# Renyi entanglement entropy in Hubbard model within dynamical mean field theory

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(Thanking you organizer)

# Quantum Entanglement

- Strange aspects of quantum mechanics (QM) - Superposition, Measurements …

But probably the strangest feature of QM - Entanglement

Example- Bell pair $|\psi\rangle = \frac{|01\rangle + |10\rangle}{\sqrt{2}}$

Two qubits perfectly correlated
➡ "True quantum correlation"

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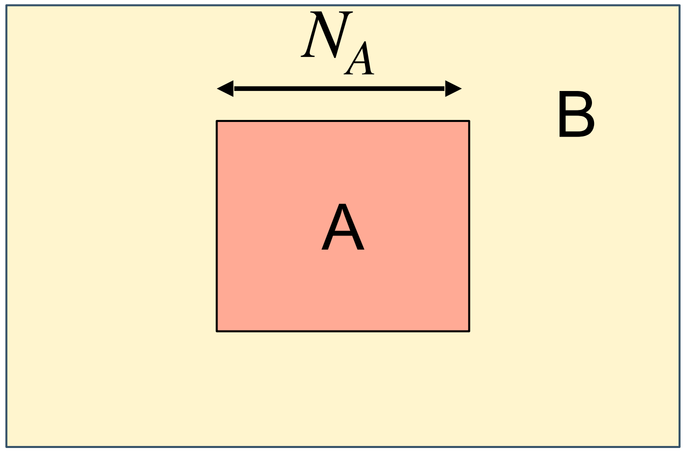
Measure of Entanglement - Entanglement entropy

For state $\rho$ (pure or mixed) - the subsystem reduced density matrix

$$\rho_A = \mathrm{Tr}_B[\rho]$$




Von Neumann entanglement entropy : $S_A = \mathrm{Tr}_A(\rho_A \ln \rho_A)$

$n$-th Renyi entropy : $S^{(n)} = \frac{1}{1-n} \ln \mathrm{Tr}_A[\rho_A^n]$

# Why care about entanglement in condensed matter systems ?

- Entanglement measures can be used to characterize the "true quantum nature" of various symmetry broken, critical and topological (ground) states

$S_A \sim$ Area law $(L^{d-1})$ + Correction

| Physical state | Entropy | Example |
|---|---|---|
| Gapped (brok. disc. sym.) | $aL^{d-1} + \ln(\text{deg})$ | Gapped XXZ [143] |
| $d = 1$ CFT | $\frac{c}{3} \ln L$ | $s = \frac{1}{2}$ Heisenberg chain [21] |
| $d \geq 2$ QCP | $aL^{d-1} + \gamma_{\text{QCP}}$ | Wilson–Fisher O($N$) [136] |
| Ordered (brok. cont. sym.) | $aL^{d-1} + \frac{n_G}{2} \ln L$ | Superfluid, Néel order [147] |
| Topological order | $aL^{d-1} - \gamma_{\text{top}}$ | $\mathbb{Z}_2$ spin liquid [159] |

N. Laflorencie, Phys. Rep. (2016)

* Topological entanglement entropy – one of the unambiguous ways to define and detect topological order

- Entanglement and dynamics- MBL, new paradigm in Entanglement transitions (in unitary and non unitary circuit etc).

Bao et al. (2019); Jian et al. (2019), Skinner et al. PRX (2019), ...

# How do we compute entanglement entropy ?

➡ Difficult to compute entanglement entropy

- Non-interacting system- Correlation matrix approch
- Interacting system - Exact diagonalisation (ED), density matrix renormalisation group (DMRG), quantum monte carlo( QMC)… etc

➡ Limitation in system sizes or heavily numerical or sophisticated conformal field theory (CFT) techniques

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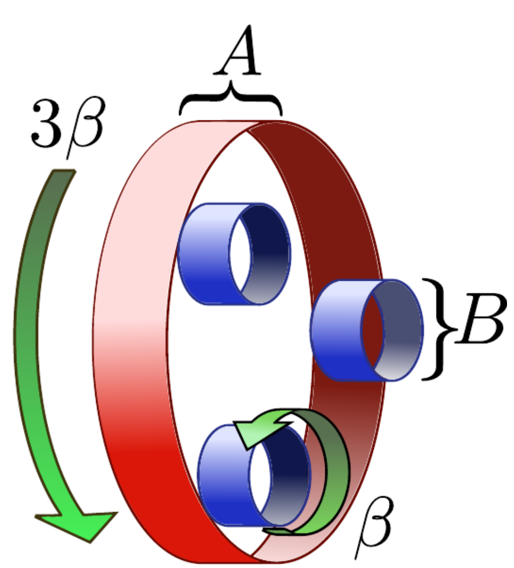
Usual replica field theory approach
(Cardy, Calabrese et al. )

