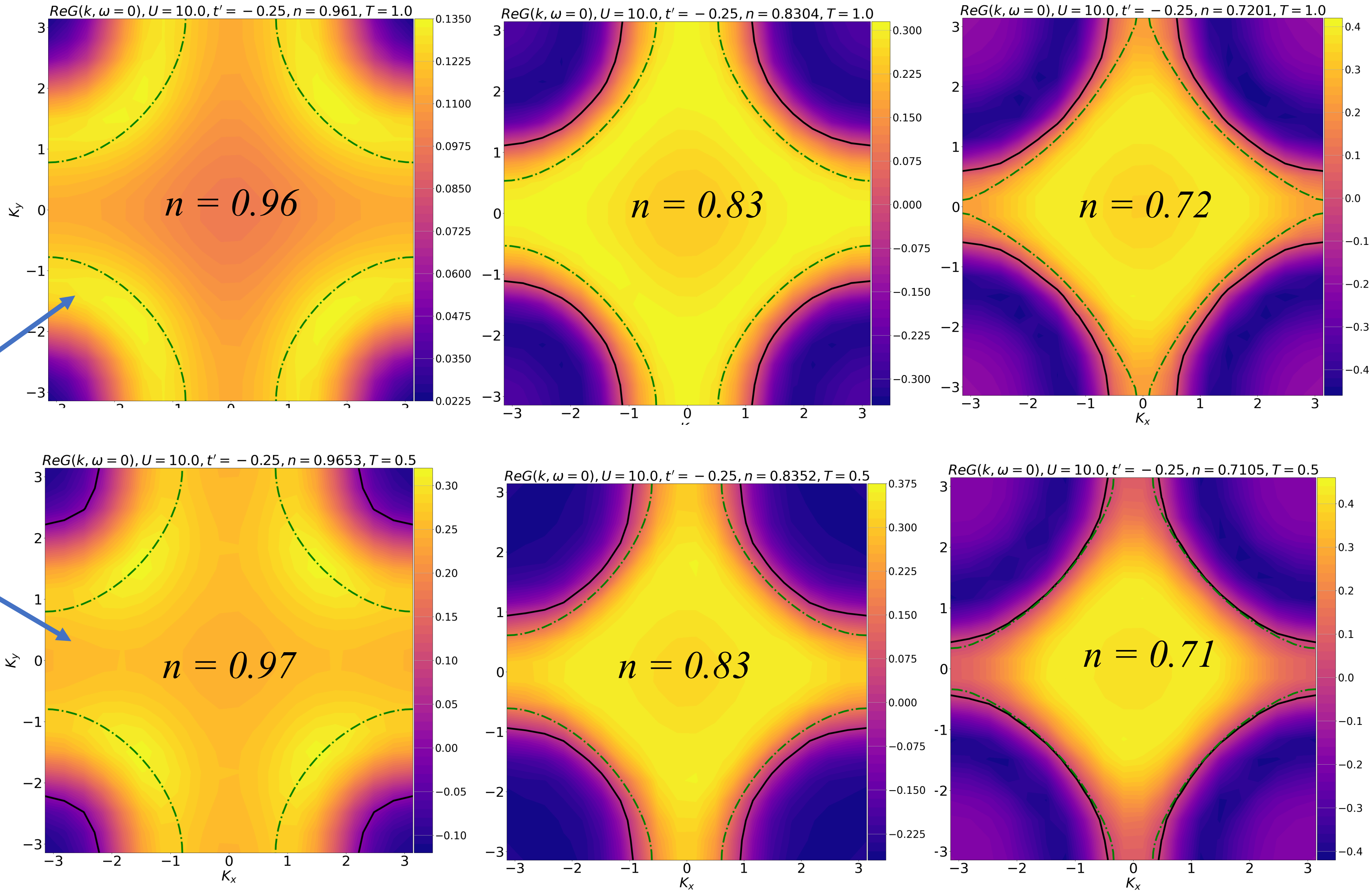


# Effect of next nearest neighbor hopping




U/t = 10, T/t = 1.0

U/t = 10, T/t = 0.5

