Dynamical mean-field theories for Rényi entanglement entropy of Fermi and non-Fermi liquids

Sumilan Banerjee

Centre for Condensed Matter Theory, Department of Physics,
Indian Institute of Science

Fractionalization and Emergent Gauge Fields in Quantum Matter, ICTP
December 5, 2023

Surajit Bera
(Physics, IISc Bangalore)

Arijit Haldar
(S N Bose Centre, Kolkata)

S. Bera, A. Haldar & SB, arXiv:2302.10940 (2023).

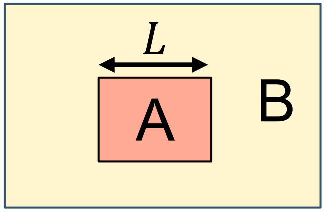
A. Haldar, S. Bera & SB, Phys. Rev. Research (2020)

IISc startup, research support

SERB ECR, CRG grants

Quantum Entanglement

Pure state $|\psi\rangle$



- Reduced density $\rho_A = Tr_B(|\psi\rangle\langle\psi|)$

- von-Neumann Entanglement entropy (EE) $S_A = -Tr_A(\rho_A \ln \rho_A)$

n-th Renyi entropy $S_A^{(n)} = \dfrac{1}{1-n} \ln Tr_A[\rho_A^n]$ $\quad S_A^{(n \to 1)} = S_A$

Second Renyi entropy $S_A^{(2)}$

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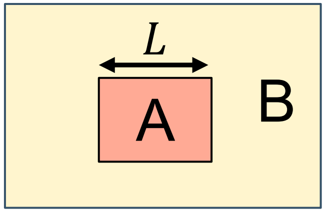

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But, why care about entanglement in condensed matter physics?

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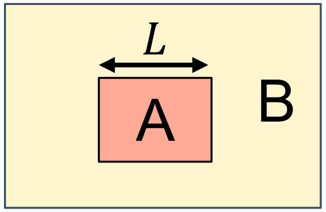

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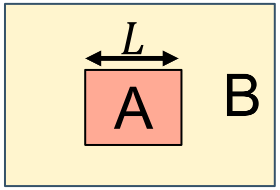
But, why care about entanglement in condensed matter physics?

Entanglement can characterize "intrinsic quantum nature" of various symmetry broken, critical and topological (ground) states.

○ Gapped systems*

$$S_A \sim \text{Area Law}\left(L^{d-1}\right) + \text{corrections}$$



Topological order, e.g. spin liquids

$$\text{corrections} \sim -\gamma_{topo} + \ldots$$

Topological entanglement entropy

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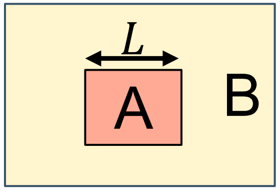

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Topological entanglement entropy

○ Universal (logarithmic) violation of area law

➢ Gapless/critical bosonic or fermionic systems in 1D (1+1 D CFT)

$$S_A^{(n)} = \frac{1}{2}\left(1+\frac{1}{n}\right)\left(\frac{c}{6}\right)\ln L + \cdots$$

Central charge c

(spinless) free fermions or Luttinger liquid $c = 2$

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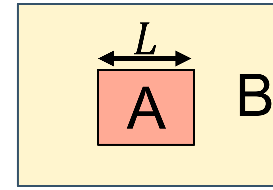

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➢ Free fermions in higher dimension $d > 1$

Gioev & Klich, PRL (2006)

Swingle, PRL (2010);Swingle, PRB (2012)

$$S_A^{(n)} \sim L^{d-1} \ln L + \cdots$$

Fermi liquids, Weyl fermions in magnetic field, certain non-Fermi liquids, Bose metals

How do we calculate entanglement of many-body states?

Entanglement measures are typically computed numerically

- Non-interacting – Correlation matrix approach
- Interacting – Exact diagonalization (ED), density matrix renormalization (DMRG) & matrix product states (MPS), Quantum Monte Carlo (QMC) , ...

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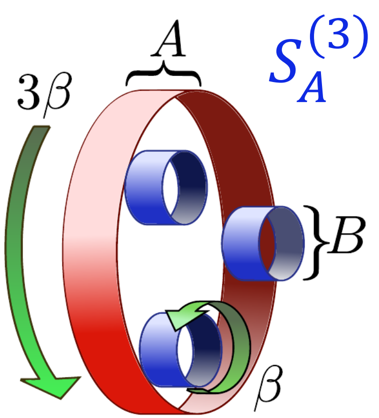
- Path integral and quantum field-theory approach for entanglement

Replica field theory



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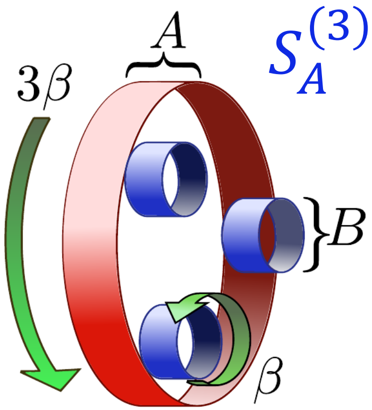

Problem of computing entanglement

Time-evolution in a complicated space-time manifold with non-trivial boundary conditions.

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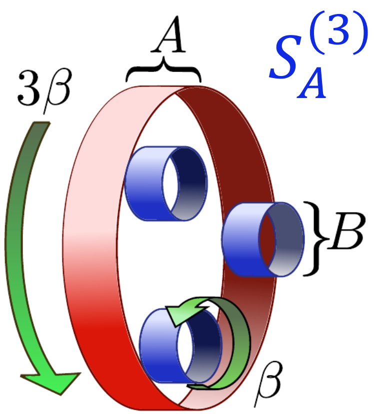

Problem of computing entanglement

⬇

Time-evolution in a complicated space-time manifold with non-trivial boundary conditions.

- Conformal field theory (CFT)

Calabrese & Cardy (2004,2009), ..

⇒ 1D gapless fermions and critical systems

Simpler representation for applying to general quantum many-body techniques/ approximations (Saddle point, RPA, RG, ..) for entanglement like for thermodynamic, spectral and transport properties

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New path integral/field theory method

- Bosonic systems -- A. Chakraborty & R. Sensarma, PRL (2021)
- Fermionic systems -- A. Haldar, S. Bera & SB, PRR (2020), S. Moitra and R. Sensrama, PRB (2020)

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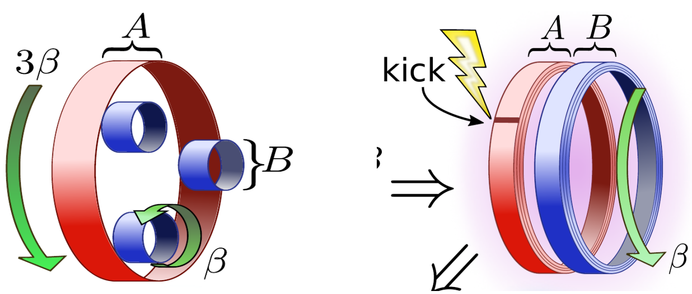
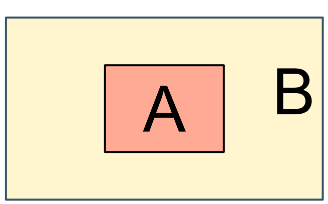
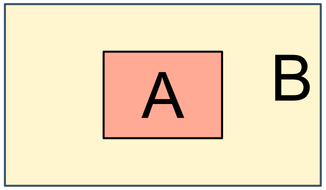
$S_A^{(3)}$



Usual boundary conditions on the fields



○ Second Renyi entropy of subsystem *A*



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Grassmann numbers $\{\bar{\xi}_i, \xi_i\}_{i\in A}$

Fermionic displacement operator

$$D_N(\xi) = e^{\sum_{i\in A} c_i^\dagger \xi_i} e^{-\sum_{i\in A} \bar{\xi}_{i\in A} c_i}$$

Fermionic Wigner characteristic function $\chi_N(\xi_A) = Tr[\rho D_N(\xi_A)]$

Gaussian factor $f_N(\xi, \eta) = 2^N e^{-\left(\frac{1}{2}\right) \sum_{i\in A}(\bar{\xi}_i \xi_i + \bar{\eta}_i \eta_i - \bar{\xi}_i \eta_i + \bar{\eta}_i \xi_i)}$

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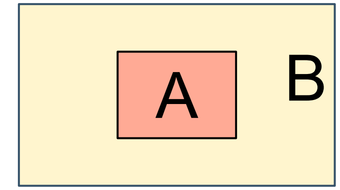

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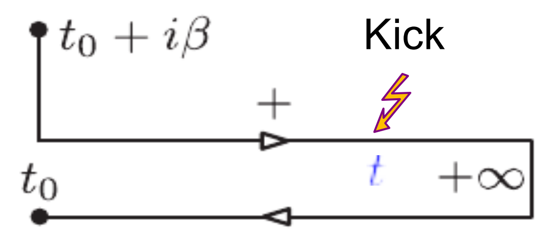

Keldysh contour *C*

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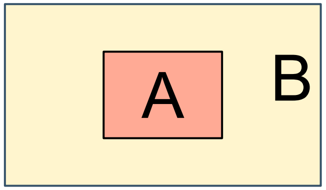

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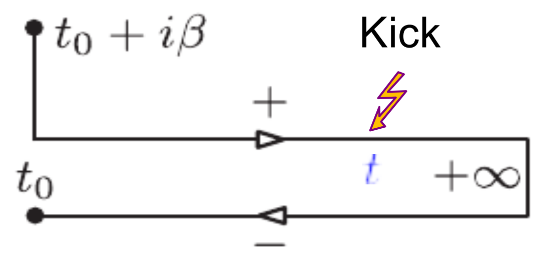


Keldysh contour *C*

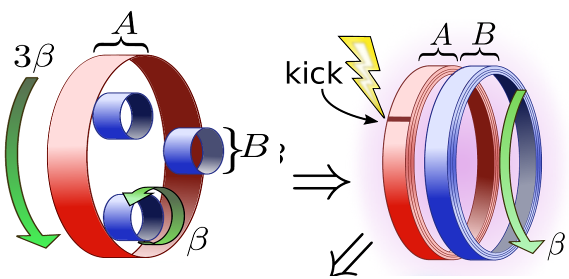
⇒ All the known expressions for Renyi entropies of non-interacting fermions

$S_A^{(n)} = \frac{1}{1-n} Tr_A \ln[(1-C)^n + C^n]$ Correlation matrix $C_{ij} = \langle c_i^\dagger(t) c_j(t)\rangle$

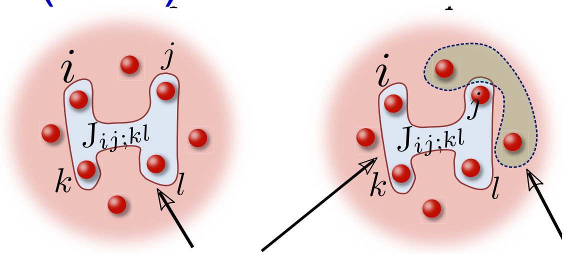
A. Haldar, S. Bera & SB, PRR (2020)

Rest of the talk

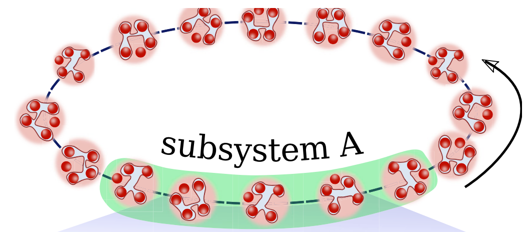
○ Entanglement entropy of correlated metallic states described by Dynamical mean field theories (DMFT) (local self energy).



