Moment formation in the repulsive Hubbard model

Sayantan Roy[1]

Collaborators

Sameed Pervaiz[1], Abhisek Samanta[1], Thomas Hartke[2], Martin Zweirlein[2],
Thereza Paiva[3] and Nandini Trivedi[1]

[1]Ohio State University, [2] Massachussetts Institute of Technology,
[3]UFRJ Brazil

Roadmap

- Background(Hubbard Model, experiments)
- Definition of correlators
- Probing moment formation
- Comparison with experiments
- Summary

Repulsive Fermi Hubbard model

- Hubbard model – parent model for high T_c cuprate superconductors

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

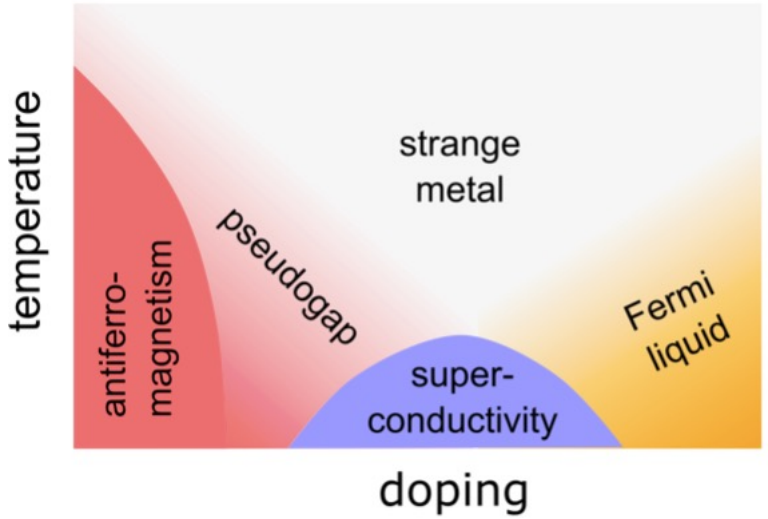
Two characteristic energy scales

Charge fluctuations: Δ_C

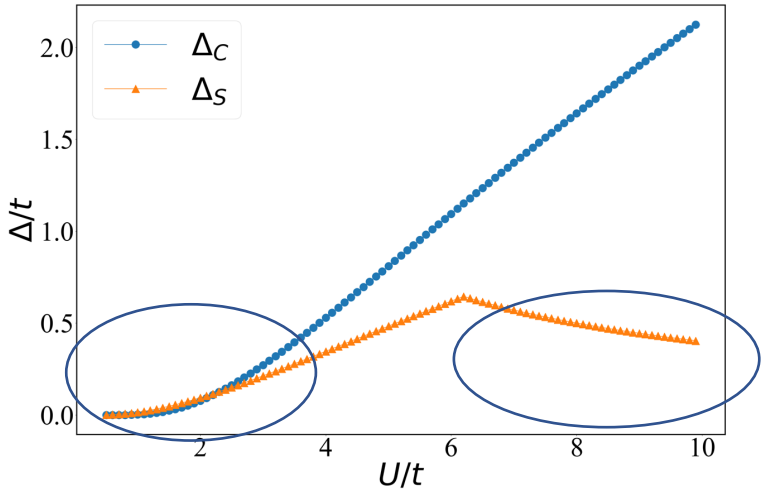
(Motion of doublon/holon)

Spin fluctuations: Δ_S

(Amplitude and phase fluctuations of moments)



I. Weak coupling



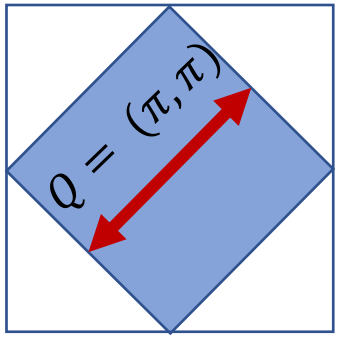
Band instability (RPA)

Local moments (t/U expansion)

Susceptibilities at half filling – Perfect nesting!

$$\chi^{00}_{RPA}(q,\omega) = \frac{\chi^{00}_0(q,\omega)}{1 + U\chi^{00}_0(q\omega)}$$

$$\chi^{ij}_{RPA}(q,\omega) = \frac{\chi^{00}_0(q,\omega)}{1 - U\chi^{00}_0(q\omega)}\delta_{ij}$$

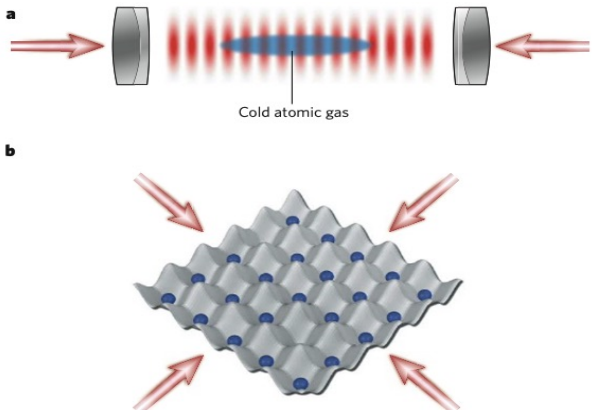


II. Strong coupling?

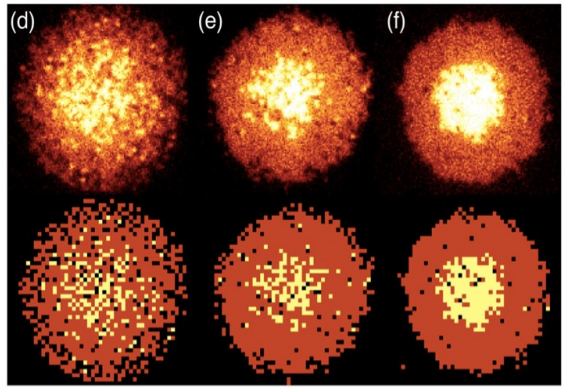
AFM Heisenberg, *t-J* model ….

Local moment formation, AFM order and correlations

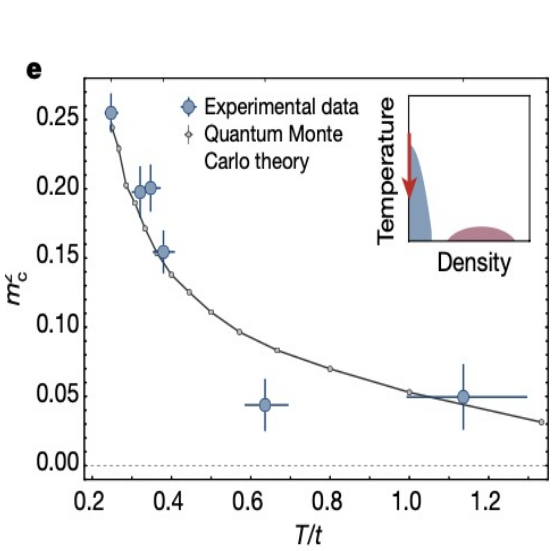
Experiments (Cold atom emulators)

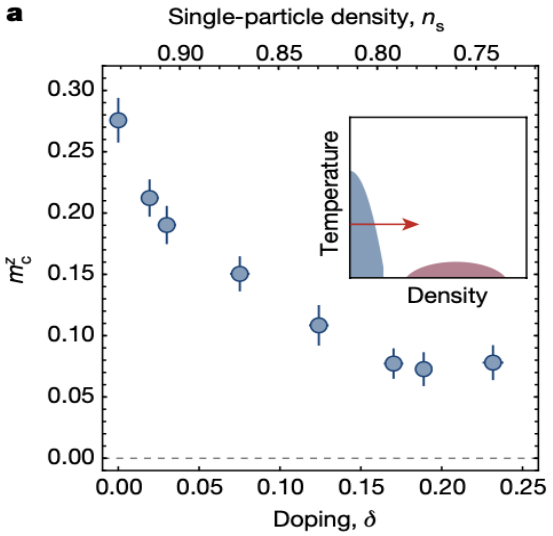


I. Bloch, Nature Physics **1**, pages 23–30 (2005)



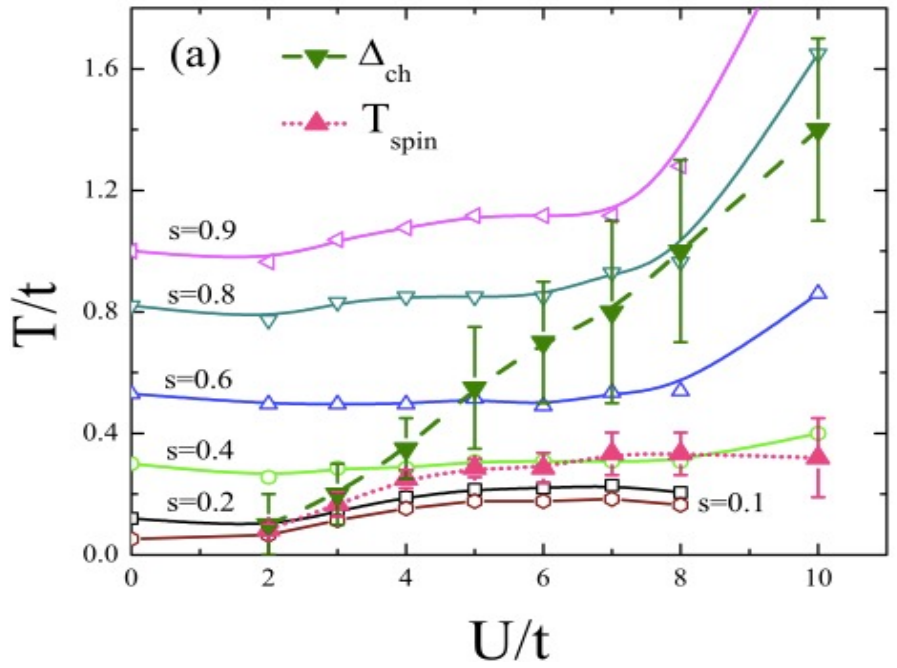
T. Hartke, B.Oreg, N. Jia, and M. Zwierlein Phys. Rev. Lett. **125**, 113601 (2020)