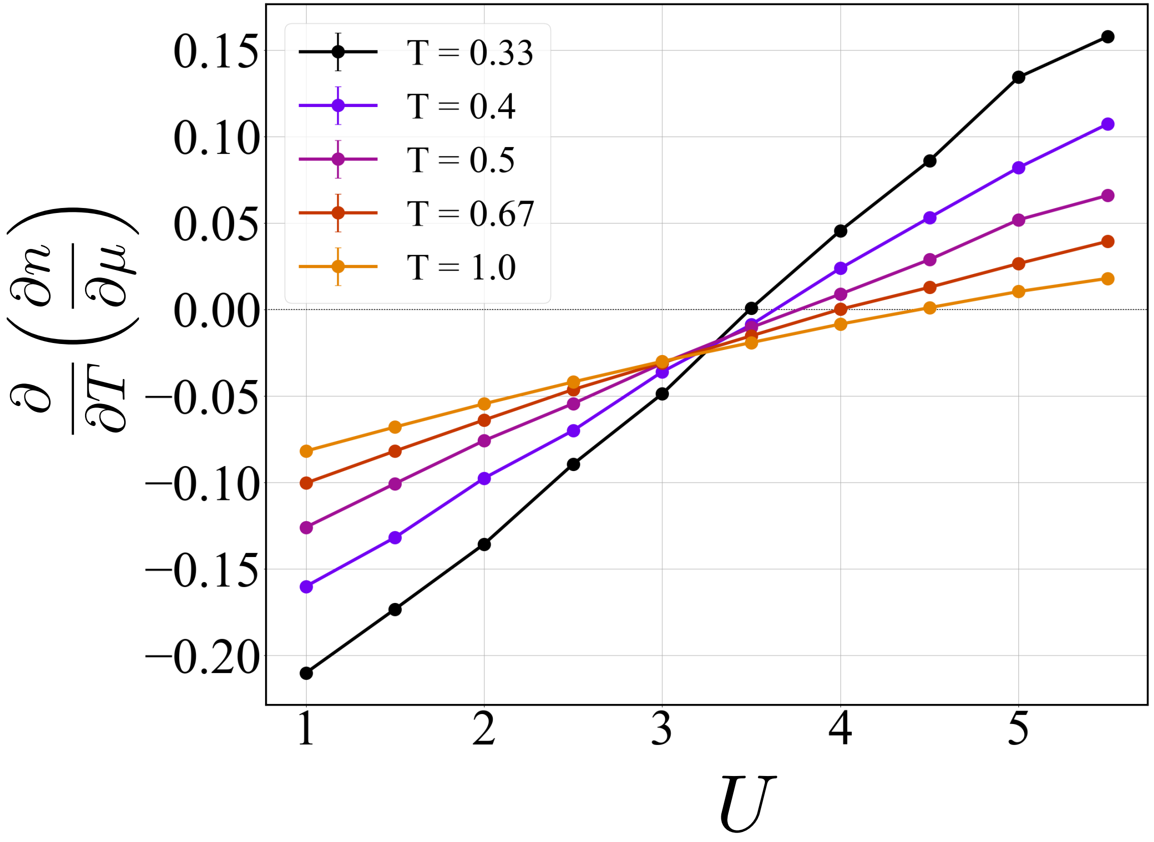



Breaking particle hole symmetry preserves Luttinger theorem violation!