Sachdev-Ye-Kitaev (SYK) NFL and FL

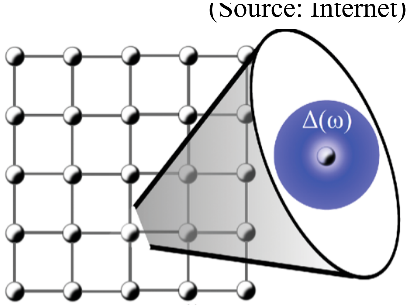


Interacting diffusive metal

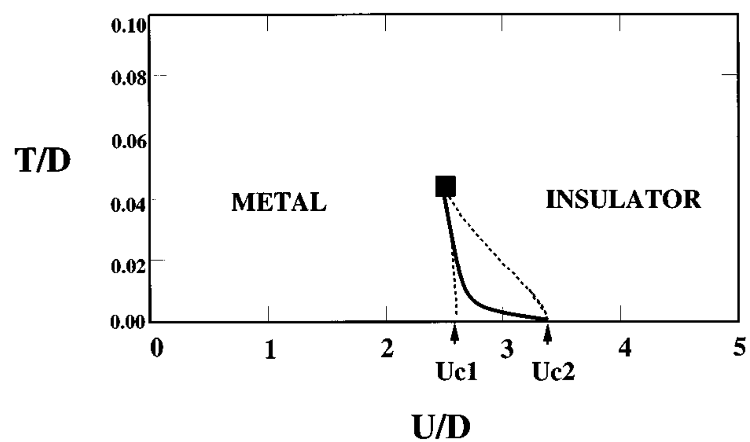


DMFT Metallic state in Hubbard model

(Source: Internet)



DMFT: Impurity problem in self-consistent bath



Second Renyi entropy for interacting fermions

- Interacting fermions $H = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_{ijkl} U_{ijkl} c_i^\dagger c_j^\dagger c_k c_l$

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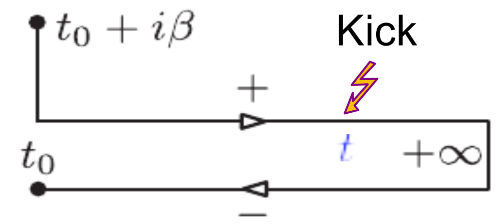

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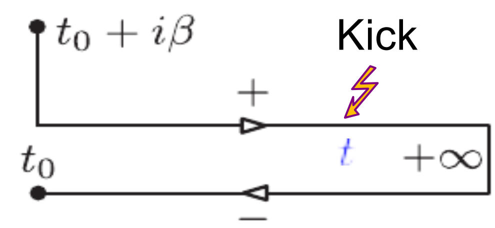

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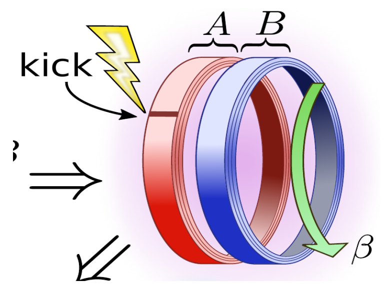
Integrate out the auxiliary fields first

Two replicas $\alpha = 1,2$



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$$S_{eff} = \int_C dz dz' \sum_{ij\alpha\beta} \bar{c}_{i\alpha}(z) G^{-1}_{0,i\alpha,j\beta}(z, z') c_{j\beta}(z') - \cdots$$

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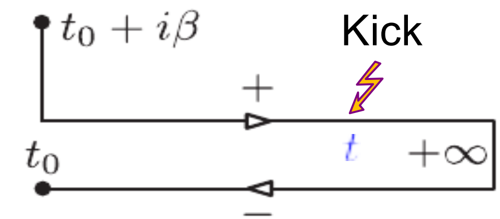

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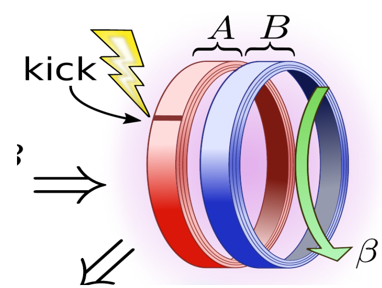

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$$G^{-1}_{0,i\alpha,j\beta}(z, z') = [(i\partial_z + \mu)\delta_{ij} - t_{ij}] \delta_C(z, z') \delta_{\alpha\beta} - \delta_{i\in A} \delta_{ij} M_{\alpha\beta}(z, z')$$

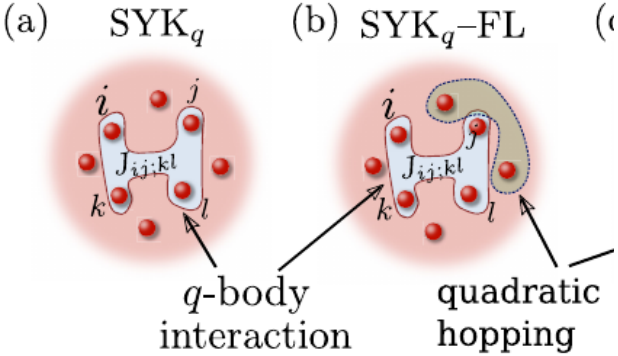
$$\underbrace{\boldsymbol{M}(\tau, \tau') = \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \delta_C(z, t^+ +) \delta_C(z', t+)}_{\text{Self-energy kick}}$$

Self-energy kick

*Can be used for QMC

SYK Non-Fermi (NFL) and Fermi (FL) liquids

$$H_{SYK} = \frac{1}{(2N)^{3/2}} \sum_{ijkl} J_{ijkl} c_i^\dagger c_j^\dagger c_k c_l$$



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Fu & Sachdev, PRB (2016)

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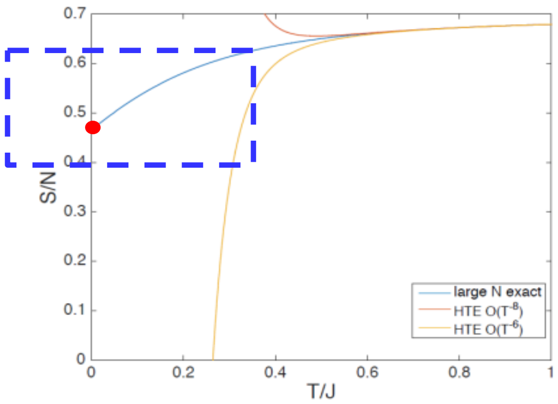
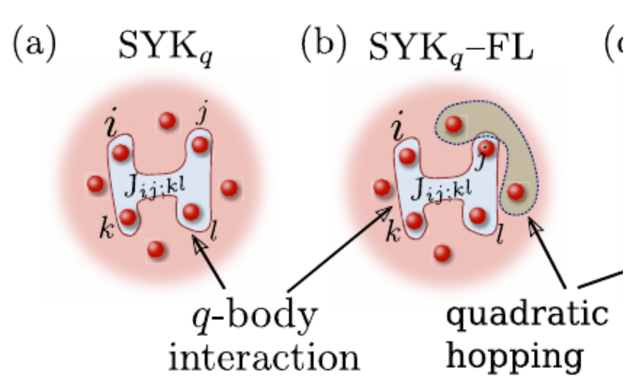
Non Fermi liquid $\quad \Sigma_R(\omega) \sim \sqrt{J\omega} \gg \omega \quad$ as $\omega \to 0$

Extensive *T=0* residual entropy S_0 (for *T→0, N→∞*)





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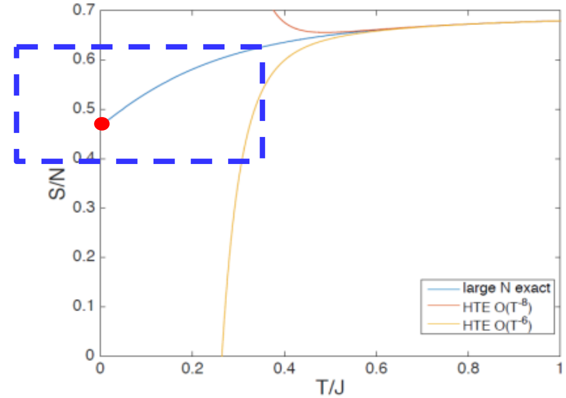
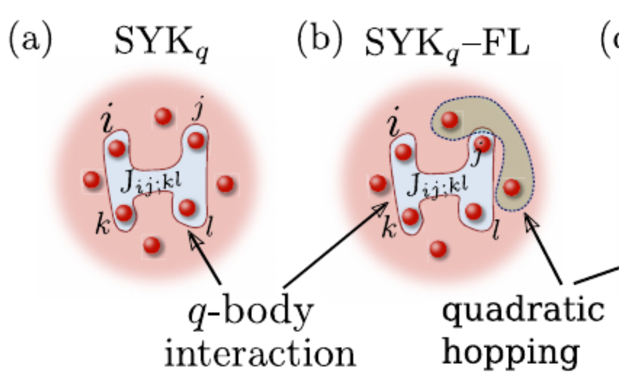


- Fermi liquid, add a quadratic term

$$H = \frac{1}{(2N)^{3/2}} \sum_{ijkl} J_{ijkl} c_i^\dagger c_j^\dagger c_k c_l + \frac{1}{\sqrt{N}} \sum_{ij} t_{ij} c_i^\dagger c_j \qquad P(t_{ij}) \sim e^{-|t_{ij}|^2/t_h^2}$$



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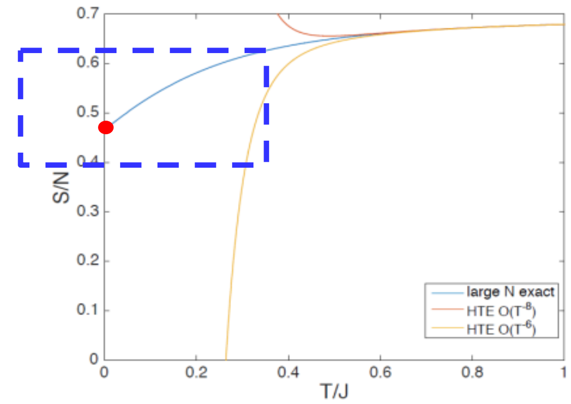
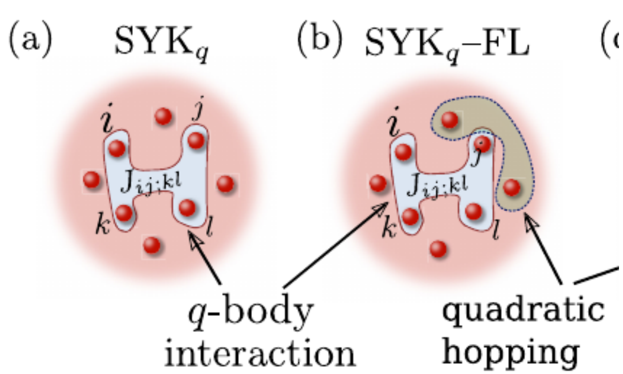
Extensive $T=0$ residual entropy S_0 (for $T \to 0$, $N \to \infty$)