A. Mazurenko, C. S. Chiu, G. Ji, M. F. Parsons, M. Kan´asz-Nagy, R. Schmidt, F. Grusdt, E. Demler, D. Greif, and M. Greiner- Nature **545**, pages 462–466 (2017)

Simulations(DQMC)

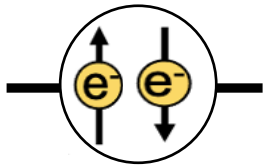


T. Paiva, R.Scalettar, M. Randeria, and N. Trivedi, Phys. Rev. Lett. **104**, 066406 (2010)

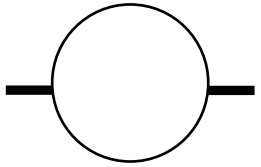
- Correlation functions can map out phase by varying U, T, δ
- Correlations can be verified in experiments.
- Behavior of correlation functions wrt to T and U ?
- Propose new correlators for understanding local moment formations?

Moments, Doublons and Holons

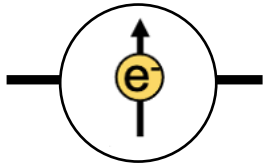
- Doublon: $d_i = n_{i\uparrow} n_{i\downarrow}$



- Holon: $h_i = (1 - n_{i\uparrow})(1 - n_{i\downarrow})$
  $= 1 - n_i + d_i$

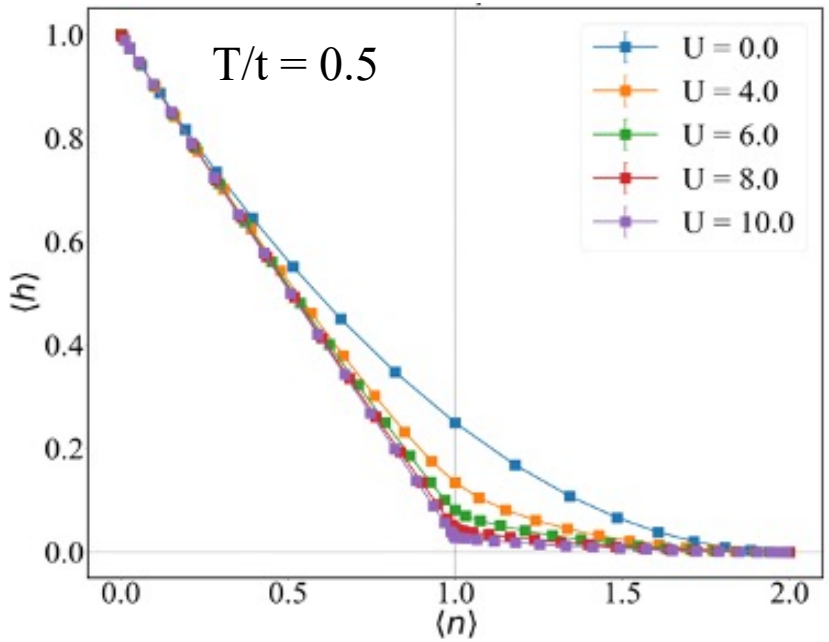


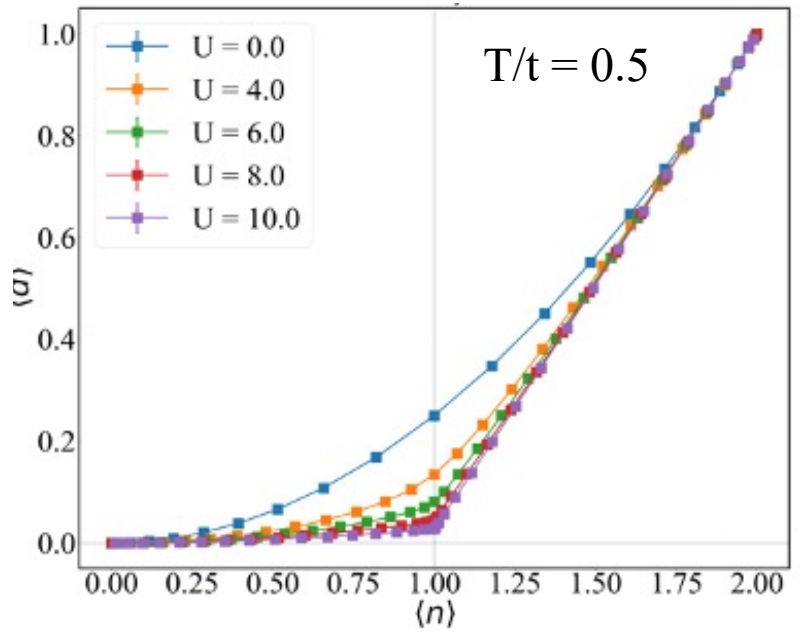
- Local moment: $m_i^2 = (n_{i\uparrow} - n_{i\downarrow})^2$
  $= n_i - 2d_i$

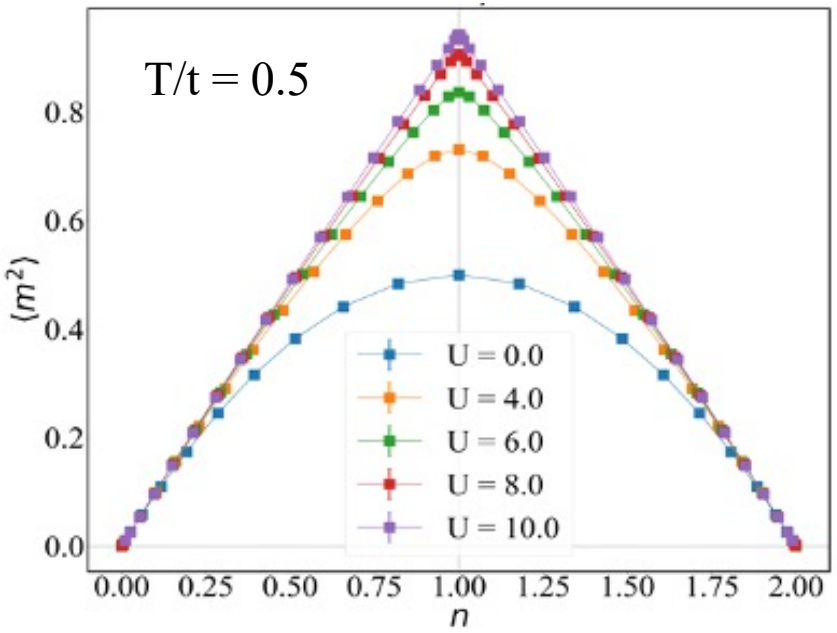


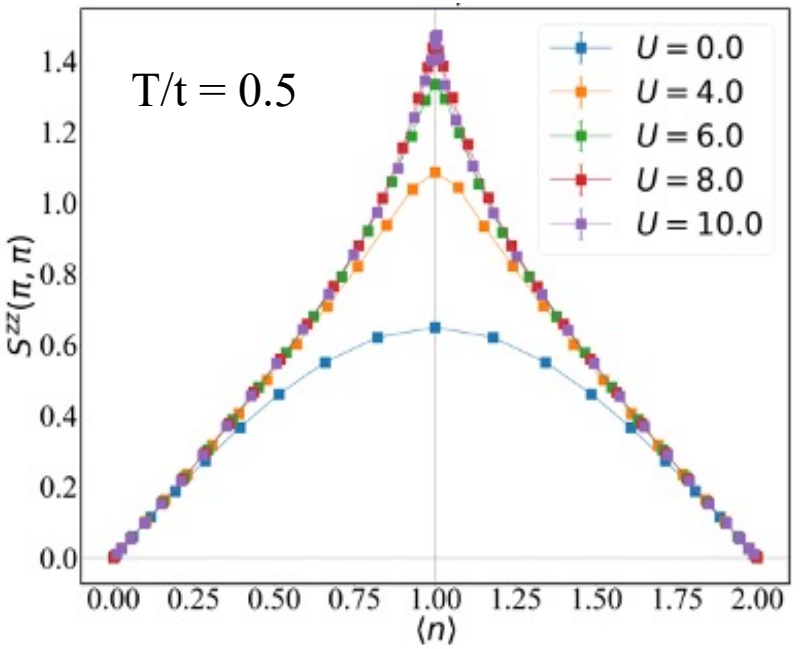
- Magnetic order characterized by

$$S^{zz}(q) = \sum_r e^{iqr} \langle S^z(r) S^z(0) \rangle$$









Correlation functions

With $h_i = 1 - n_i + d_i \ , \quad m_i^2 = n_i - 2d_i$

$$\langle h_i d_j \rangle_C = \langle h_i d_j \rangle - \langle h_i \rangle \langle d_j \rangle$$

$$\langle n_i n_j \rangle_C = \langle d_i d_j \rangle_C + \langle h_i h_j \rangle_C - 2\langle h_i d_j \rangle_C$$