# Estimation of many body and single particle gaps

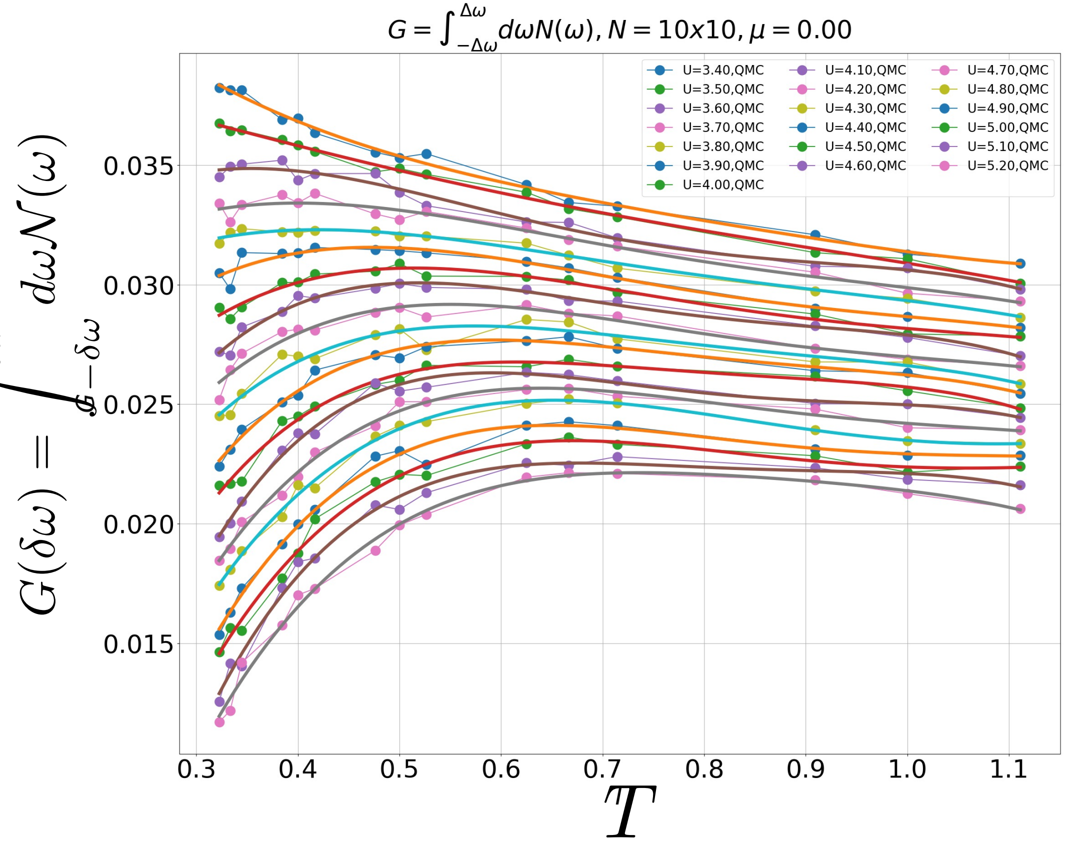
## Many body gap – from compressibility

$$\frac{\partial}{\partial T}\left(\frac{\partial