- Fermi liquid, add a quadratic term

$$H = \frac{1}{(2N)^{3/2}} \sum_{ijkl} J_{ijkl} c_i^\dagger c_j^\dagger c_k c_l + \frac{1}{\sqrt{N}} \sum_{ij} t_{ij} c_i^\dagger c_j \qquad P(t_{ij}) \sim e^{-|t_{ij}|^2/t_h^2}$$

Heavy Fermi liquid for $t_h \ll J$, $\quad T_{coh} \sim t_h^2/J \qquad \Sigma(\omega) \sim \omega^2, \quad \omega \to 0$



SYK Non-Fermi (NFL) and Fermi (FL) liquids

Fu & Sachdev, PRB (2016)

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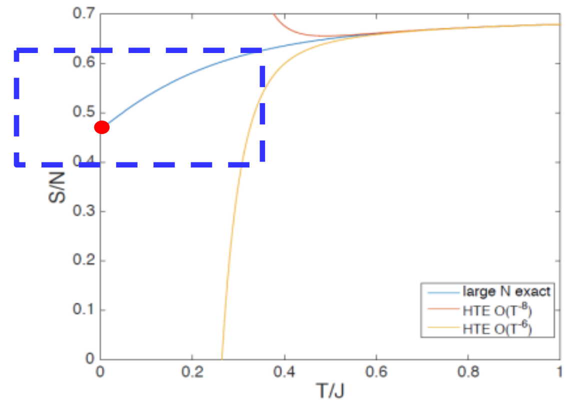

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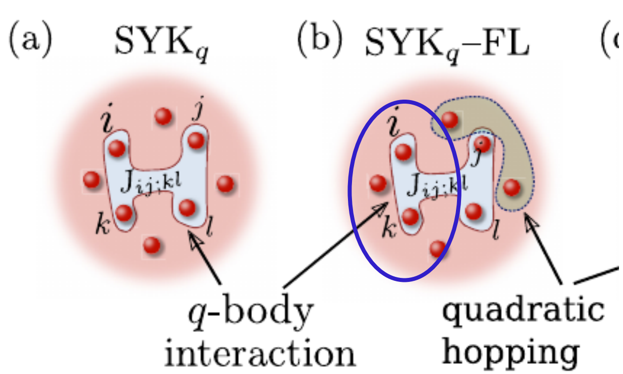
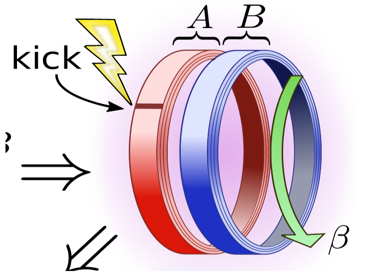


Subsystem *A* – choose any N_A sites out of *N* sites

$$S_A^{(2)}\left(p = \frac{N_A}{N}\right)$$

Subsystem (second) Renyi entropy in the large N limit

Thermal state, $\rho = e^{-\beta H}/Z$ (Also, for pure state $|\psi\rangle \sim e^{-\beta H}|\psi_0\rangle$)



- Try to approach ground state entanglement by taking $T \to 0$ after $N \to \infty$ limit

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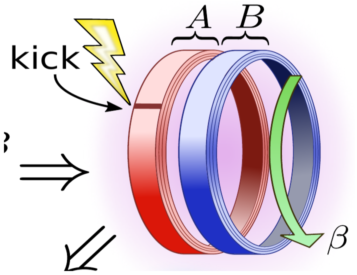

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$$S_A^{(2)} = -\overline{\ln(Tr_A \rho_A^2)}$$

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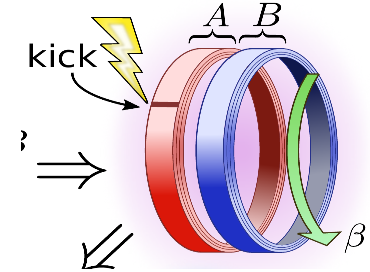

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- Large-N saddle point for Renyi entropy field theory

$$\boldsymbol{G} = -(1-p)(\boldsymbol{\partial}_\tau + \boldsymbol{\Sigma})^{-1} - p(\boldsymbol{\partial}_\tau + \boldsymbol{\Sigma} + \boldsymbol{M})^{-1}$$

$$\Sigma_{\alpha\beta}(\tau_1,\tau_2) = -J^2 G_{\alpha\beta}^2(\tau_1,\tau_2) G_{\beta\alpha}(\tau_2,\tau_1) + t_h^2 G_{\alpha\beta}(\tau_1,\tau_2)$$

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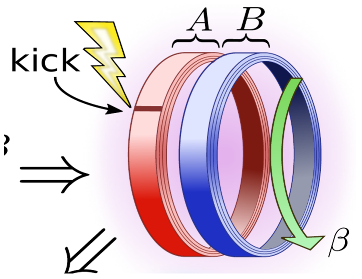

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$$\underbrace{\boldsymbol{M}(\tau_1, \tau_2) = \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \delta(\tau_1 - \tau_0^+)\delta(\tau_2 - \tau_0)}_{\text{Self-energy kick}}$$

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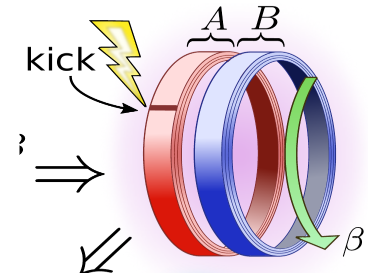

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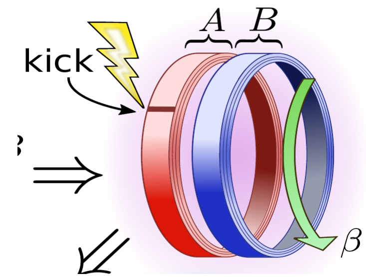

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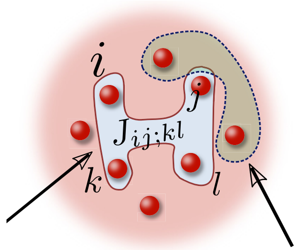
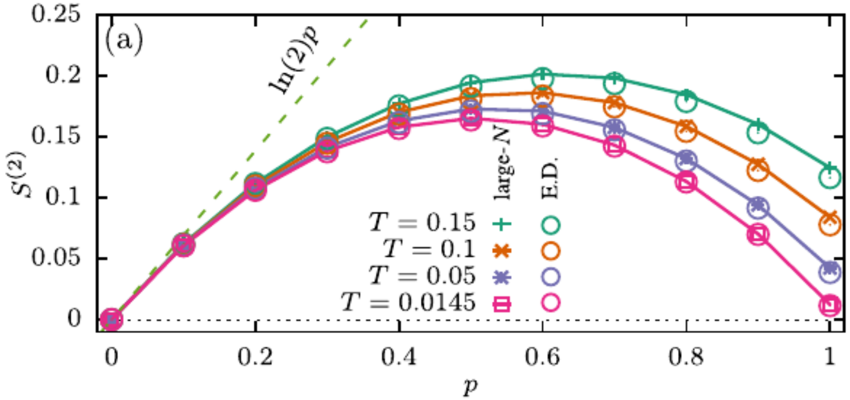
Need to solve self consistently

Discretize over (τ) time and solve self-consistently numerically

Fermi liquid and heavy Fermi liquid ($J, t_h \neq 0$)



$$S_A^{(2)}\left(p = \frac{N_A}{N}\right)$$



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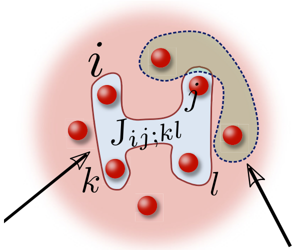

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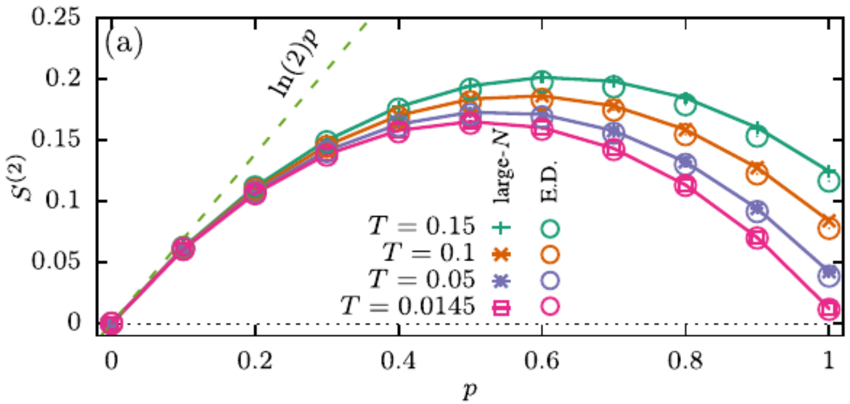
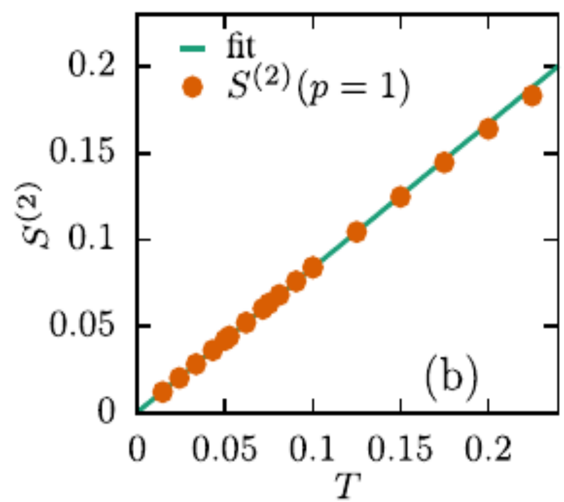


- Large N, $p=1$ value approaches zero as $T \to 0$
- ED results for $N=8, 10$ matches perfectly with $N \to \infty$ limit!

→ Finite-N corrections are very small for entanglement entropy.