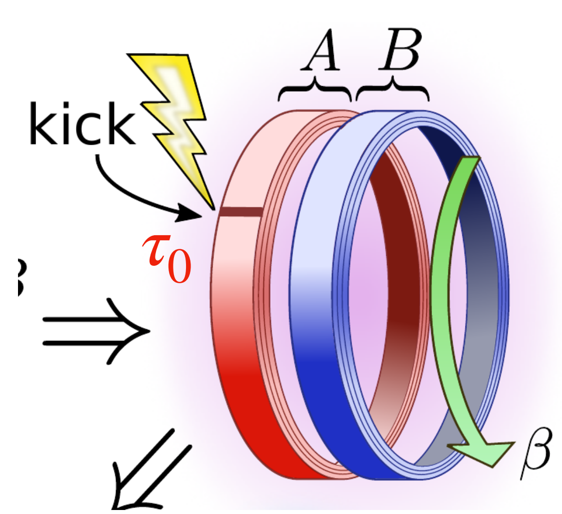
Complicated boundary conditions

$S_A^{(3)}$




New path integral method

Usual antiperodic boundary conditions on fermionic fields




A. Haldar, S. Bera & SB, Phys. Rev. Research (2020)

# Second Renyi entropy $S_A^{(2)}$ of Interacting fermions

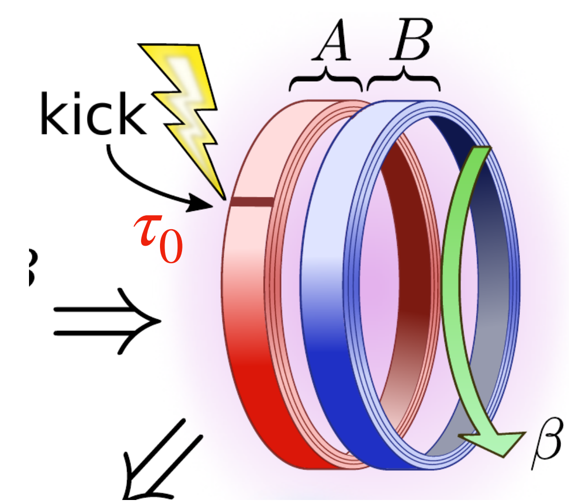
For example- Hubbard Model: $H = -\sum_{<ij>} t_{ij} c_i^\dagger c_j + U \sum_i n_{i\uparrow} n_{i\downarrow}$

New path integral for $S_A^{(2)}$: $$e^{-S_A^{(2)}} = \frac{Z^{(2)}}{Z^2} = \frac{1}{Z^2}\int D[\bar{c}, c] e^{-S}$$ $$Z^{(2)} = \mathrm{Tr}_A[\rho_A^2]$$

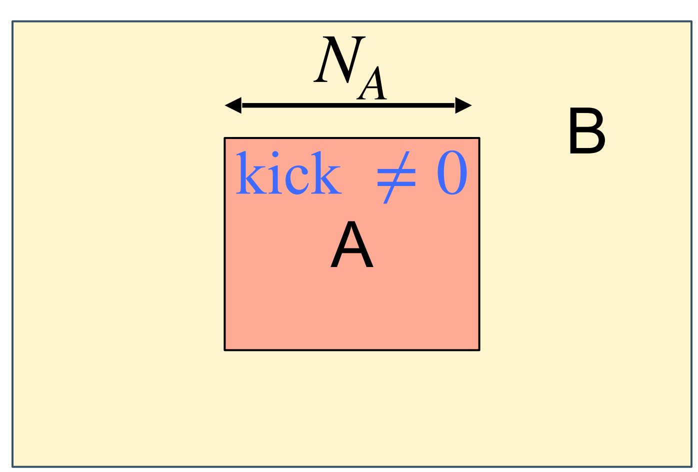
Entanglement action for Hubbard Model: $S(\lambda) = S_U + \lambda S_{\mathrm{kick}}$, $S = S(\lambda = 1)$

$S_U \rightarrow$ The usual imaginary time action for Hubbard Hamiltonian

$$S_{\mathrm{kick}} = \int d\tau d\tau' \sum \bar{c}_{i\alpha}(\tau)\delta_{i\in A} M_{\alpha\beta}(\tau,\tau') c_{j\beta}(\tau')$$




where $$M_{\alpha\beta}(\tau,\tau') = \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}_{\alpha\beta} \delta(\tau' - \tau_0^+)\delta(\tau - \tau_0)$$




A. Haldar, S. Bera & SB, Phys. Rev. Research (2020)

# Extraction of $S_A^{(2)}$ using "kick term" integration

Path integral of $S_A^{(2)}$: $$e^{-S_A^{(2)}} = \frac{Z^{(2)}}{Z^2} = \frac{1}{Z^2}\int D[\bar{c}, c] e^{-[S_U + \lambda S_{\text{kick}}]}$$

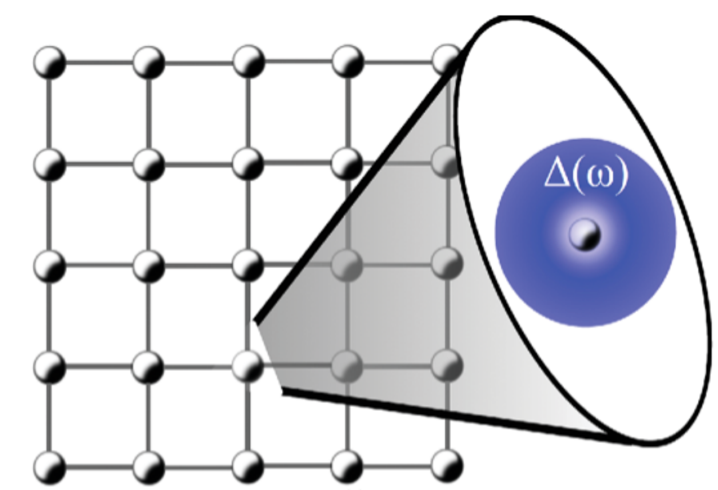
$S_A^{(2)} = -\ln(Z^{(2)}) + 2\ln Z \rightarrow$ Leads to calculation of thermodynamic potential (very difficult )

Noble way to extract by employing strength of kick term, we get - $S_A^{(2)} = \int_0^1 d\lambda < S_{\text{kick}} >_{Z^{(2)}(\lambda)}$

$$< S_{\text{kick}} >_{Z^{(2)}(\lambda)} = \sum_{i,\alpha,\beta} \delta_{i\in A} M_{\alpha\beta} G^{\lambda}_{ii,\beta\alpha}(0,0^+)$$

- $G^{\lambda}_{ab}(\tau, \tau')$ can be computed within DMFT
- We use Iterated Perturbation Theory (IPT) as impurity solver

★ More sophisticated impurity solver like continious time quantum monte carlo (CTQMC) can be used