n}{\partial \mu}\right) = 0$$




## Single particle gap – from LDOS

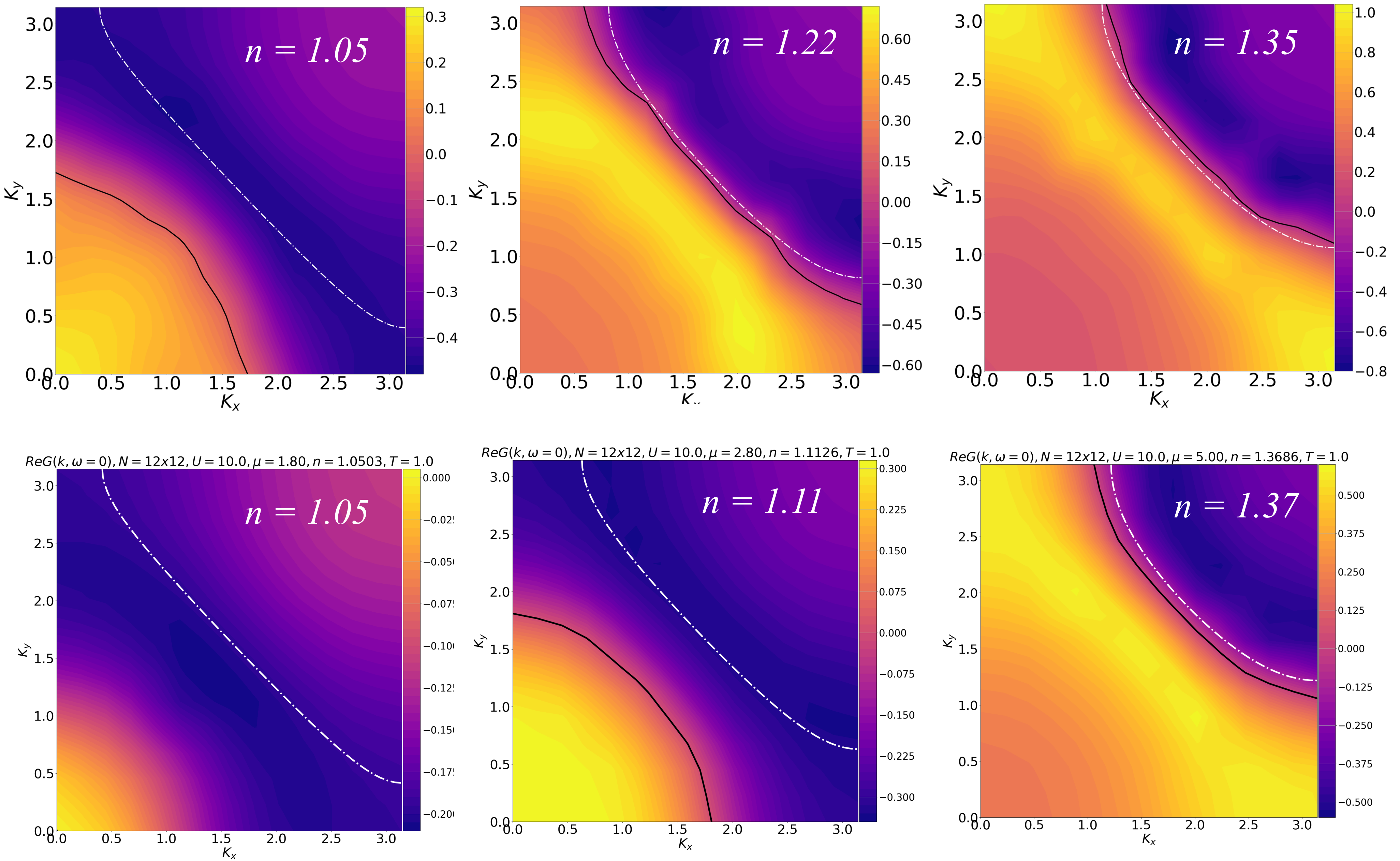
$$\frac{\partial \mathcal{N}(0)}{\partial T} = 0$$