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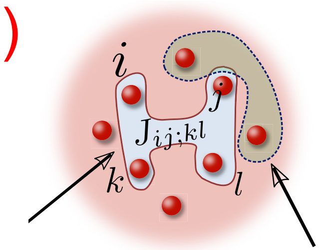

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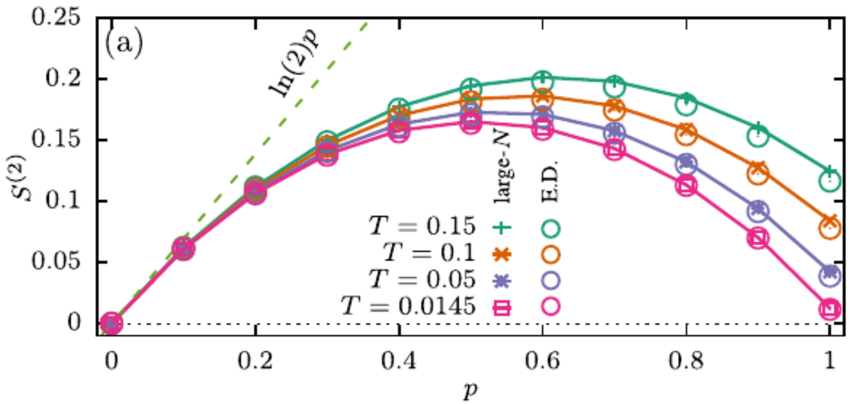

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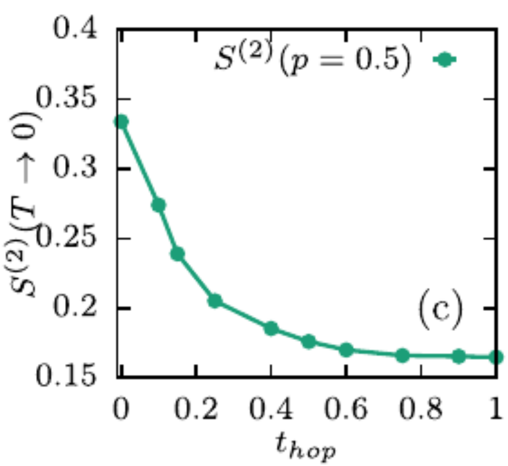
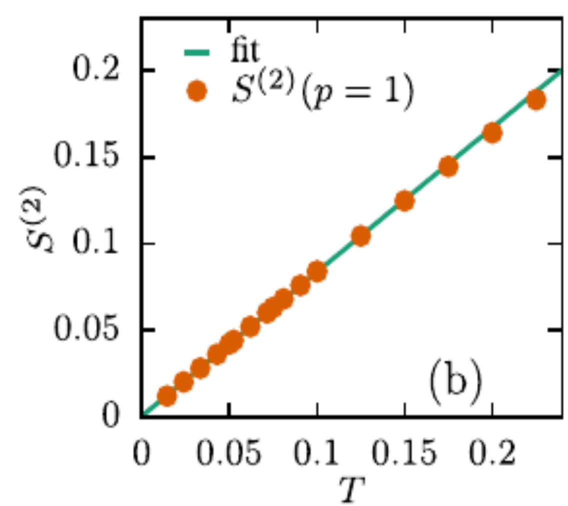
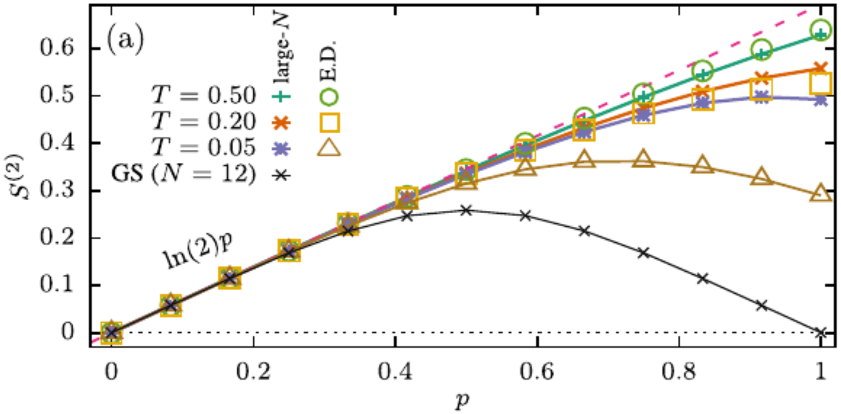




Bipartite ($p=1/2$) entanglement entropy

Heavy Fermi liquid → *weakly interacting FL*

Pure SYK model ($t_h = 0$)



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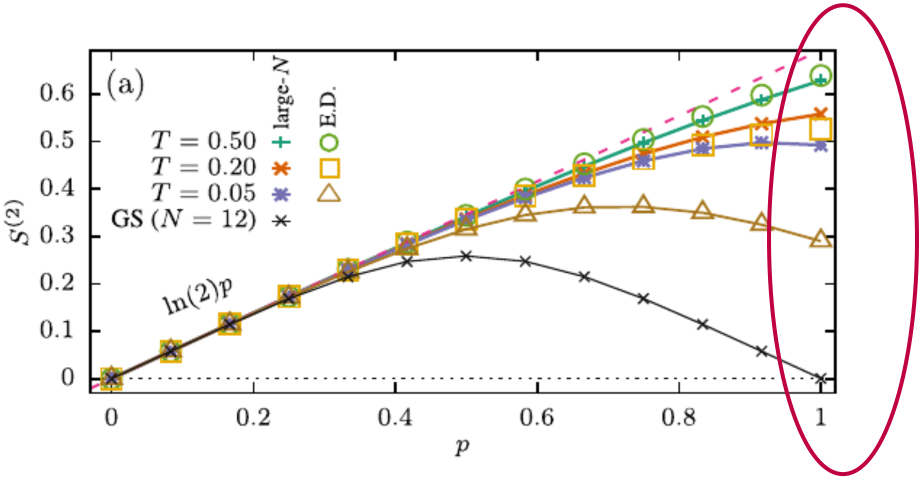

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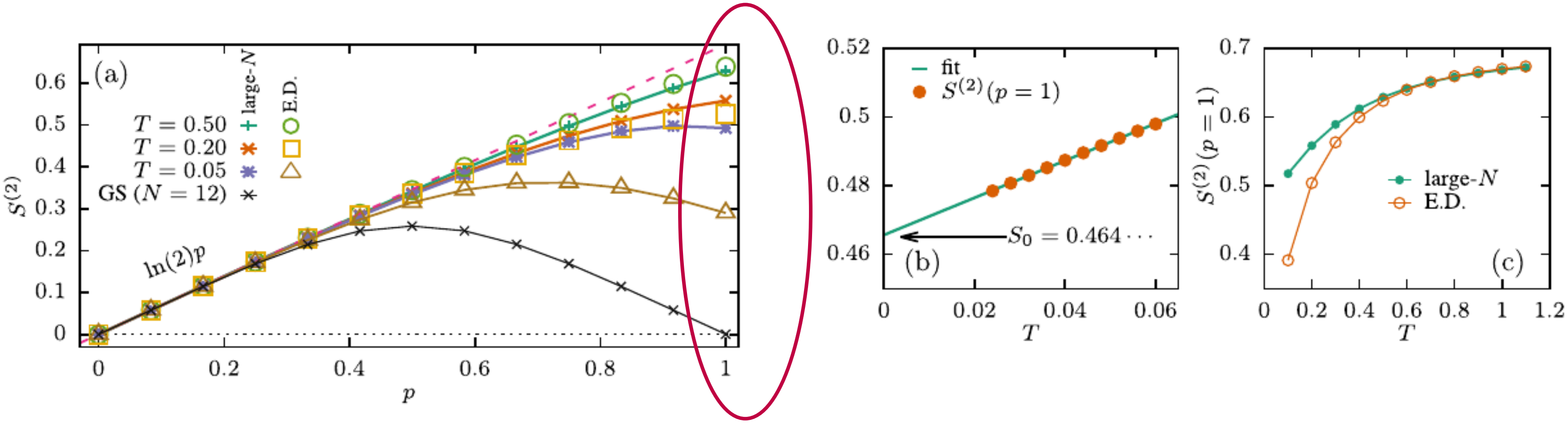

- Large *N, p=1* value does not approach zero as *T→0*
- It can be shown $S_A^{(2)}(p \to 1, T = 0) = S_0$

Residual entropy

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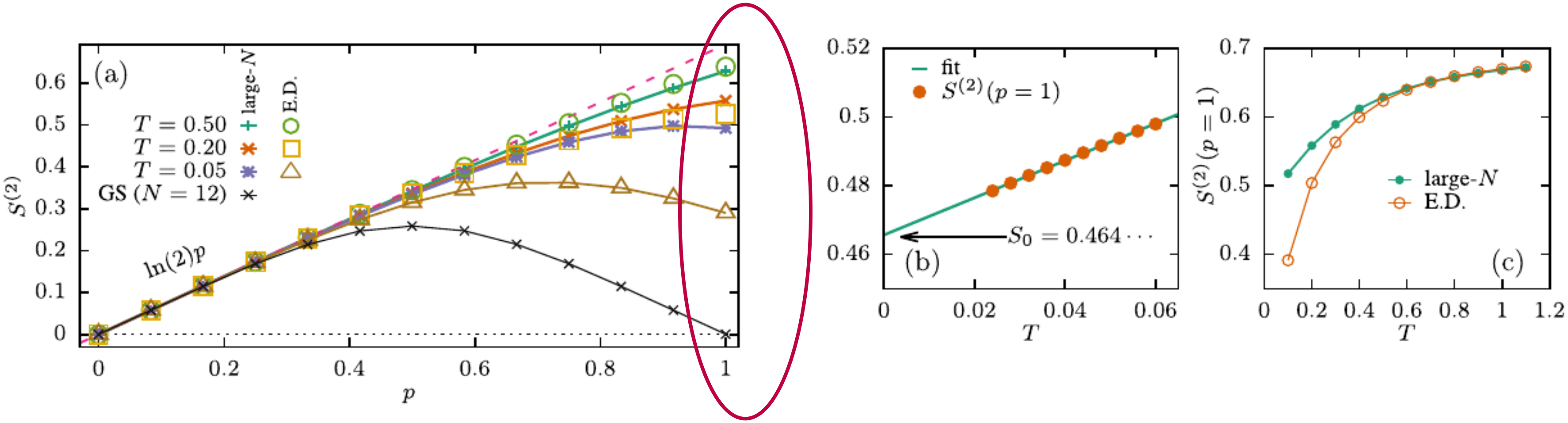

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Residual entropy

Quantum entanglement of the SYK NFL ground-state cannot be extracted in the large-*N* limit from $T \to 0$ limit.

Entanglement in interacting diffusive metal

$$H = \underbrace{\sum_{xx',ij} t_{xi,x'j} c^{\dagger}_{xi} c_{x'j}}_{\text{Inter-dot hopping}} + \underbrace{\sum_{x,ij} J_{x,ijkl} c^{\dagger}_{xi} c^{\dagger}_{xj} c_{xk} c_{xl}}_{\text{Intra-dot hopping}} \qquad i = 1, \ldots, N$$

Gu et al. (2017),
Davison et al. (2017),
...
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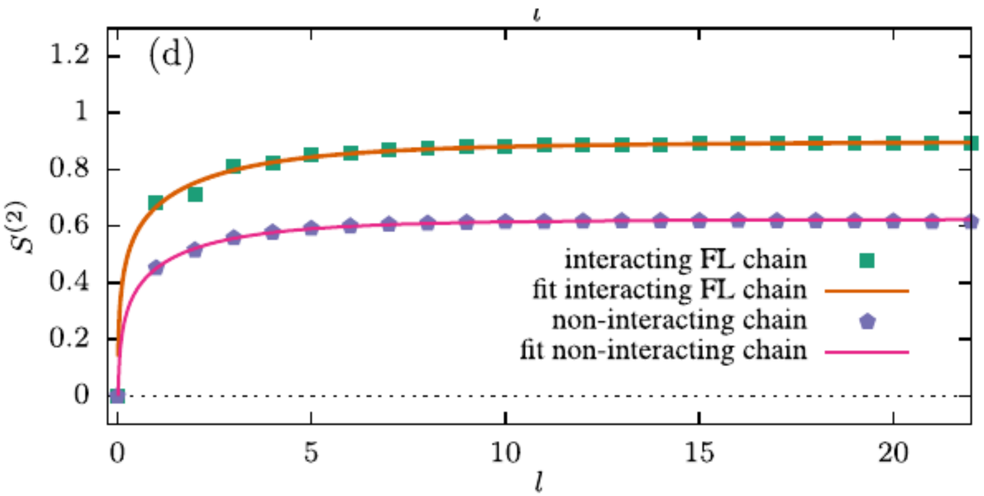