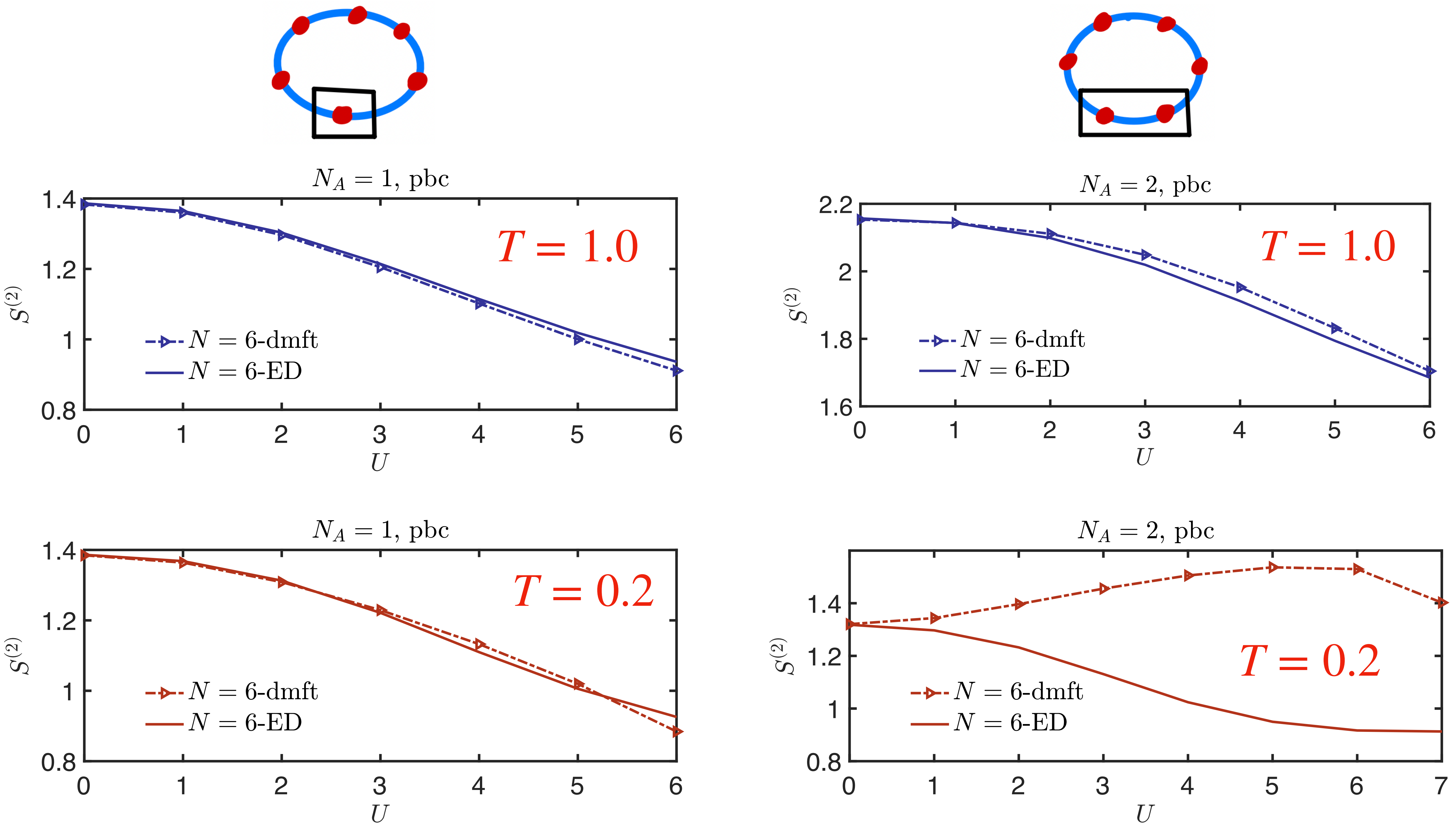



DMFT: Impurity problem in self-consistent bath

(Source: Internet)

To get entanglement, we need to compute $S_A^{(2)}(T)$ and take $T \rightarrow 0$ extrapolation