# Spectral functions on Fermi surface

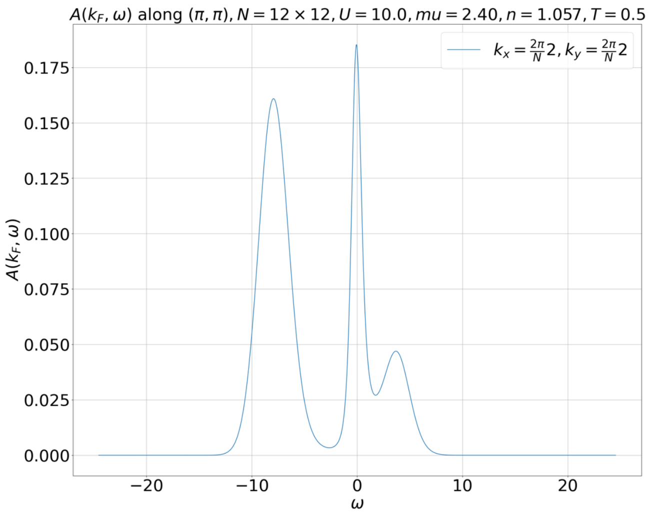
U/t = 10, T/t = 0.5

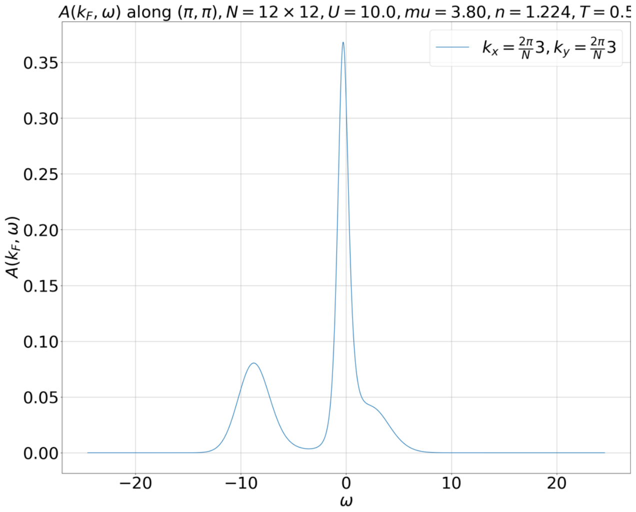
U/t = 10, T/t = 1.0

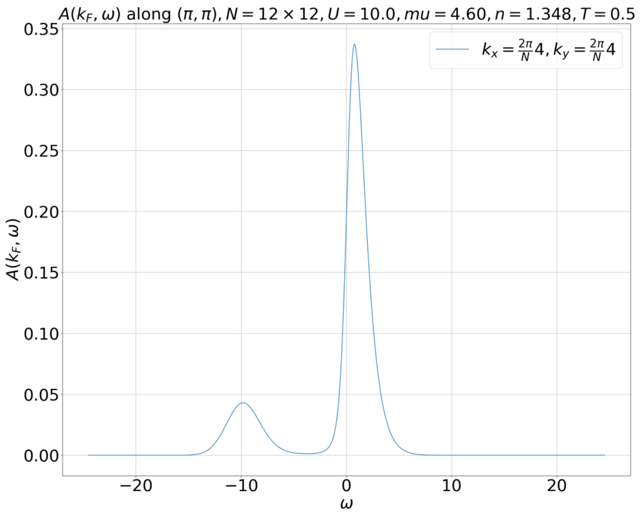


# Spectral functions on Fermi surface

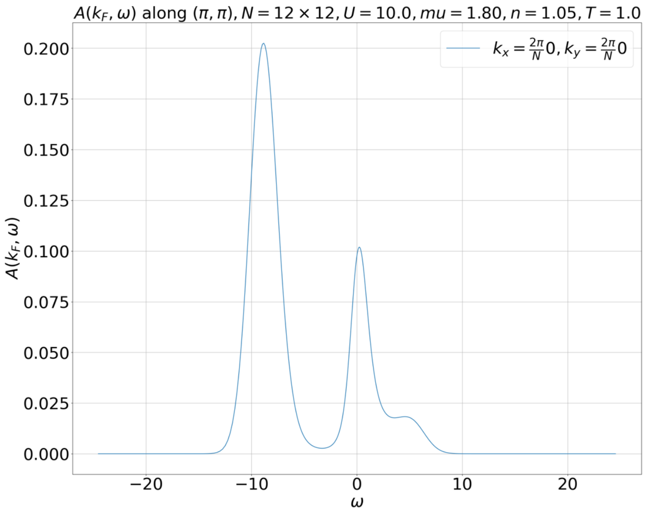
U/t = 10, T/t = 0.5