Hartke et al(2020)

$$\langle m_i^2 m_j^2 \rangle_C = \langle n_i n_j \rangle_C + 4\langle h_i d_j \rangle_C$$

$$\langle S_i^z S_j^z \rangle_C = \langle S_i^z S_j^z \rangle - \langle S_i^z \rangle \langle S_j^z \rangle$$

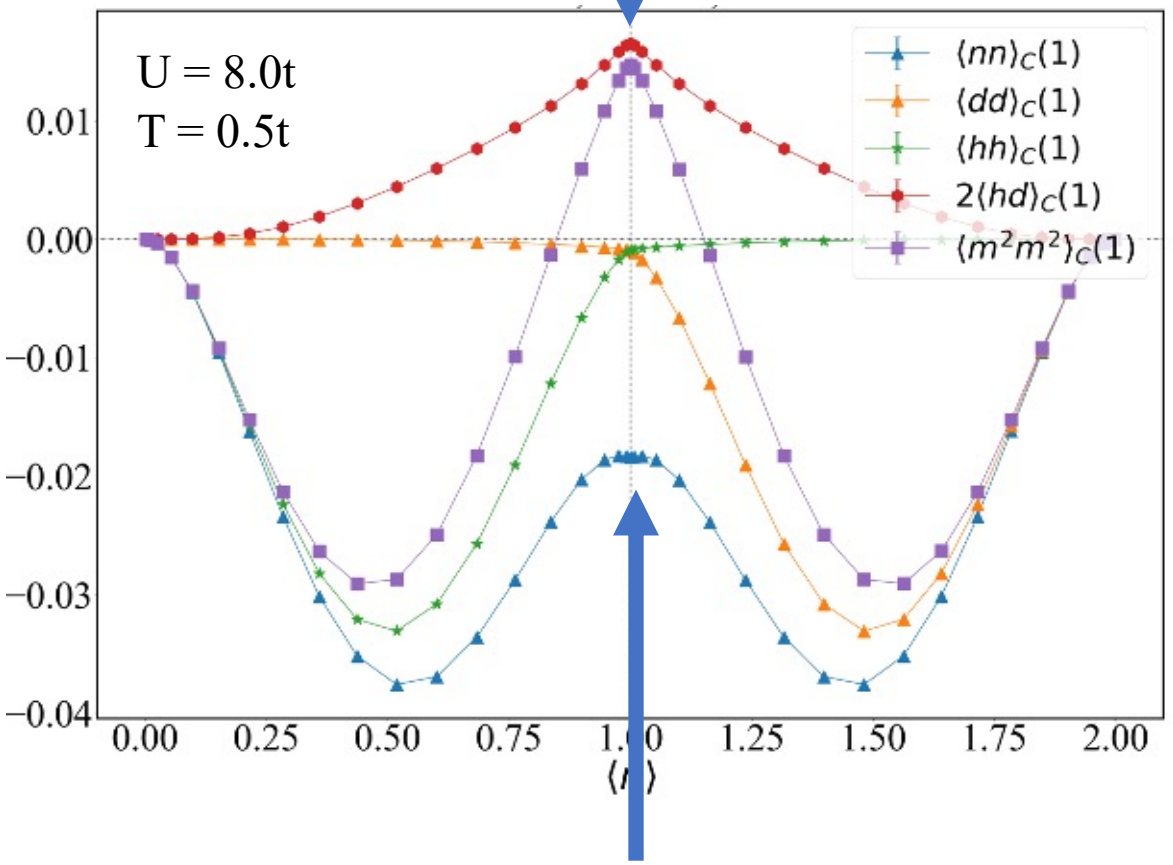
Cold atom experiments [Mazurenko et al(2016), Cheuk et al(2016)..]

$$\langle m_i^2 d_j \rangle_C = \langle n_i d_j \rangle_C - 2\langle d_i d_j \rangle_C$$

$$\langle m_i^2 h_j \rangle_C = 3\langle n_i d_j \rangle_C - 2\langle d_i d_j \rangle_C - \langle n_i n_j \rangle_C$$

$\langle m_i^2 d_j \rangle_C$ and $\langle m_i^2 h_j \rangle_C$ indicate local charge fluctuations destroying local moments

Formation of local moments enhanced



Mott gap opens

Moment correlation function

- Local moment formation – characterized by

$$\langle m_i^2 m_j^2 \rangle_c = \langle m_i^2 m_j^2 \rangle - \langle m_i^2 \rangle \langle m_j^2 \rangle$$

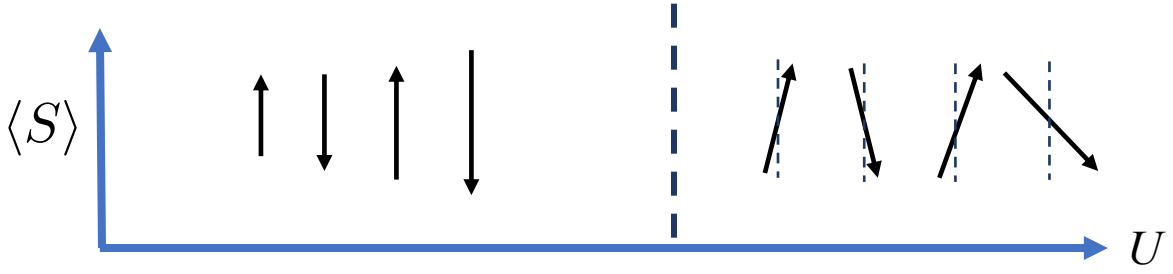
Region I – Formation of local moments due to low no of d_i ,h_i