# Comparision with Exact Diagonalisation (ED) in 1d Hubbard Model

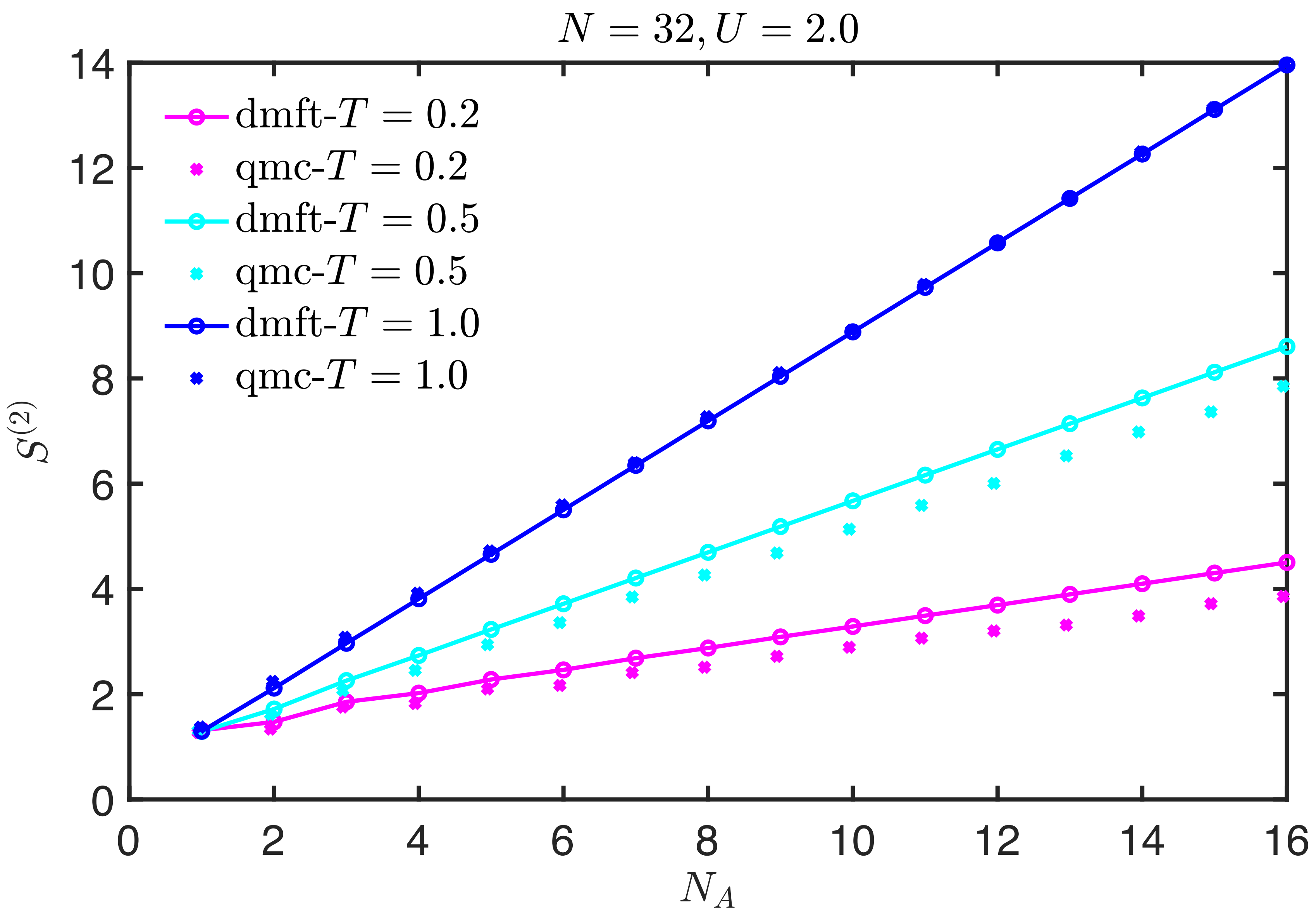



Spectral properties in ED and DMFT for such small systems for 1d are very different

# Comparision with QMC in 1d Hubbard Model

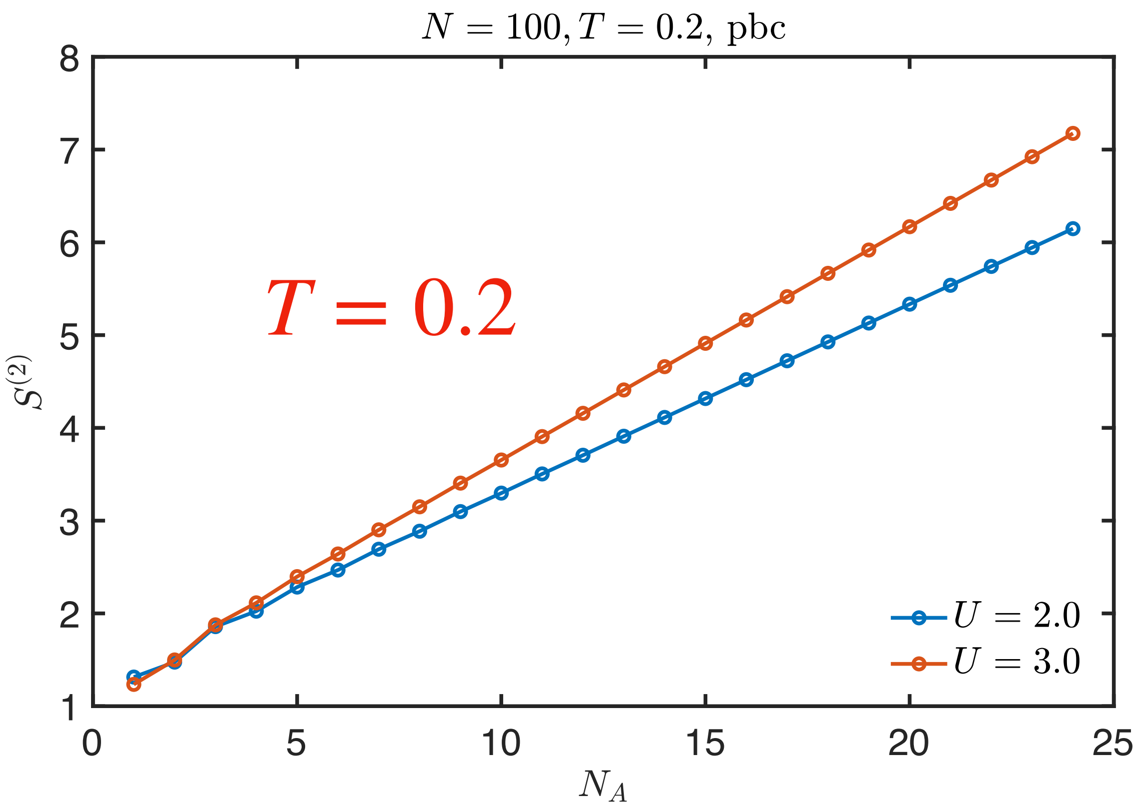
QMC →

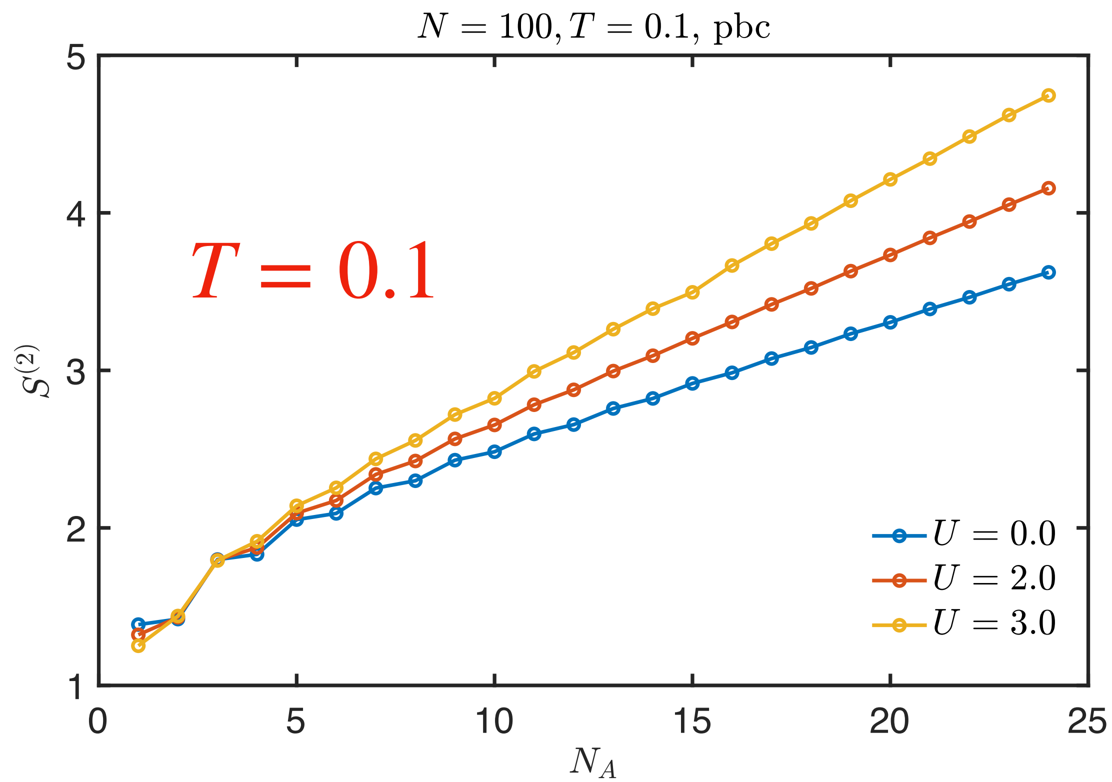
(P. Broecker & S Trebst)