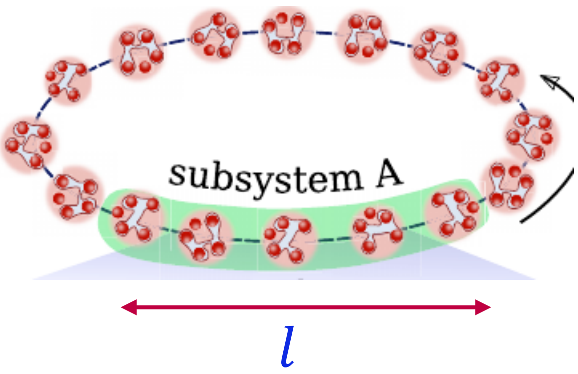

Lattice of SYK dots

Entanglement in interacting diffusive metal

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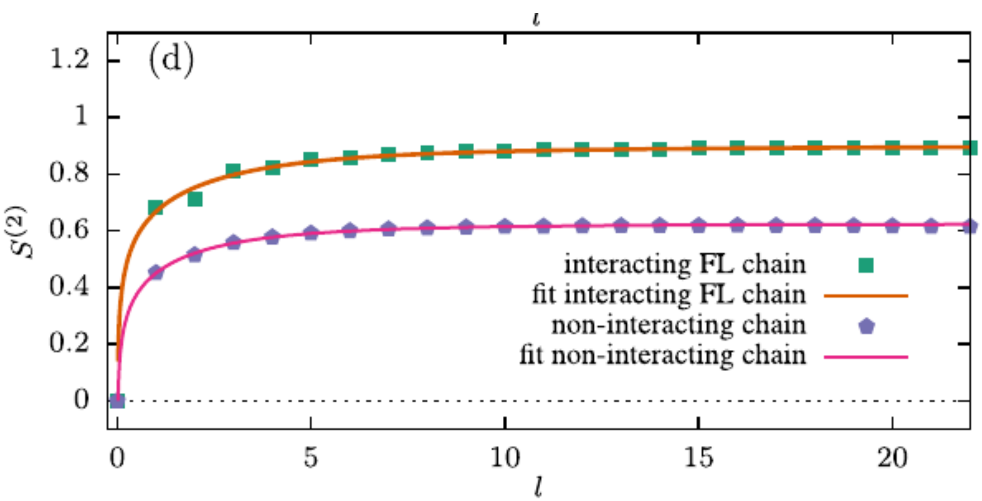

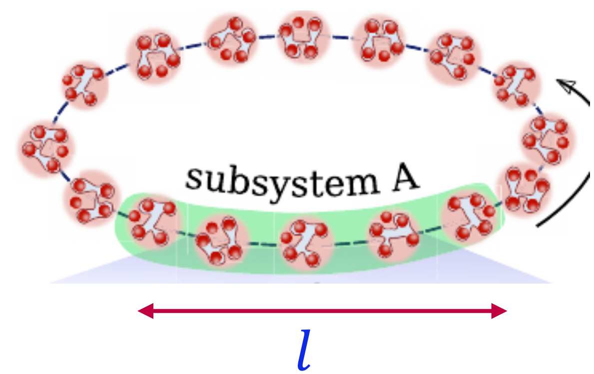

Lattice of SYK dots

- Renyi entropy initially grows like $\ln l$, but then saturates.

→ Modified growth law $S_A^{(2)} \sim \frac{c_{eff}}{8} \ln\left(\frac{1}{\sqrt{l^{-2} + l_0^{-2}}}\right)$

A. Potter, arxiv (2014)

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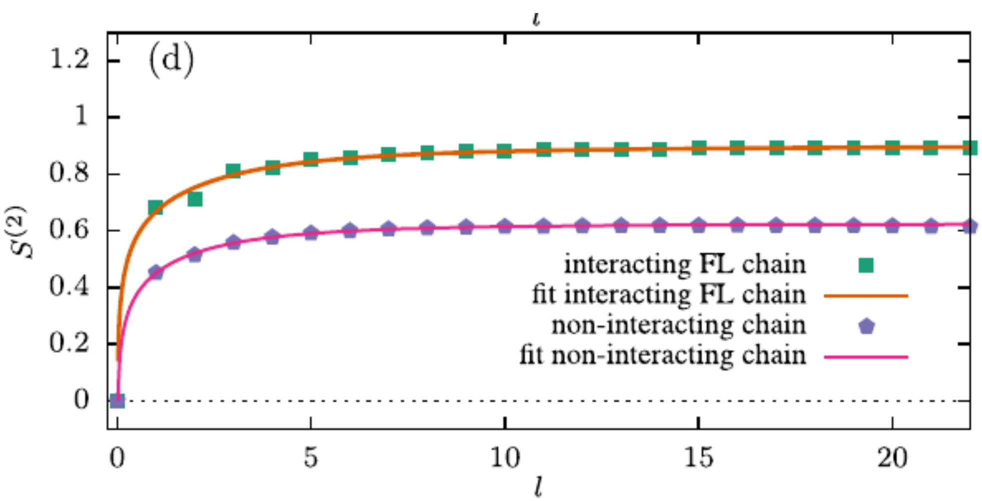

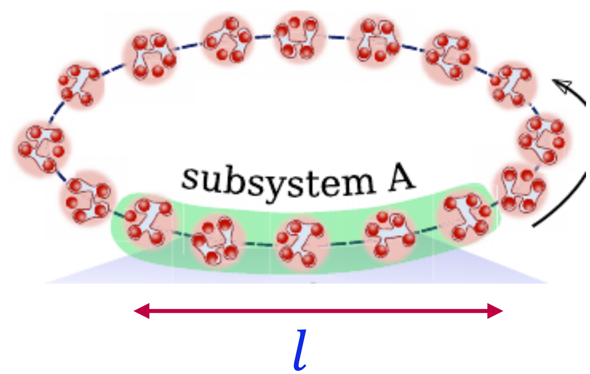

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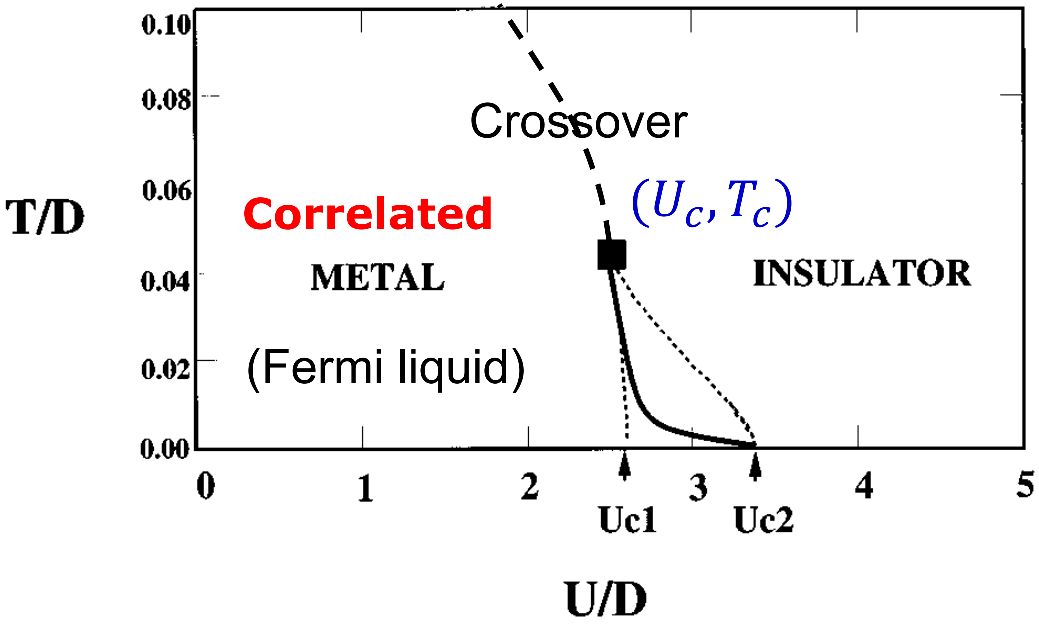
→ Emergent length scale, "mean free path" l_0

c_{eff} changes with interaction

A. Potter, arxiv (2014)

Hubbard model at half filling and Mott metal-insulator transition



$$H = -t \sum_{<ij>,\sigma} \left(c_{i\sigma}^{\dagger} c_{j\sigma} + h.c. \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

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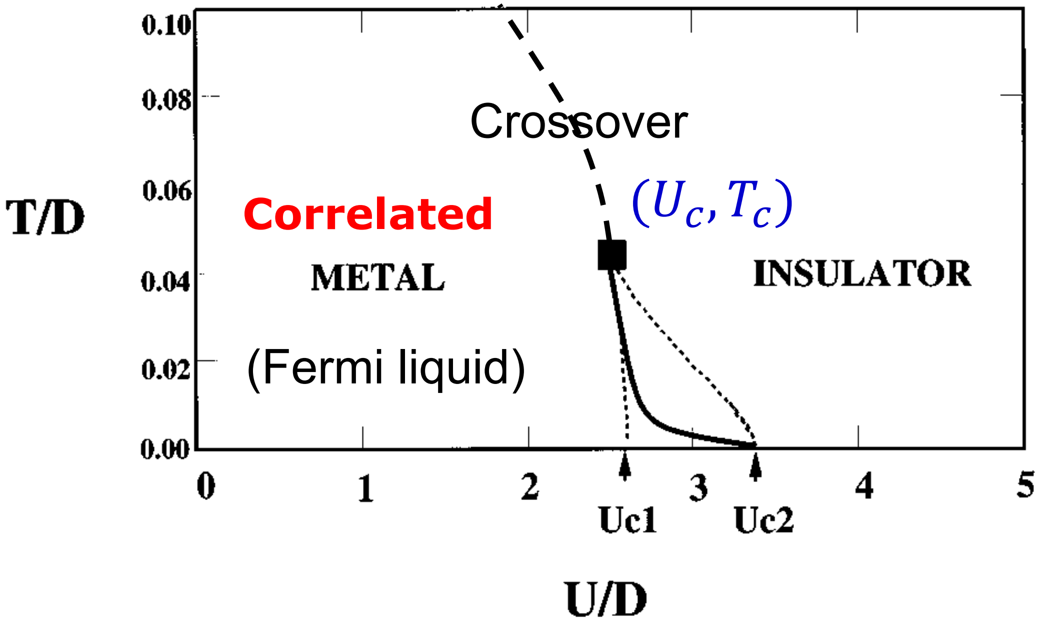

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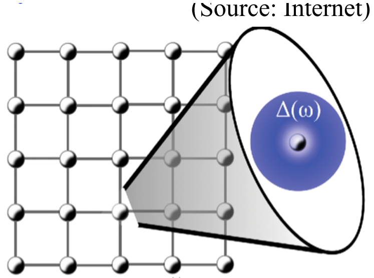
Single-site Dynamical mean-field theory (DMFT)