Region II – Suppression of local moments due to high no of d_i ,h_i

Region I: Two distinct behaviors

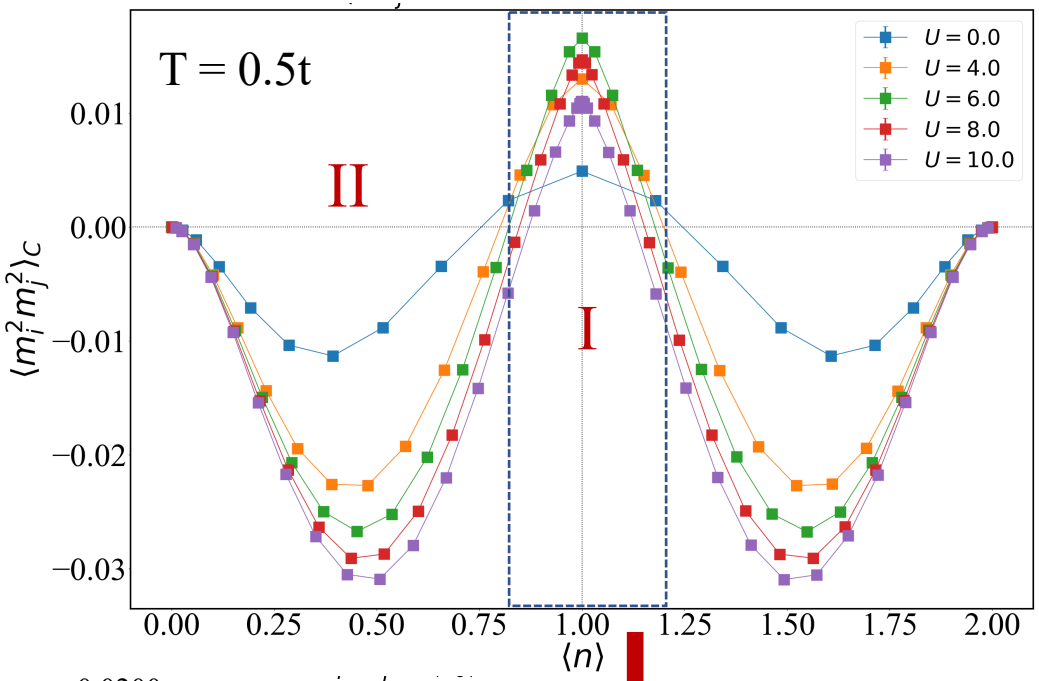
A : Amplitude fluctuations

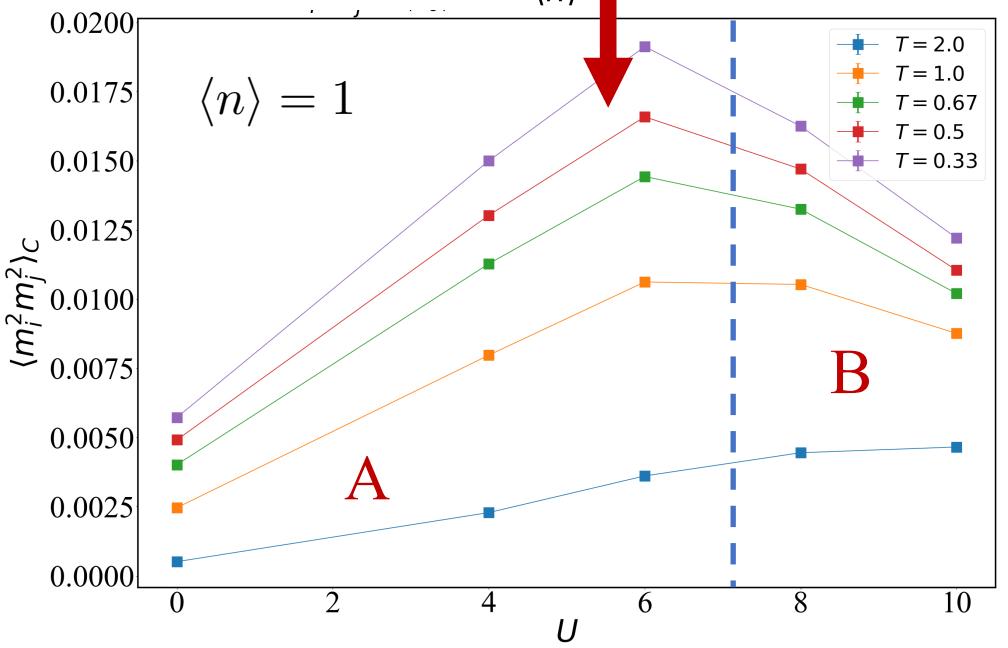
B: Phase fluctuations



- "Softening" of correlations at n=1 due to phase fluctuations!
- Correlations can track Δ_s by varying U

Region II: Suppression of moments increase monotonically with U



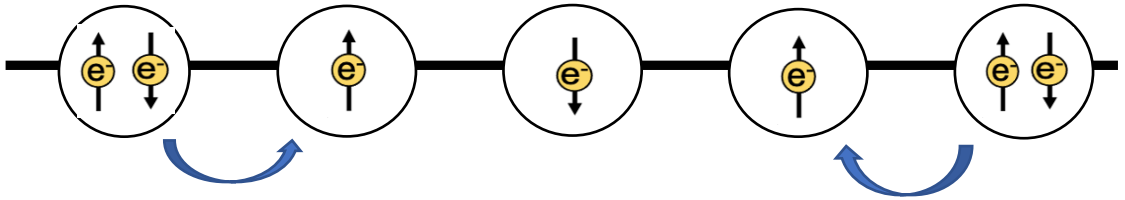


Doublon, Holon correlations and local moment formation

- Moment moment correlation has two parts

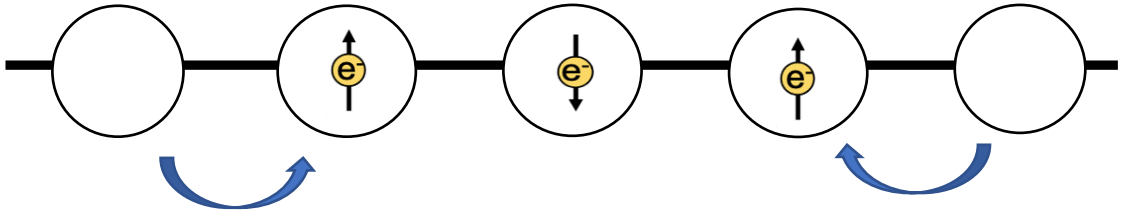
$$\langle m_i^2 m_j^2 \rangle_c = -[\langle m_i^2 d_j \rangle_C + \langle m_i^2 h_j \rangle_C]$$

$\langle m_i^2 d_j \rangle_c = \langle m_i^2 d_j \rangle - \langle m_i^2 \rangle \langle d_j \rangle$ involves fluctuations :



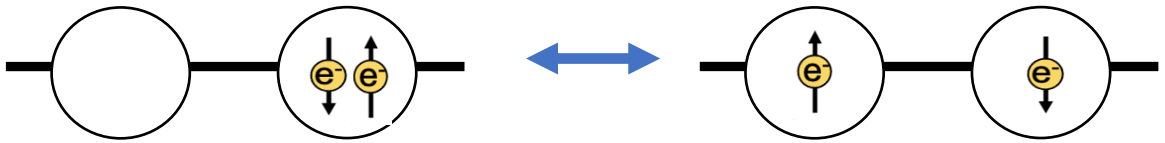
n>1, suppression by doublons!

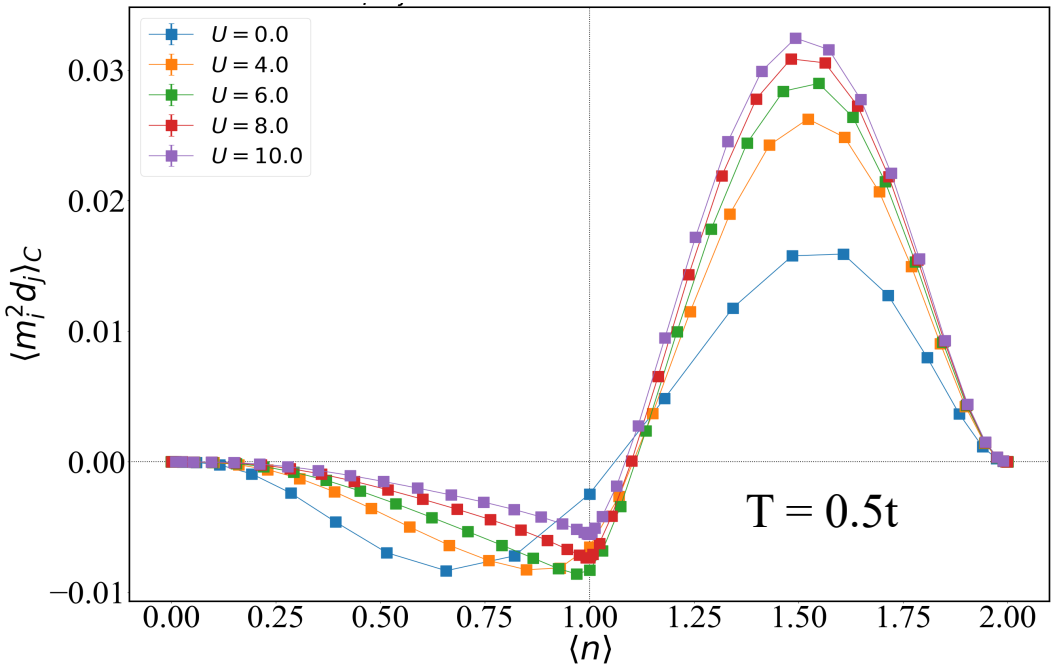
$\langle m_i^2 h_j \rangle_c = \langle m_i^2 h_j \rangle - \langle m_i^2 \rangle \langle h_j \rangle$ involves fluctuations :