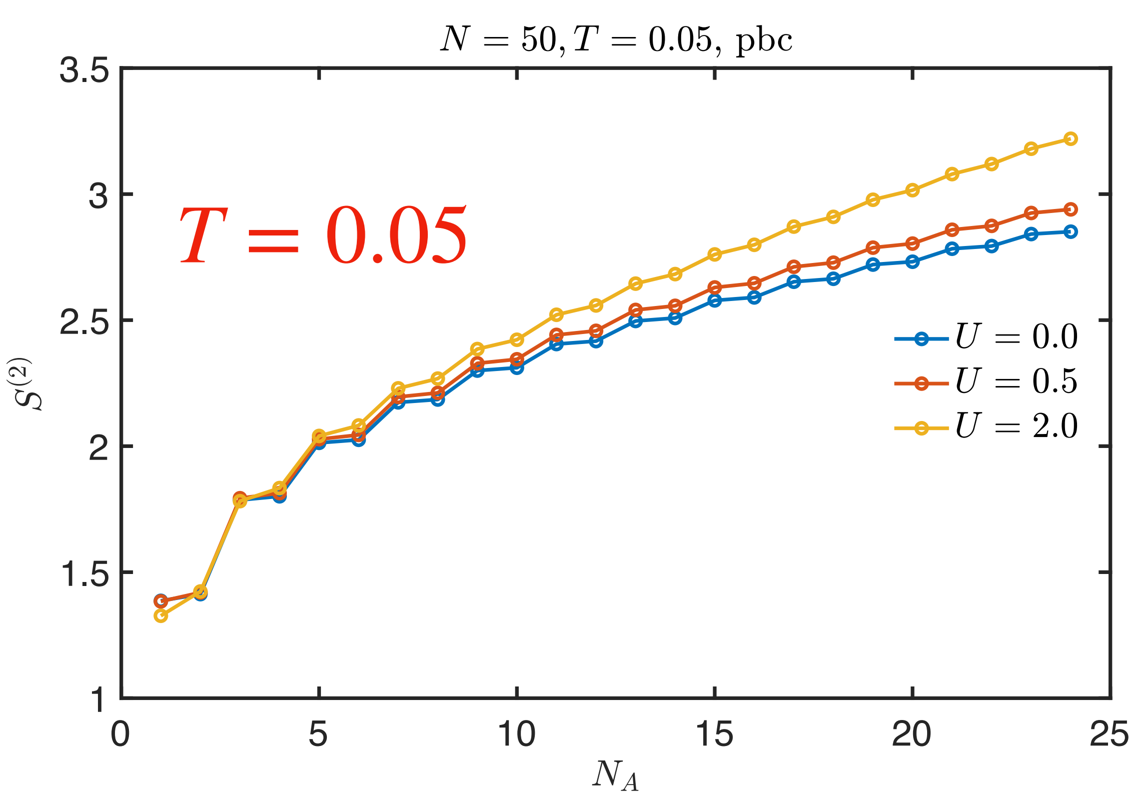



- Comparision with QMC at intermediate $T$ is quite good even in 1d

# Thermal entropy to entanglement crossover in $S_A^{(2)}(N_A, T)$




- Arc like feature: signature of more entanglement contribution
- Linear feature → more thermal entropy
- What is scaling of $S^{(2)}(N_A, T)$ ?
- How to "disentangle" entropy and entanglement ?
- How interaction affects on $S^{(2)}$ within DMFT ?

# Subsystem scaling and thermal to entanglement crossover in Fermi-liquid

From conformal field theory (CFT) -

Renyi entanglement entropy : $S_A^{(n)}(T=0,N_A) = \frac{c}{2}(1+\frac{1}{n})\log\left[\frac{N}{\pi}\sin\left(\frac{\pi N_A}{N}\right)\right] + k_n$

Logarithmic correction to boundary law

$c \rightarrow$ Central charge of CFT

For free fermi system $c = 1$

Subsystem Renyi entropy in finite temperature $(T = 1/\beta)$ :

$$S_A^{(n)}(T,N_A) = \frac{c}{2}(1+\frac{1}{n})\log\left[\frac{\beta v}{\pi}\sinh\left(\frac{\pi N_A}{\beta v}\right)\right] + k_n$$