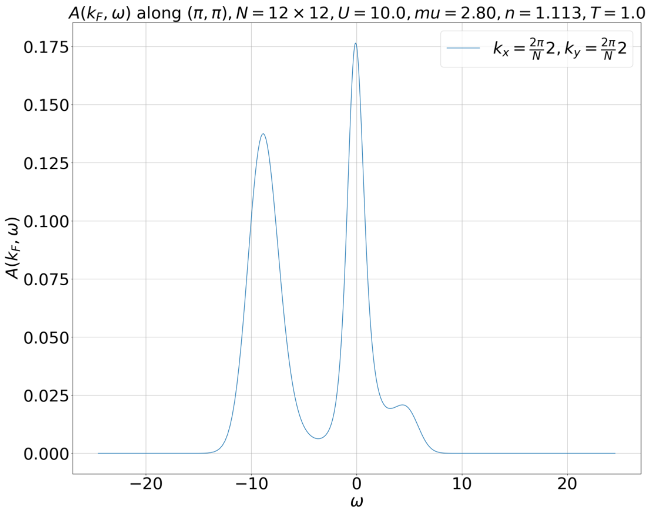


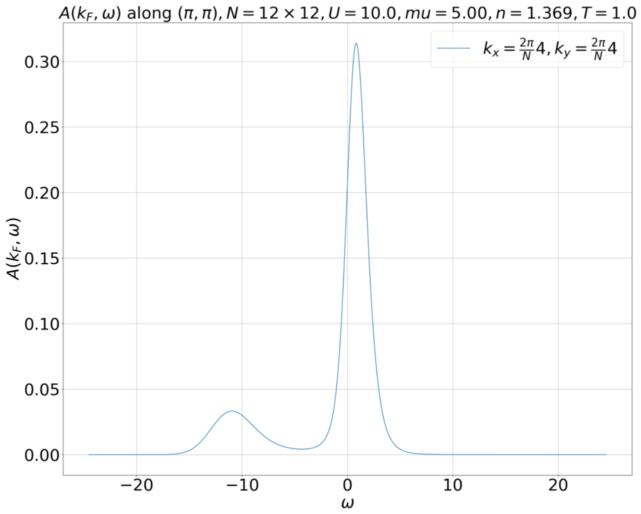




U/t = 10, T/t = 1.0

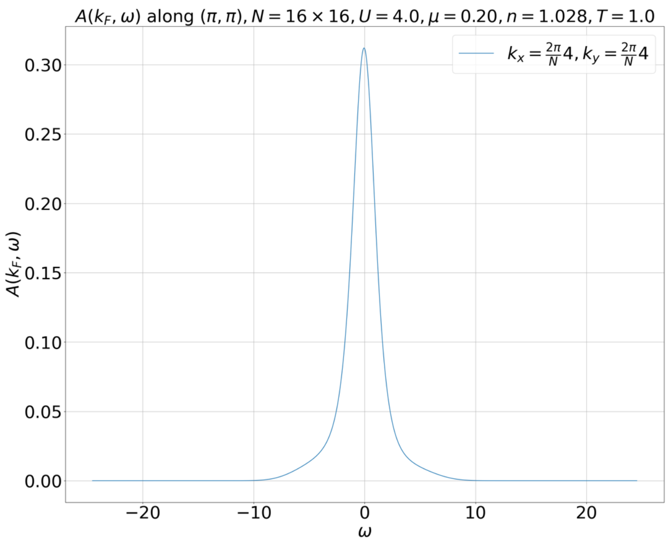


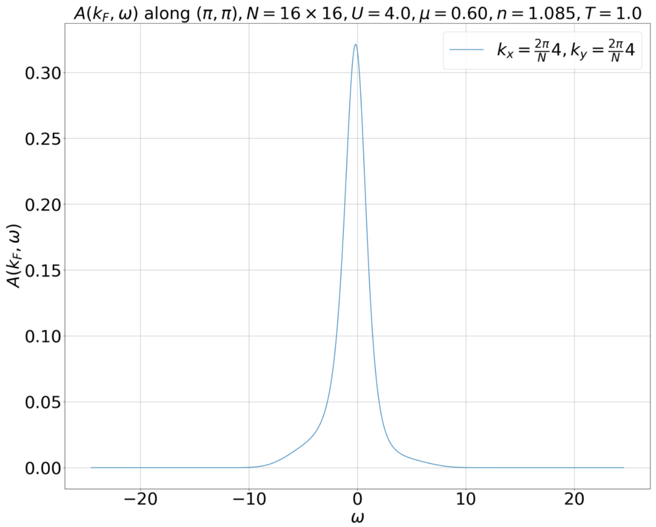



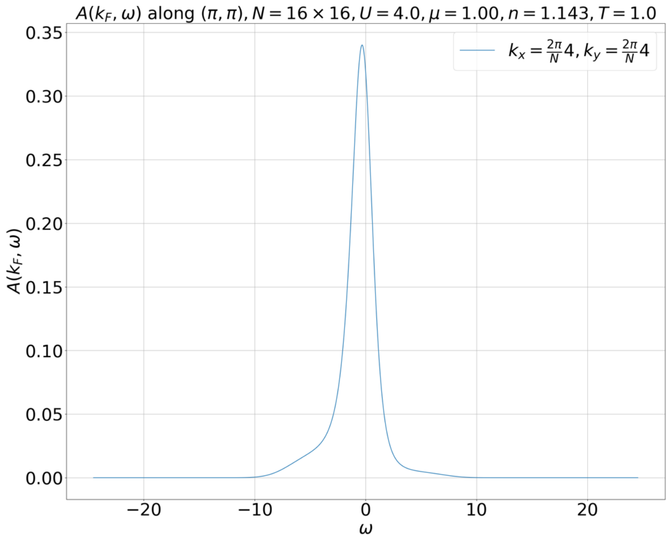



# Spectral functions on Fermi surface

U/t = 4, T/t = 1.0




U/t = 7, T/t = 1.0