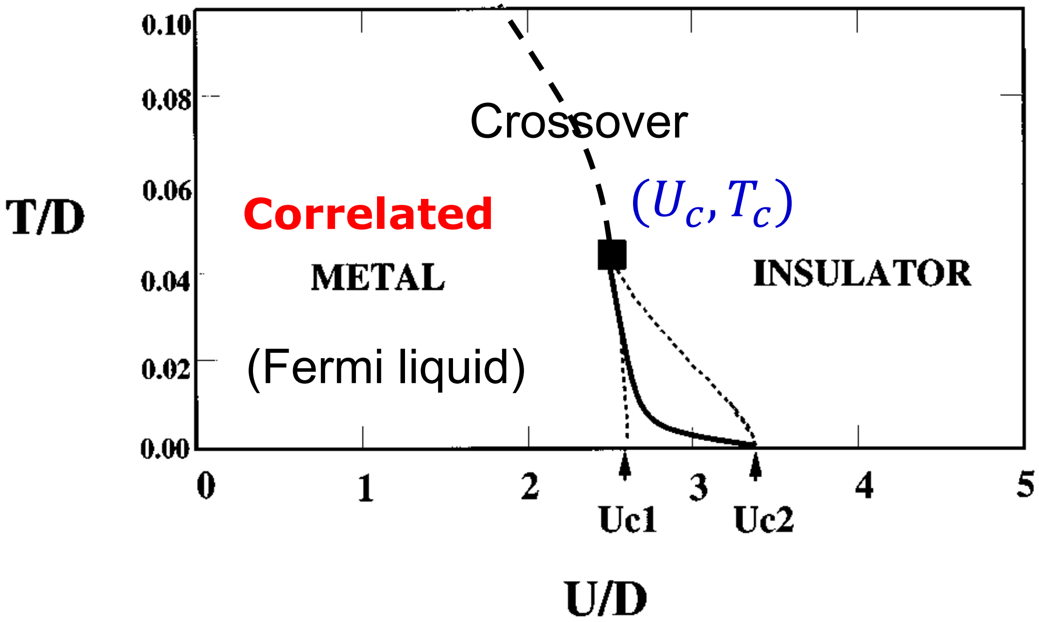
(Source: Internet)



DMFT: Impurity problem
in self-consistent bath

Georges et al. RMP (1996)

Hubbard model at half filling and Mott metal-insulator transition



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Extensions

DMFT+ CTQMC,
Cluster DMFT,
DFT +DMFT, ..

Kotliar et al., RMP (2006)

Single-site Dynamical mean-field theory (DMFT)

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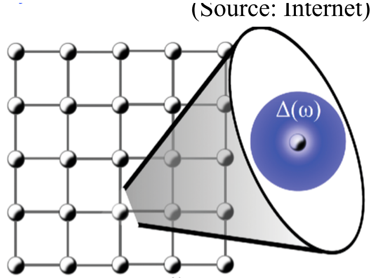

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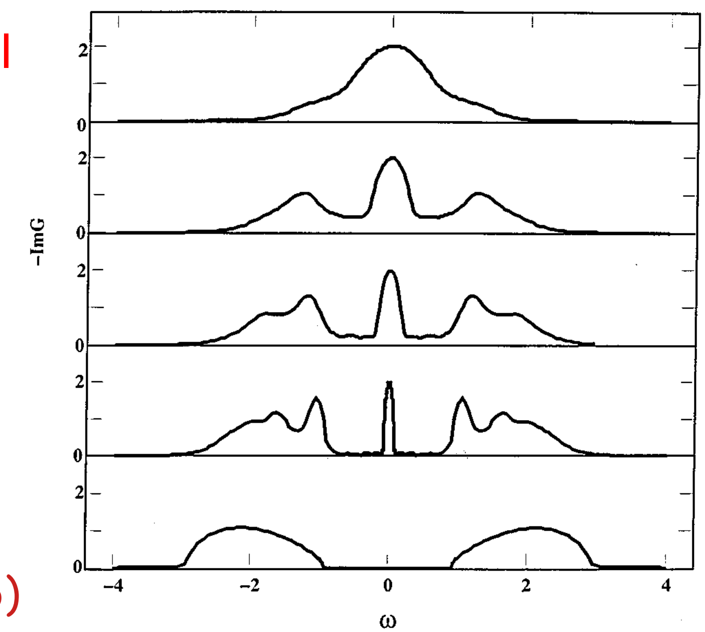
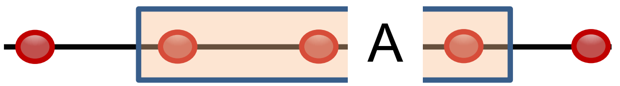
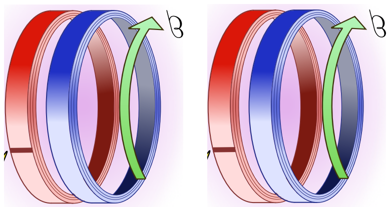


Second Renyi entropy



Not possible to extract $S_A^{(2)}$ from action directly unlike the large-N models.

Two replicas



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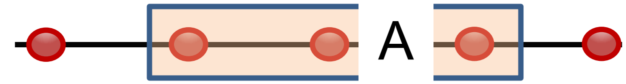

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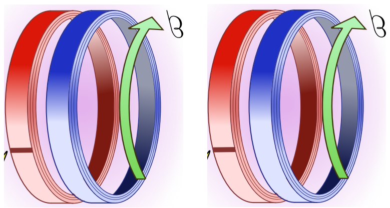
$$\exp[-S_A^{(2)}(\lambda)] \propto \int \mathcal{D}(\bar{c}, c) \exp[-(S_U + \lambda S_{kick})] \qquad \lambda = 1$$

$$S_{kick} = \int d\tau d\tau' \sum_{i\in A,\alpha,\beta=1,2} \bar{c}_{i\alpha}(\tau) M_{\alpha\beta}(\tau,\tau') c_{i\beta}(\tau')$$

Two replicas



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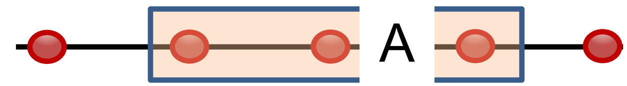

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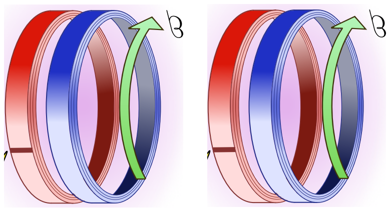
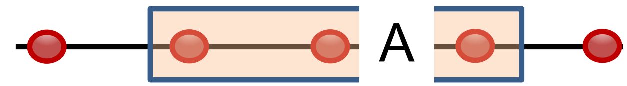
Second Renyi entropy

Two replicas





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Need only the local Green's function
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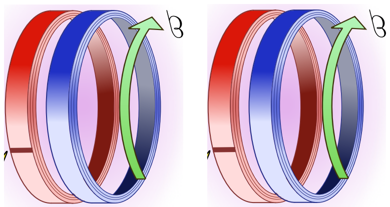

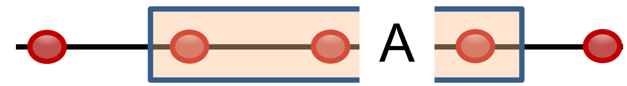

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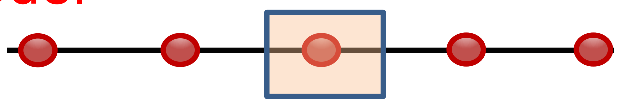
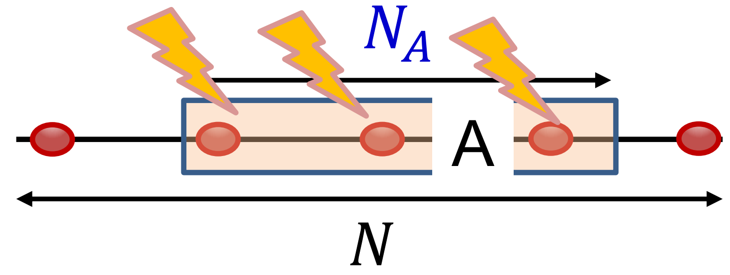
Entanglement is extracted as a 'non-equilibrium work' done due to kick perturbation

Entanglement via DMFT in Hubbard model



Space and time (τ) translation symmetries broken

Effective non-equilibrium inhomogeneous DMFT



Impurity action for i-th site

$$S_{\lambda,i} = -\int_0^\beta d\tau d\tau' \sum_{\sigma\alpha\beta} \bar{c}_{\sigma\alpha}(\tau)\mathcal{G}^{-1}_{i,\alpha\beta}(\tau,\tau')c_{\sigma\beta}(\tau') + U\int_0^\beta d\tau \sum_{\alpha} n_{\uparrow\alpha}(\tau)n_{\downarrow\alpha}(\tau)$$

$$\mathcal{G}_i^{-1}(\tau,\tau') = -(\partial_\tau-\mu)\delta(\tau-\tau') - \Delta_i(\tau,\tau') - \lambda\delta_{i\in A}M\delta(\tau-\tau_0^+)\delta(\tau'-\tau_0)$$

kick self energy

generalization of IPT impurity solver (CTQMC can be used)

+ lattice self consistency

→ recursive Green's function method on a space-time lattice

⇒ Calculate $G^{\lambda}_{ii,\alpha\beta}(\tau_0,\tau_0^+)$ to obtain $S_A^{(2)}(T)$

What do we expect for entanglement of metals (Fermi liquid)?

We calculate subsystem Renyi entropy $S_A^{(2)}(T)$

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1D $$S_A^{(2)}(T) = \left(\frac{c}{8}\right) \log\left[\frac{v_F}{\pi T} \sinh\left(\frac{\pi N_A T}{v_F}\right)\right] + \text{constant}$$

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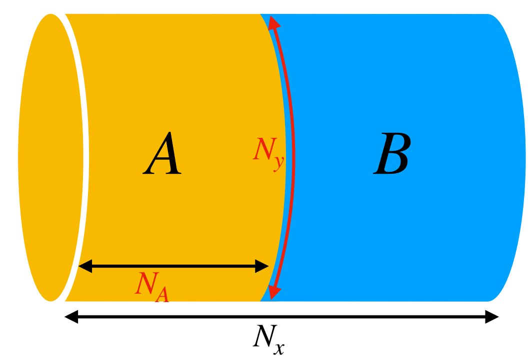

Collection of 1D gapless modes (CFTs)

Swingle, PRL (2010);

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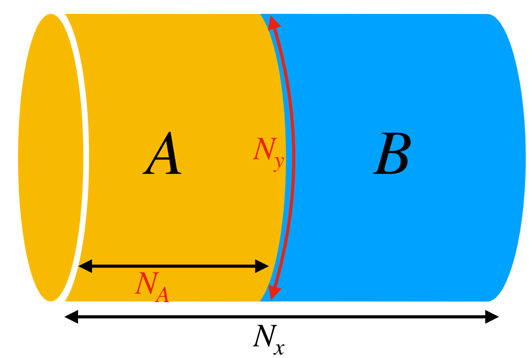

Collection of 1D gapless modes (CFTs)

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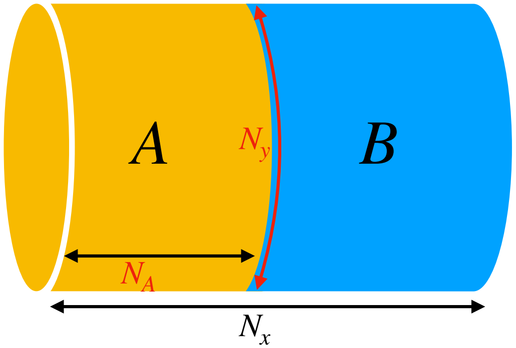
Does the correlated metallic state in Hubbard model (within DMFT) obey CFT predictions?