replace $N \rightarrow -i\beta v$

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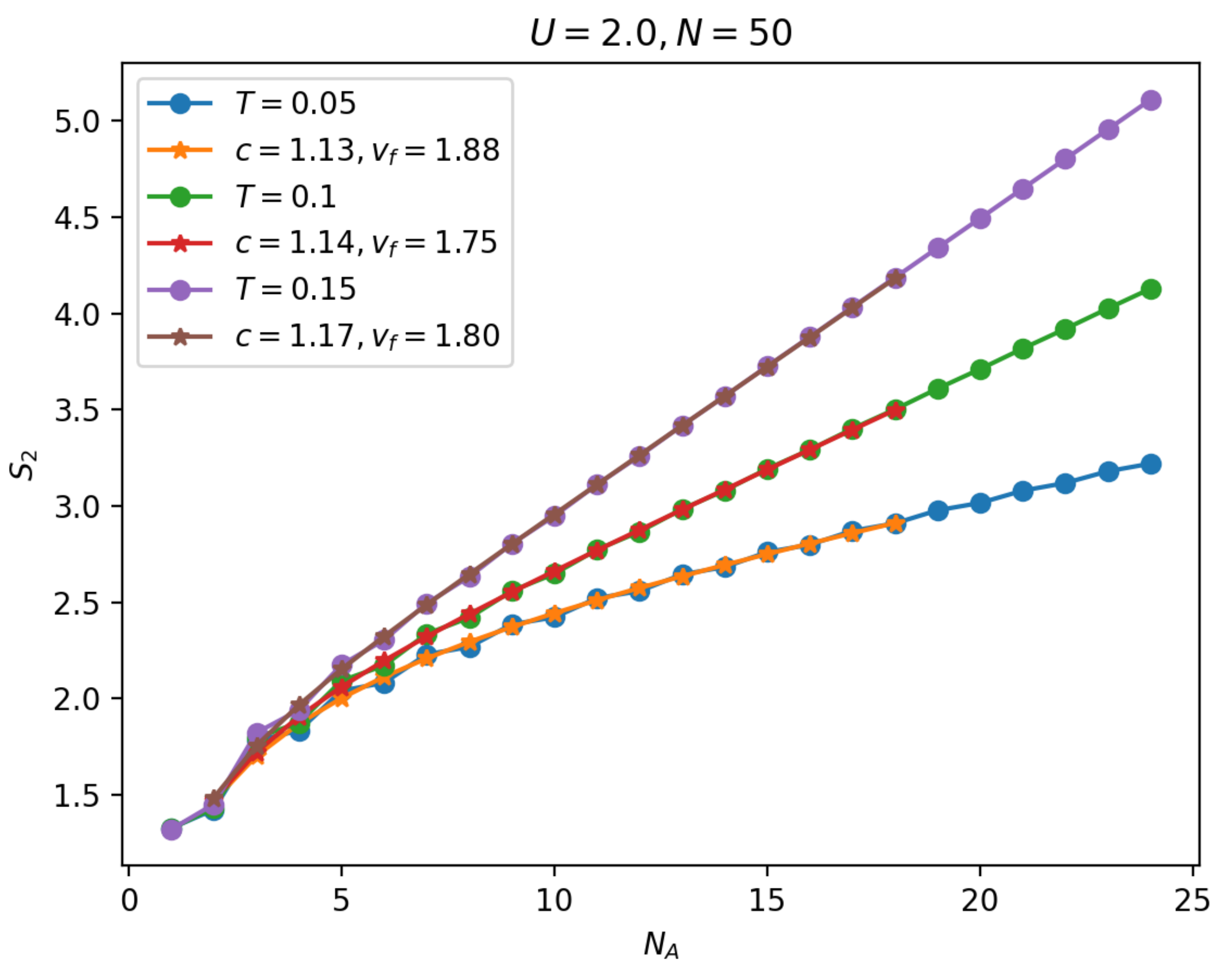
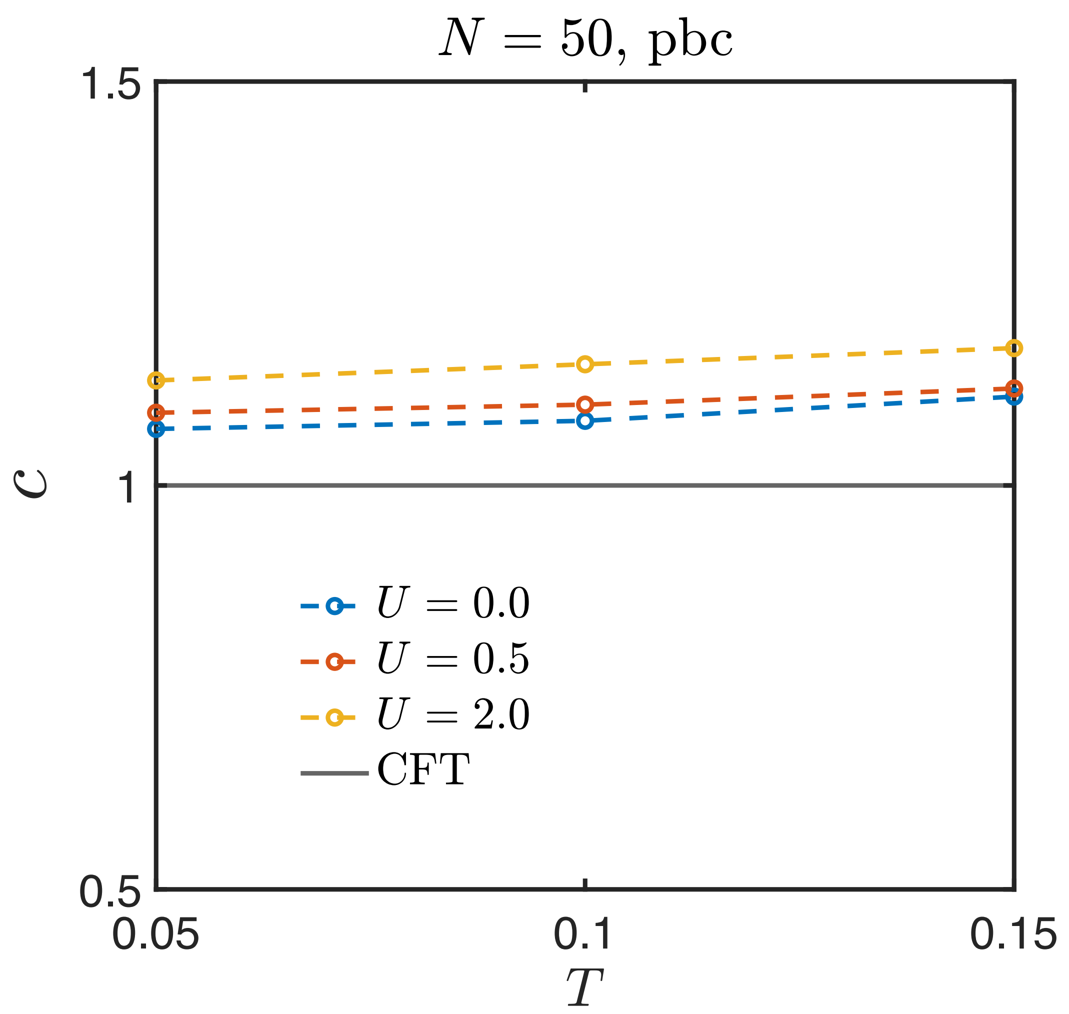
- Does the correlated metalic state in DMFT follow the above crossover formula ?