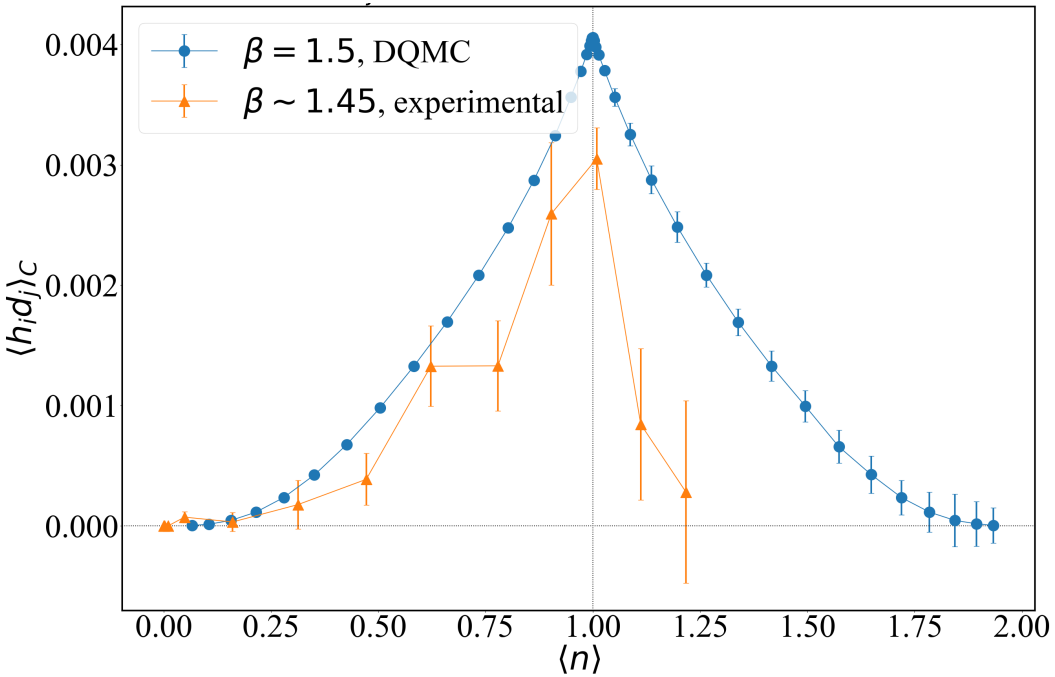


n<1, suppression by holons!

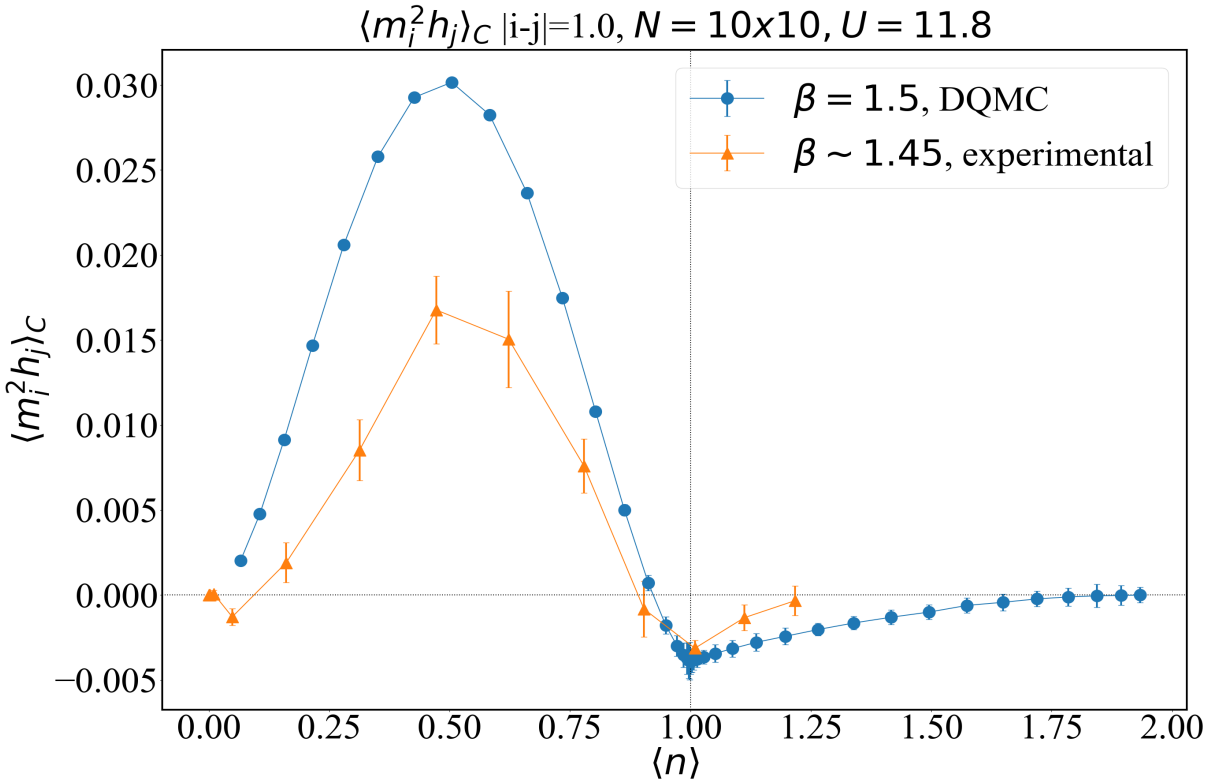
Close to half filling, system favors doublon holon fluctuations:

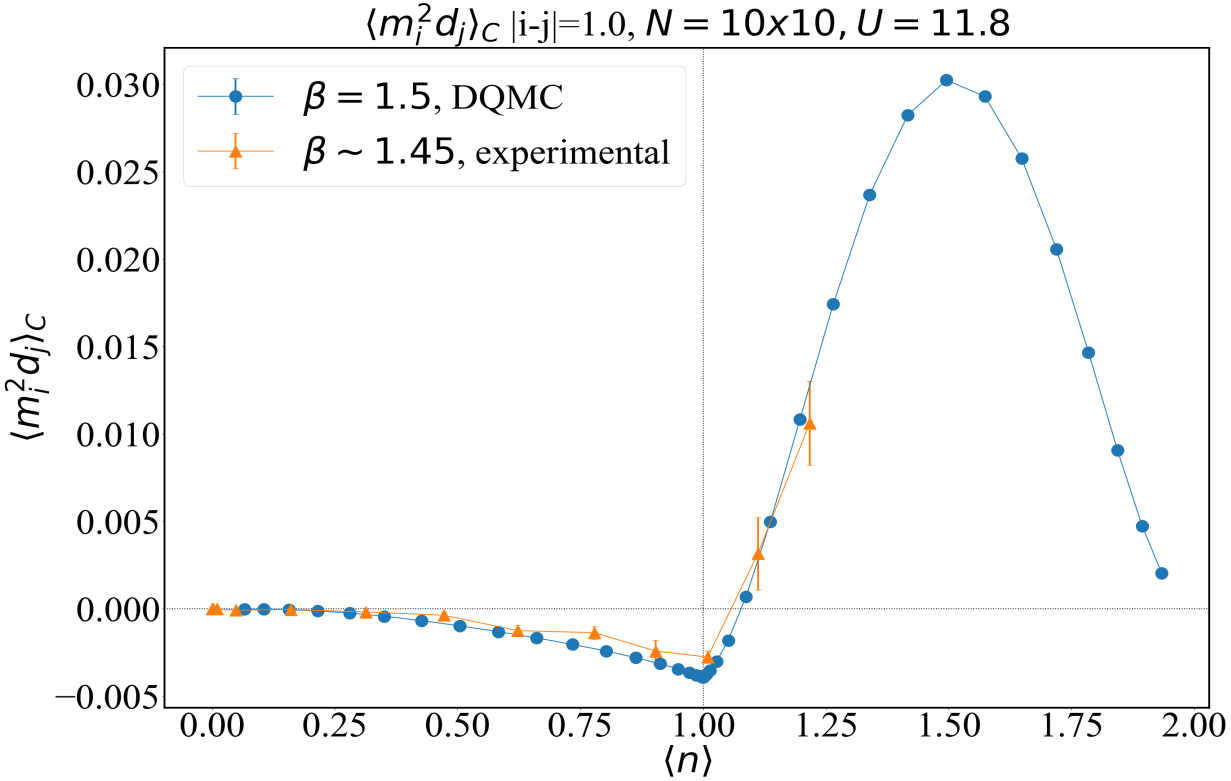






Can these correlations be observed in experiments?





Summary

- Local correlations can reveal exotic nature of ground states.
- Cold atom emulators and simulations can probe temperature and interaction strength dependence of correlators.
- In repulsive Fermi Hubbard model, spin gap can be tracked by moment moment correlation functions.
- Doublon and holons destroy local moments by charge fluctuations.
- New correlators proposed that capture local moment formation, can be verified experimentally.

Ongoing work

- Parton Mean field theory to understand correlation functions.