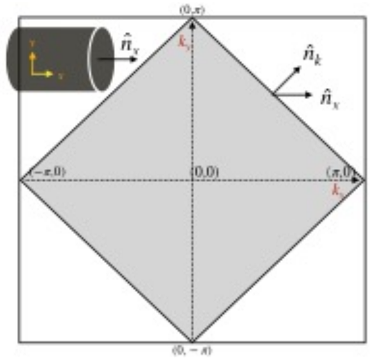
2D Hubbard Model



Widom formula

$$S_A^{(2)}(T) = WN_y\left[\left(\frac{c}{8}\right)\log\left[\frac{v_F}{\pi T}\sinh\left(\frac{\pi N_A T}{v_F}\right)\right] + \text{constant}\right]$$

$$WN_y = \frac{1}{4\pi}\int_{\partial A_x}\int_{\partial A_k} dA_x dA_k |\hat{\boldsymbol{n}}_x \cdot \hat{\boldsymbol{n}}_y|$$



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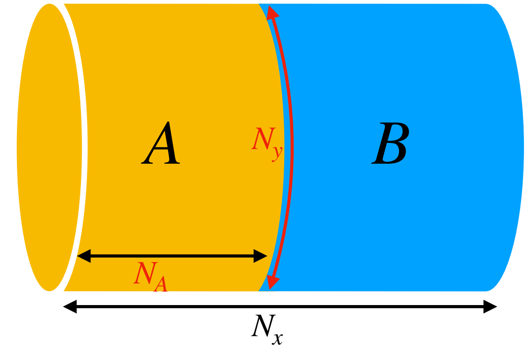

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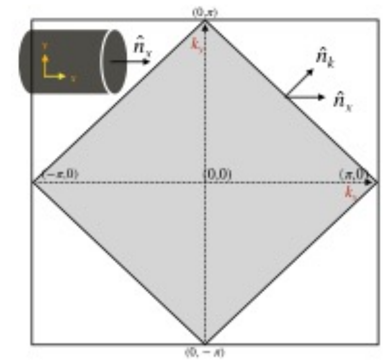

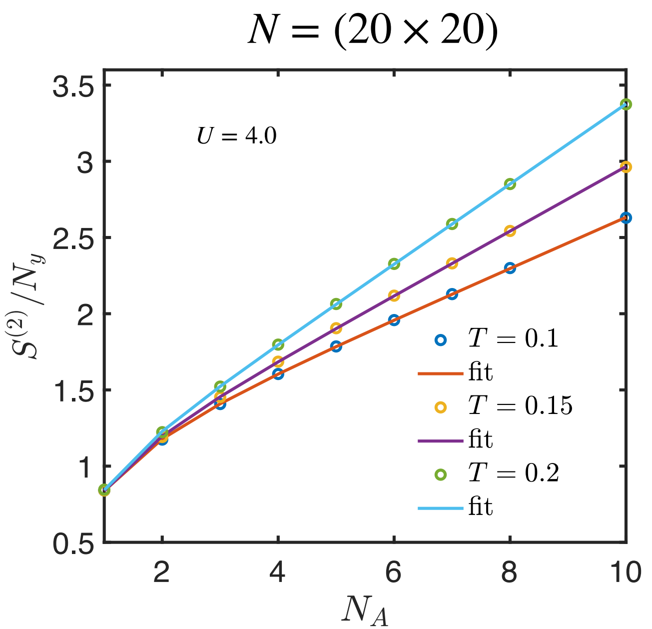

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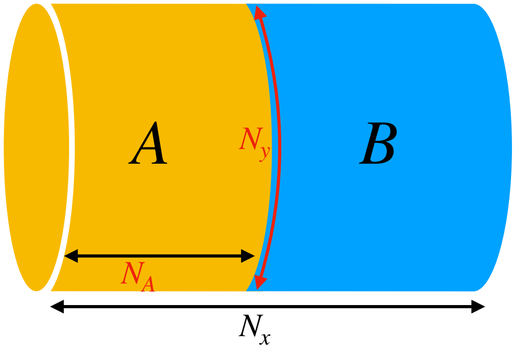

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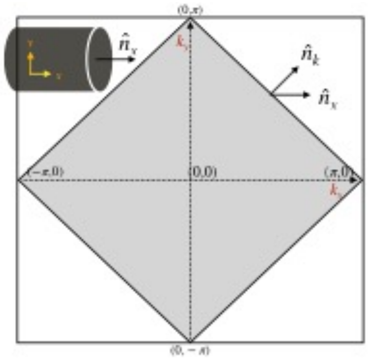

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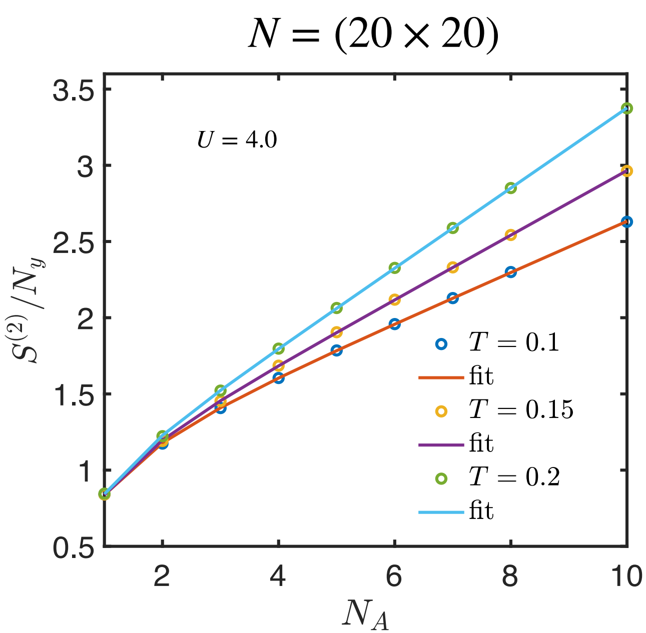

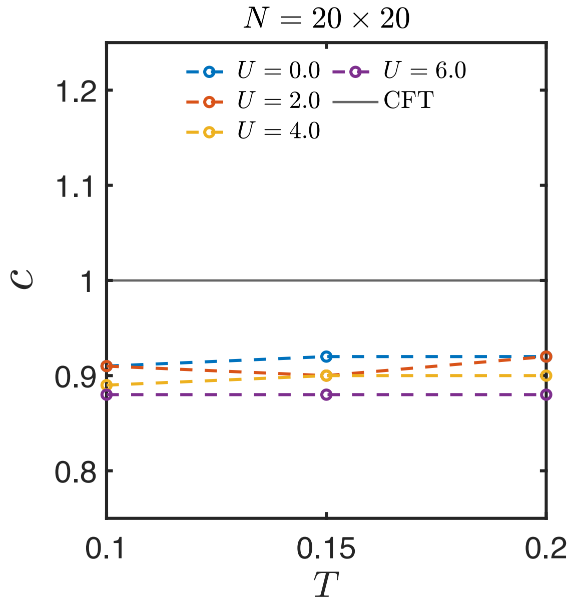

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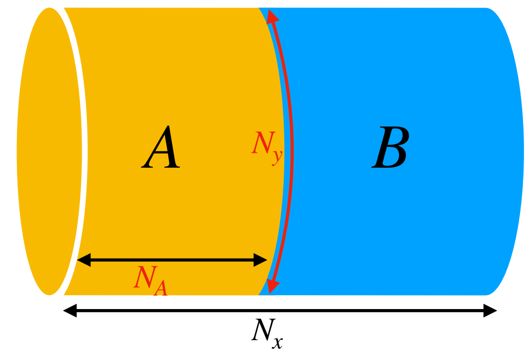

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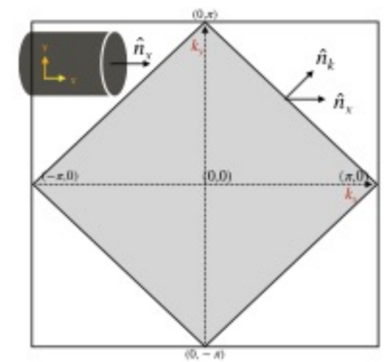
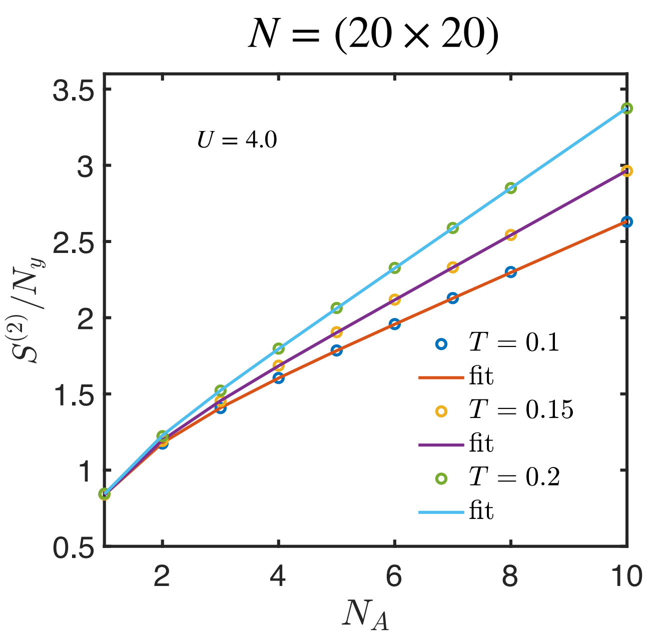
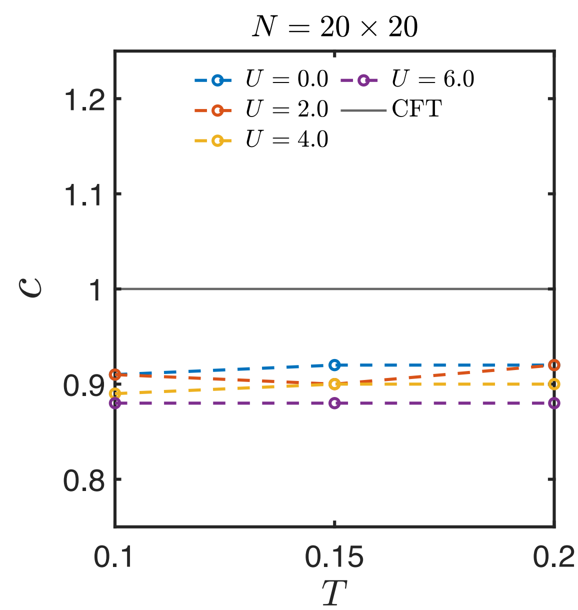