These formula are valid for $N \rightarrow \infty$. Finite $N$ and finite $T$ is not known in CFT.

(Cardy, Calabrese et al. )

# Crossover formula fitting and the effect of interaction in central charge



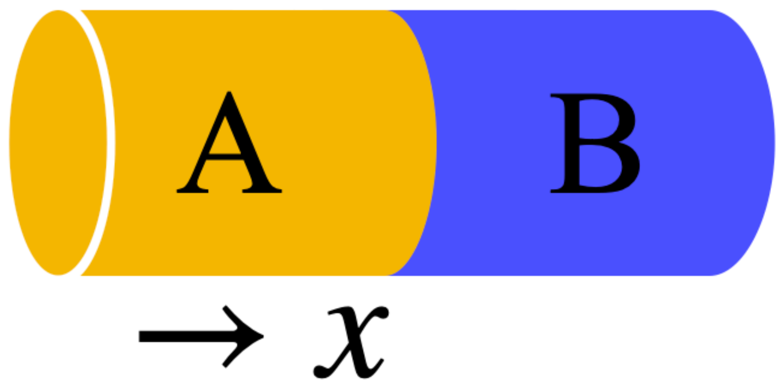




- Fits to crossover formula is reasonably well

With system size extracted $c$ very slowly tends toward CFT values

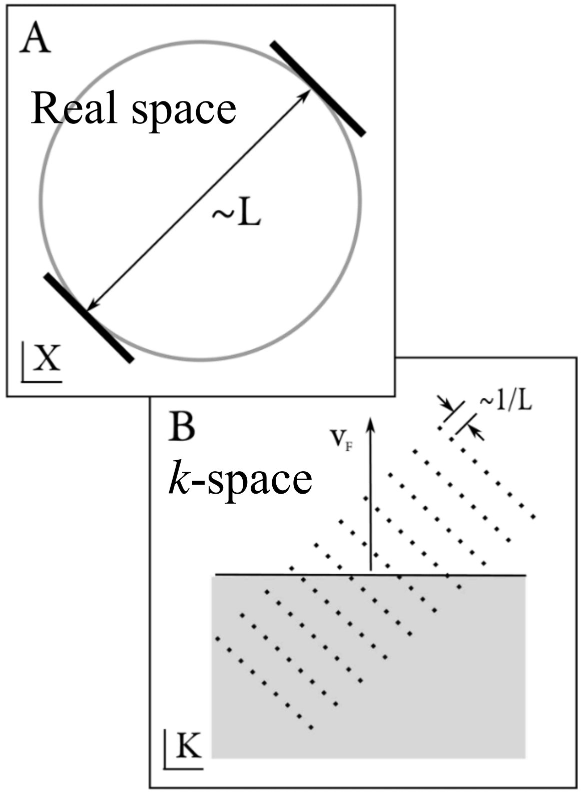
# Renyi entropy in 2d Hubbard Model

Cylindrical cut subsystem →




- What is scaling of $S^{(2)}$ in higher dimension (2d) in fermi-liquid phase ?

(B. Swingle, PRL 105, 050502 (2010) )




In Metalic phase -

Widom formula for scaling: Finite Fermi surface as collection of 1d gapless mode

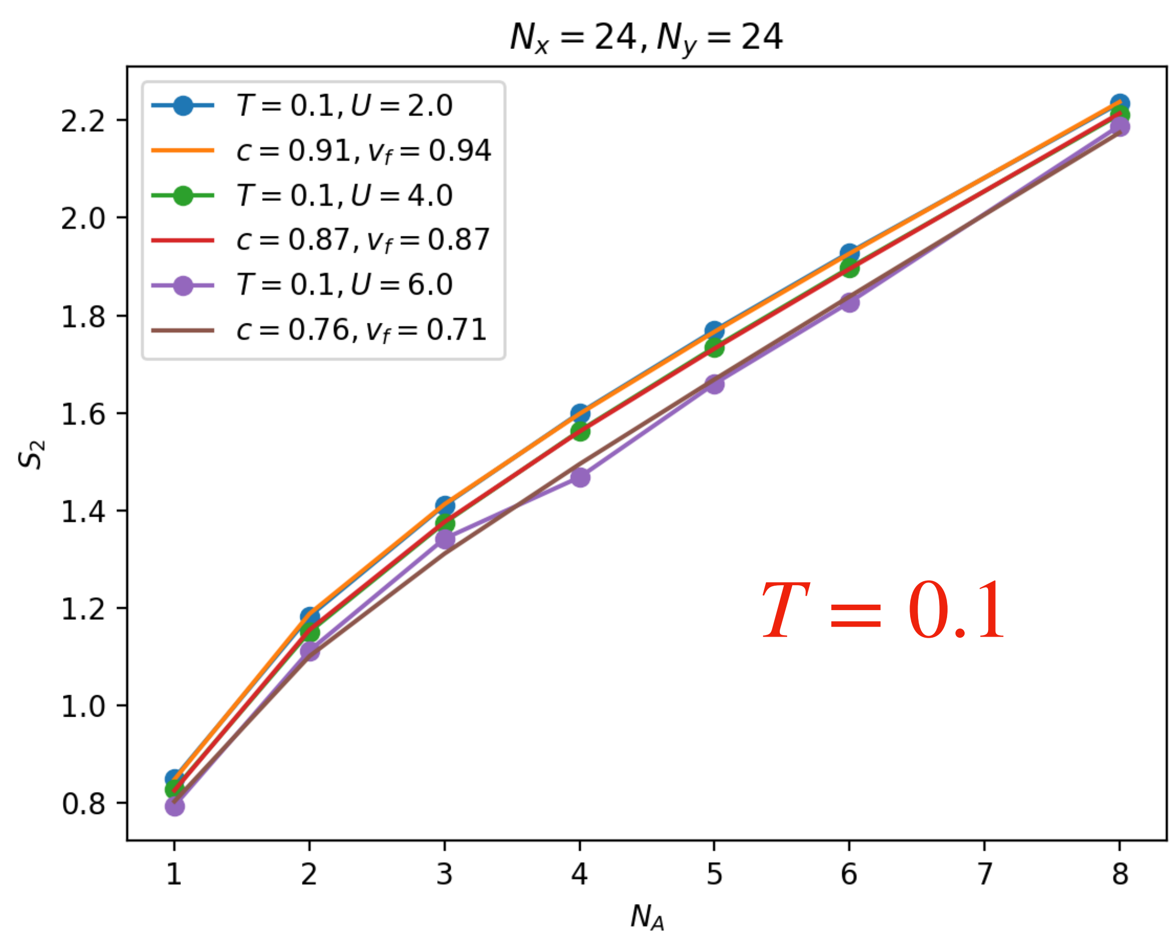
$$S_A^{(n)}(T, N_A) = \left( \frac{1}{2} \int\int \frac{dA_x dA_k}{(2\pi)^{d-1}} |n_k \cdot n_x| \right) \times \left[ \frac{c}{2}(1+\frac{1}{n})\log\left[\frac{\beta v}{\pi}\sinh\left(\frac{\pi N_A}{\beta v}\right)\right] + k_n \right]$$