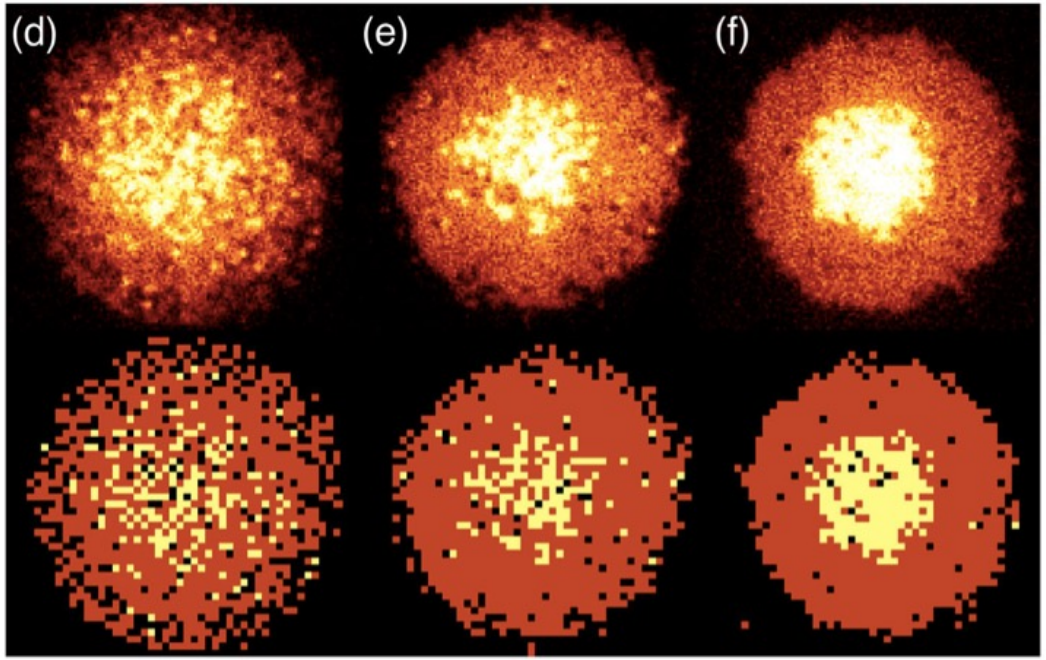
$$\left.\begin{aligned}\hat{c}^{\dagger}_{i\sigma} &= \hat{f}^{\dagger}_{i\sigma}\hat{h}_i + \sigma \hat{f}_{i\bar{\sigma}}\hat{d}^{\dagger}_i \\ \hat{c}_{i\sigma} &= \hat{h}^{\dagger}_i \hat{f}_{i\sigma} + \sigma \hat{d}_i \hat{f}^{\dagger}_{i\bar{\sigma}}\end{aligned}\right\}$$

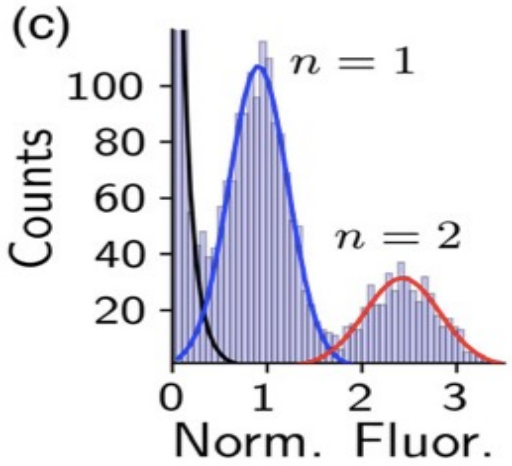
Neel ordered state: $\langle \hat{f}^{\dagger}_{i\uparrow} \rangle = b_i e^{i\theta_i}$

Backup slides

Fluctuation thermometry

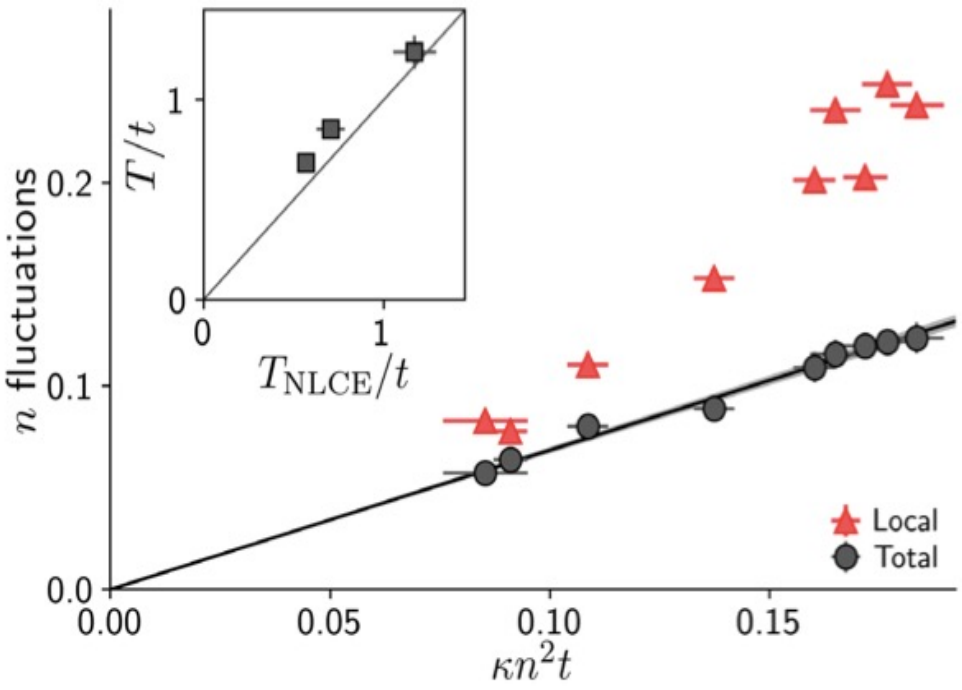
PRL 125, 113601 (2020) T.Hartke , B.Oreg , N.Jia, and M.Zwierlein



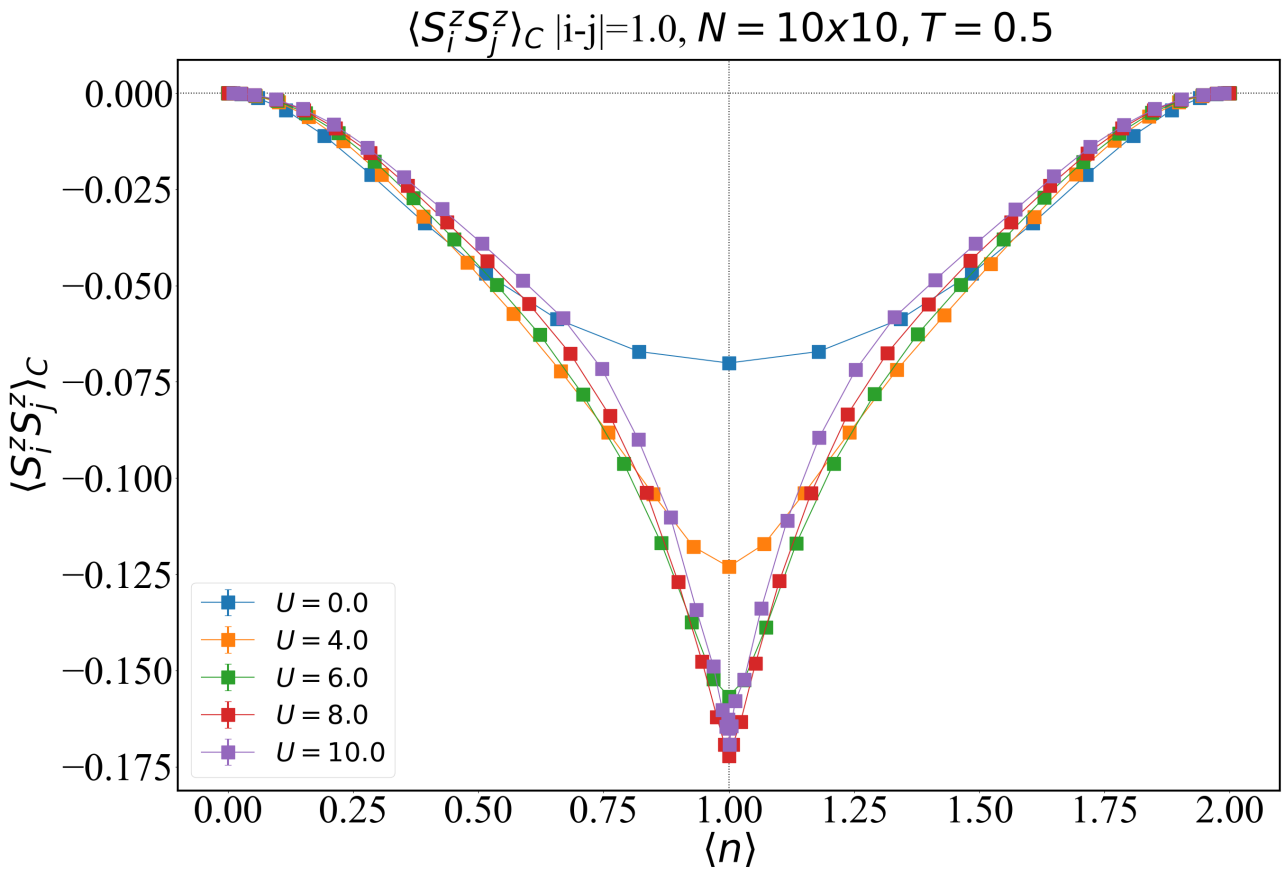


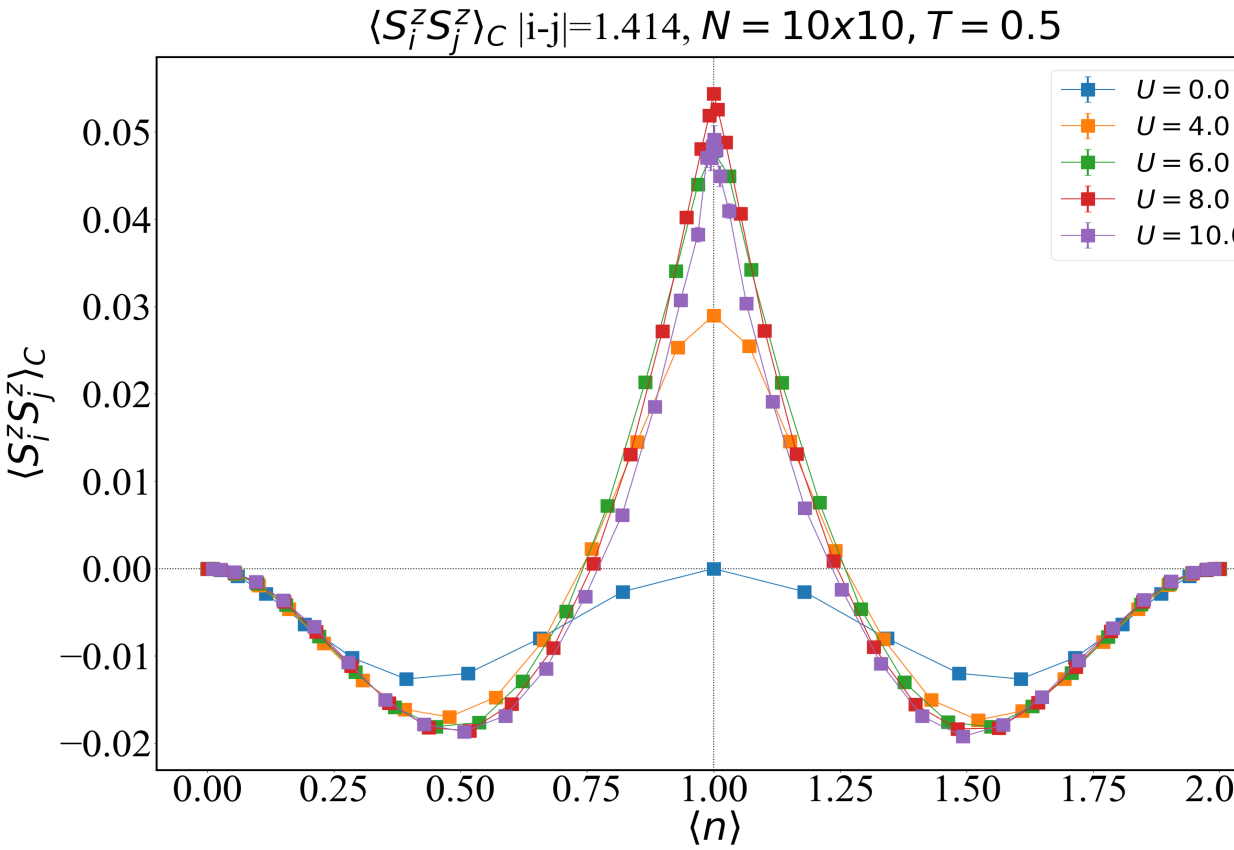
Fluctuation dissipation theorem

$$\kappa n^2 = \beta \sum_{\delta} \langle n_i n_{i+\delta} \rangle_C$$

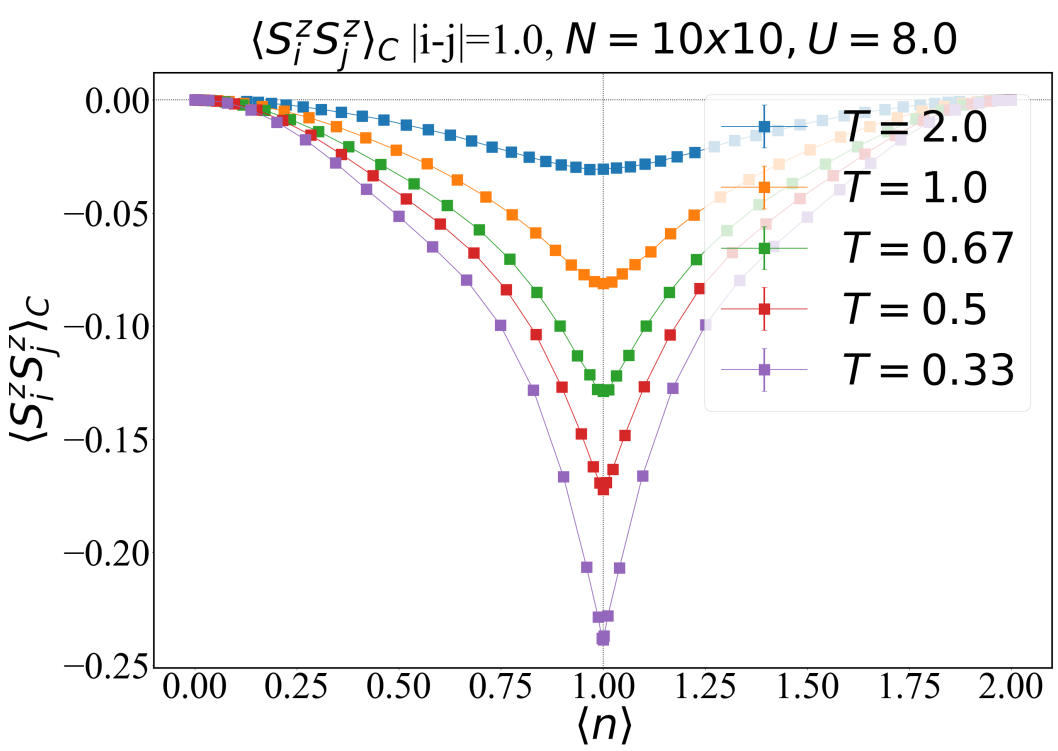


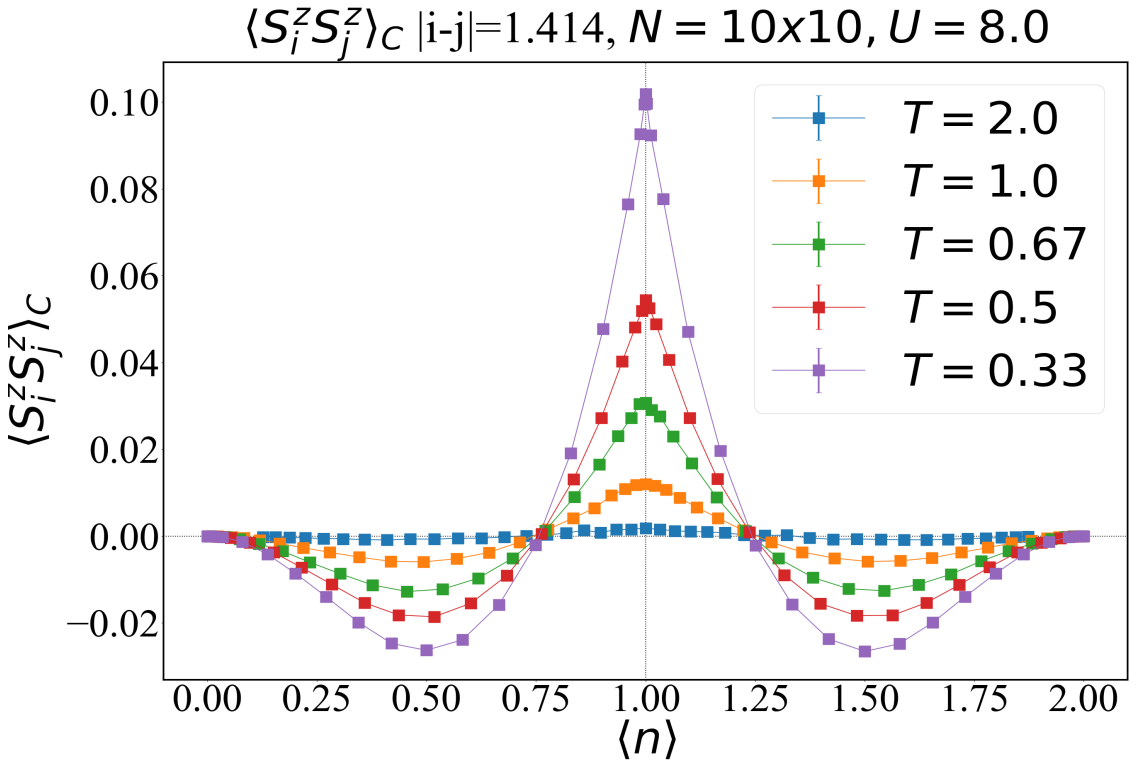
Spin spin correlation functions





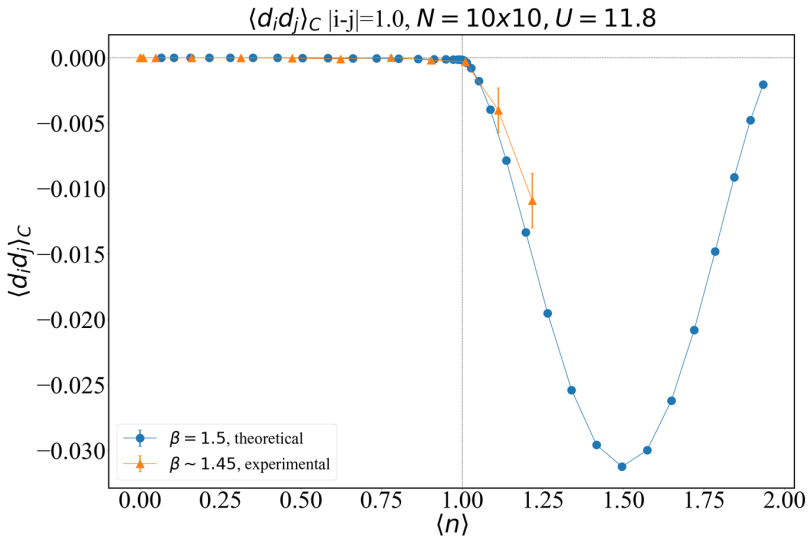
Spin spin correlation functions