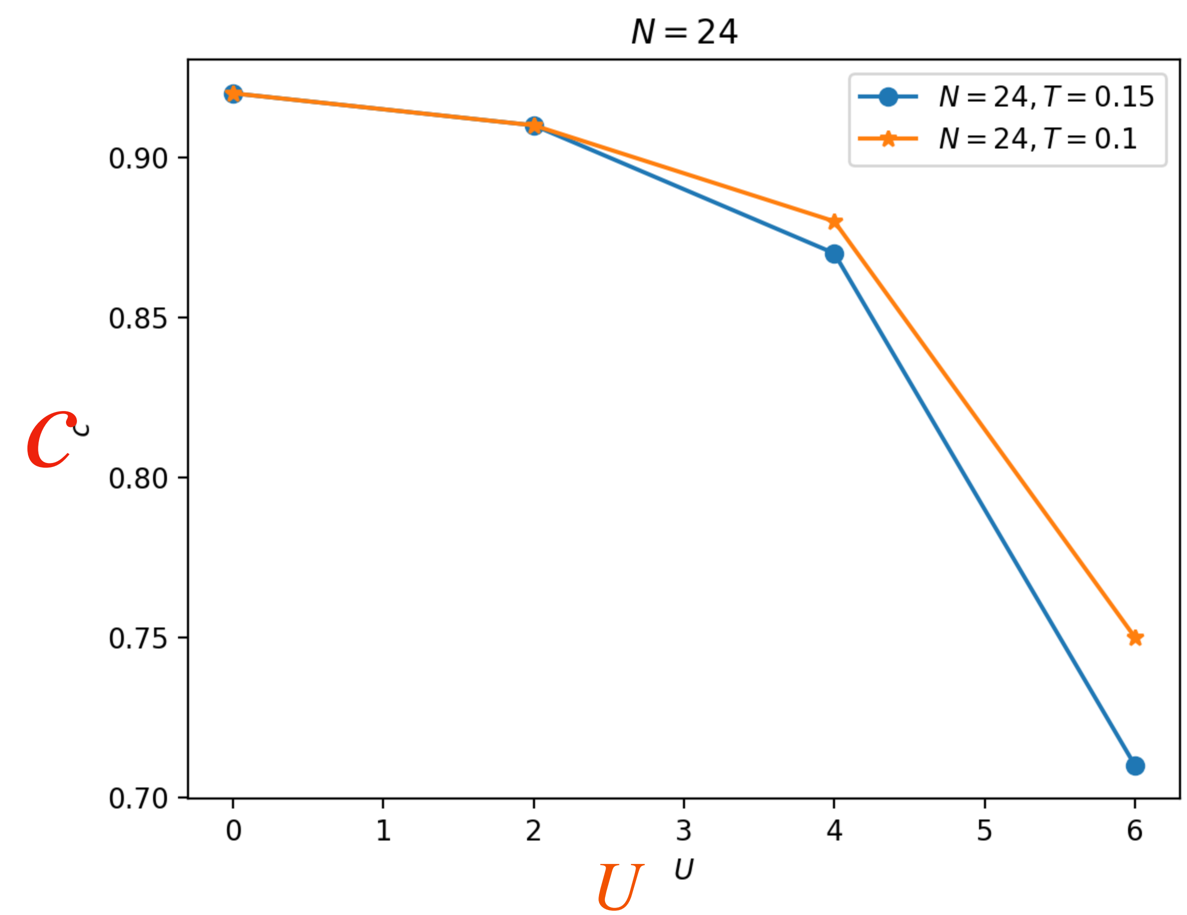
Effective no of 1d mode

1d subsystem scaling from CFT

Depends relative orientation of real and momentum space geometry

# Result: Metalic phase




- Fits to crossover formula is reasonably well

Substantial changes of $c$ for large $U$

# Summary and Conclusion

- Developed a new path integral method to compute Renyi entropy and present "kick term" integration method to extract Renyi entropy efficiently.

- Have shown computation of Renyi entropy within DMFT

- Subsystem scaling of 1d DMFT fermi-liquid phase reasonably well described by CFT but 2d DMFT correlated fermi-liquid phase is not.

- Future direction: Study of second Renyi entropy in Mott phase and study of mutual information across finite temperature metal-insulator critical point

*Thank you*