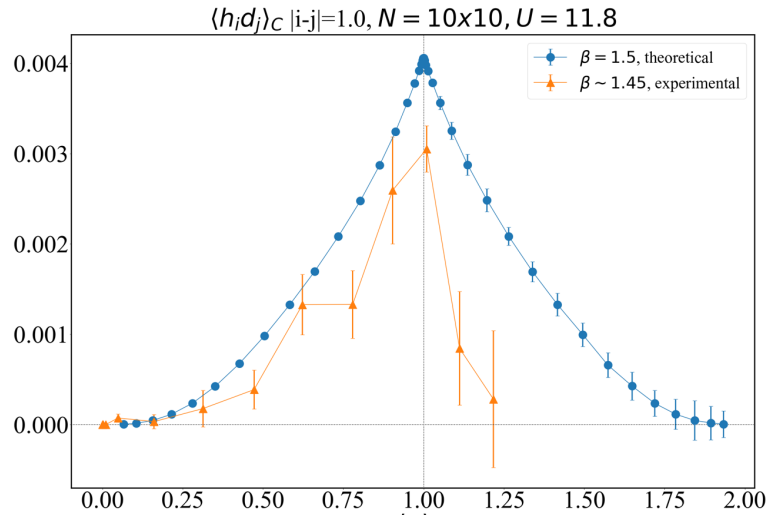


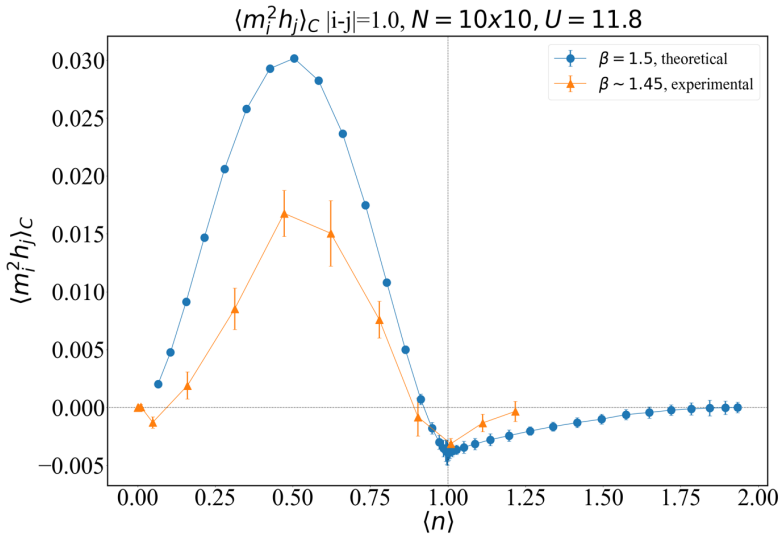


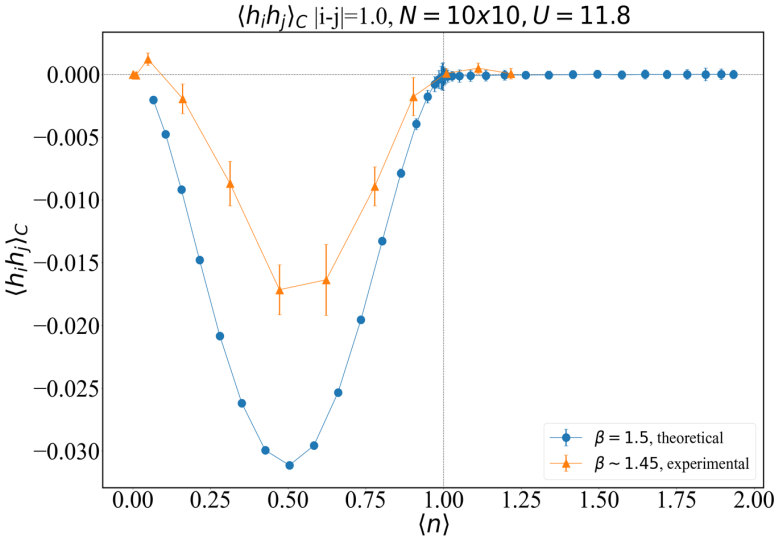
Comparison with experimental data

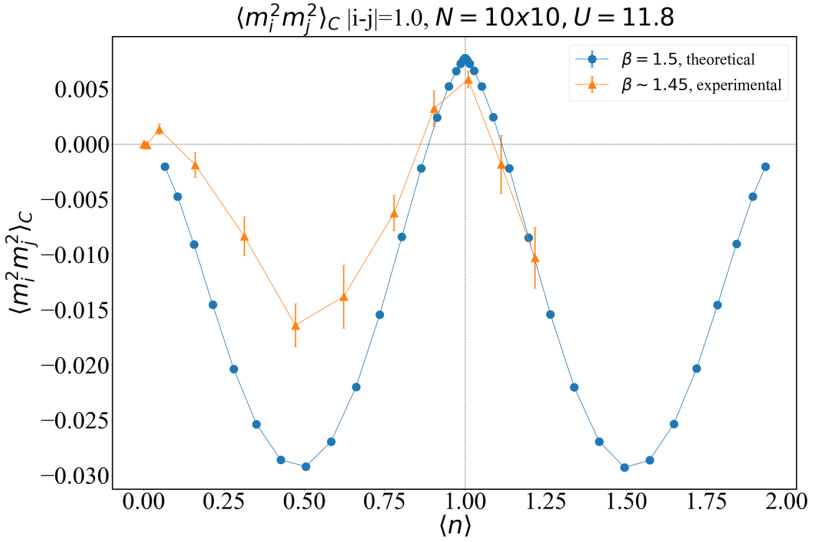
Experimental data from PRL 125, 113601 (2020) T.Hartke , B.Oreg , N.Jia, and M.Zwierlein

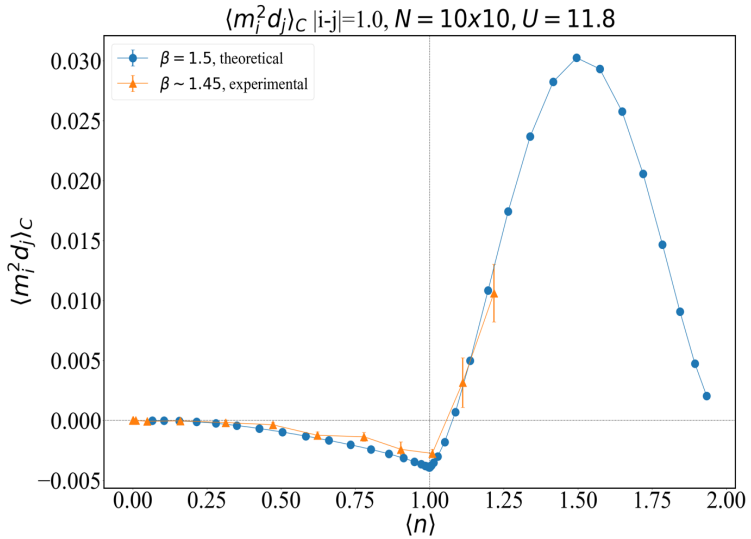












Correlators at half filling