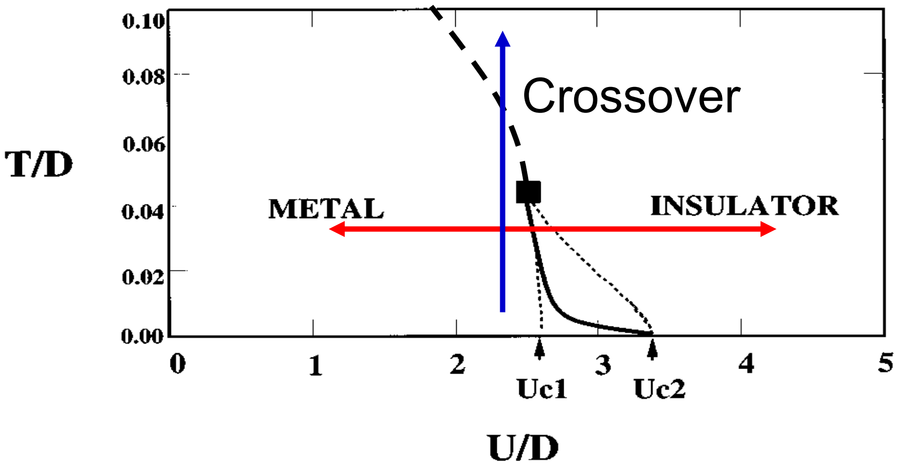


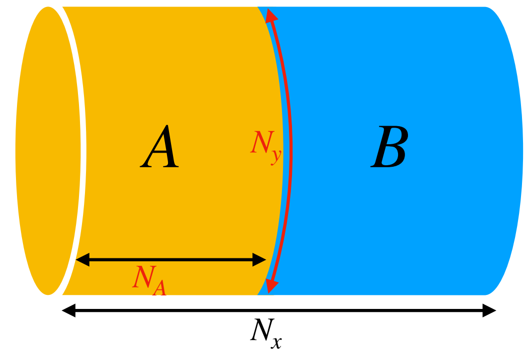


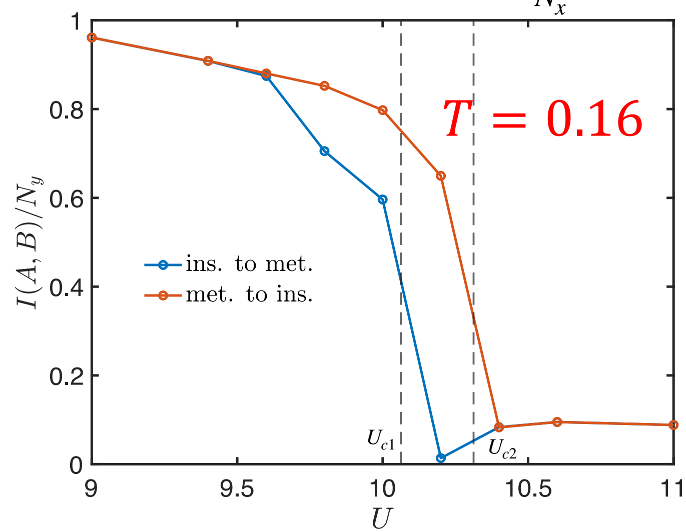
- 2D DMFT results well fitted by Widom crossover formula
- Central charge consistent with $c \approx 1$ $(\times 2)$

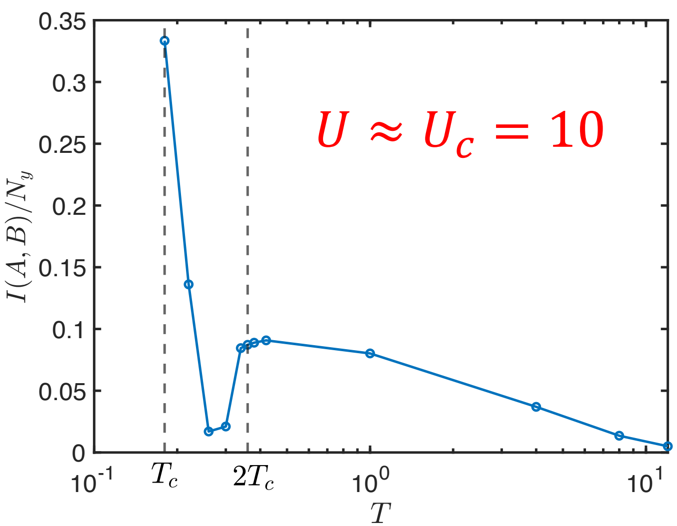
Mutual information across Mott transition

Renyi mutual information $I(A,B) = S_A^{(2)} + S_B^{(2)} - S_{A\cup B}^{(2)}$









Mutual information shows hysteresis across Mott metal-insulator transition

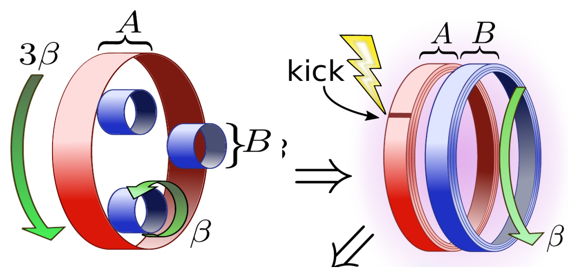
Correlation persists up to $T \lesssim W$ in the Mott insulator

Summary and outlook

○ New path integral and DMFT methods to compute entanglement in large-N models and strongly correlated systems.

⇒ SYK NFL, Heavy FL, interacting diffusive metal, metallic state in Hubbard model.

○ Metallic state in Hubbard model within local self-energy approximation is well described by CFT crossover formula.

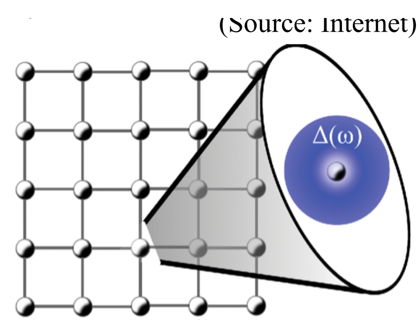


○ Entanglement of correlated systems in 3D.

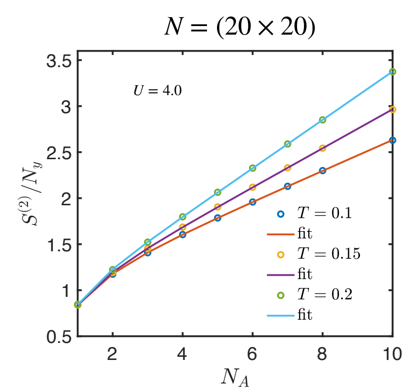
○ Extensions to CTQMC impurity solver, cluster DMFT, ..

○ Other quantum many-body approximations for entanglement -- RPA, RG, ..

○ Entanglement entropy of large-N solvable non-Fermi liquid with critical Fermi surface.



DMFT: Impurity problem in self-consistent bath



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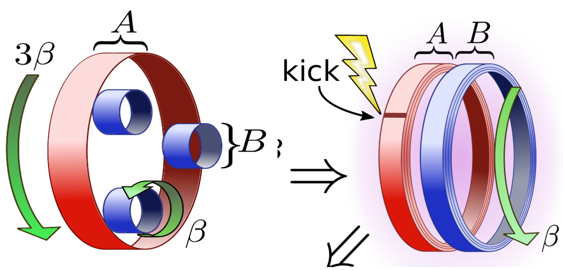

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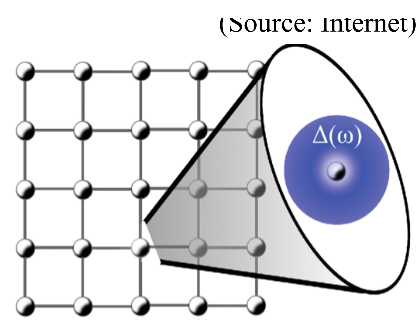

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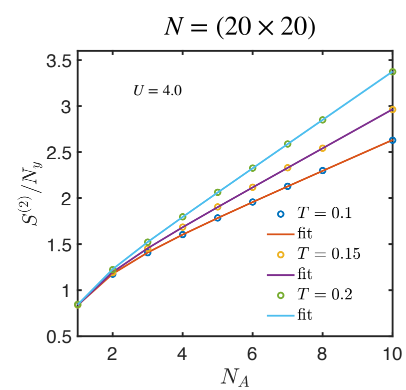
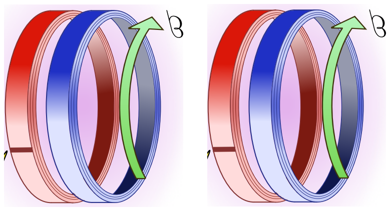
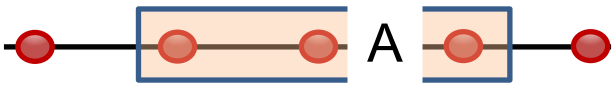


Thank You!

Two replicas



Second Renyi entropy



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$$S_A^{(2)} = \int_0^1 d\lambda \langle S_{kick}\rangle$$

$$e^{-S_A^{(2)}(\lambda)} = \frac{Z_A^{(2)}(\lambda)}{Z^2} = \frac{1}{Z^2}\int \mathcal{D}(\bar{c},c)e^{-(\mathcal{S}+\lambda\mathcal{S}_{\text{kick}})}$$

$$\langle \mathcal{S}_{\text{kick}}\rangle_{Z_A^{(2)}(\lambda)} = \sum_{i\in A,\alpha\beta\sigma} M_{\alpha\beta} G_{i\sigma\beta,i\sigma\alpha}(\tau_0,\tau_0^+)$$

$$\partial_\lambda S_A^{(2)}(\lambda) = \frac{\int \mathcal{D}(\bar{c},c)e^{-(\mathcal{S}+\lambda\mathcal{S}_{\text{kick}})}\mathcal{S}_{\text{kick}}}{\int \mathcal{D}(\bar{c},c)e^{-(\mathcal{S}+\lambda\mathcal{S}_{\text{kick}})}} = \langle \mathcal{S}_{\text{kick}}\rangle_{Z_A^{(2)}(\lambda)}$$

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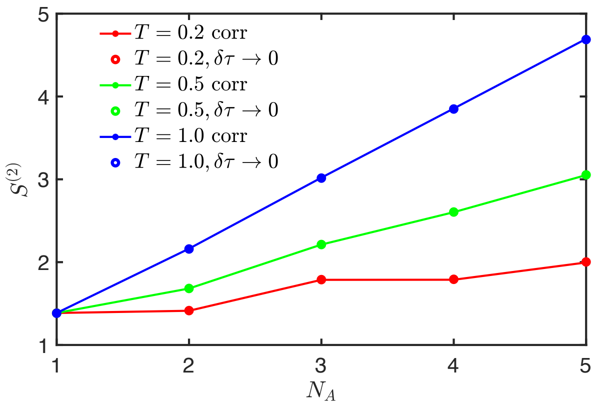
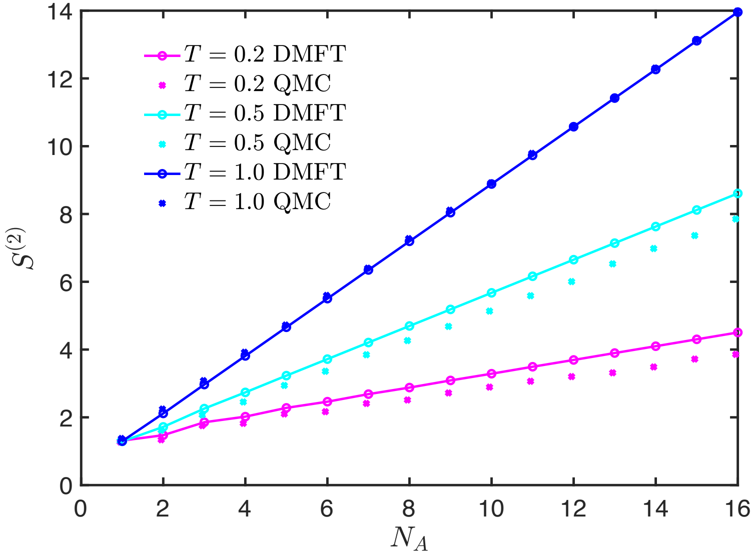
1D Hubbard Model

Non interacting, $U = 0$



○ our DMFT is exact for $U = 0$

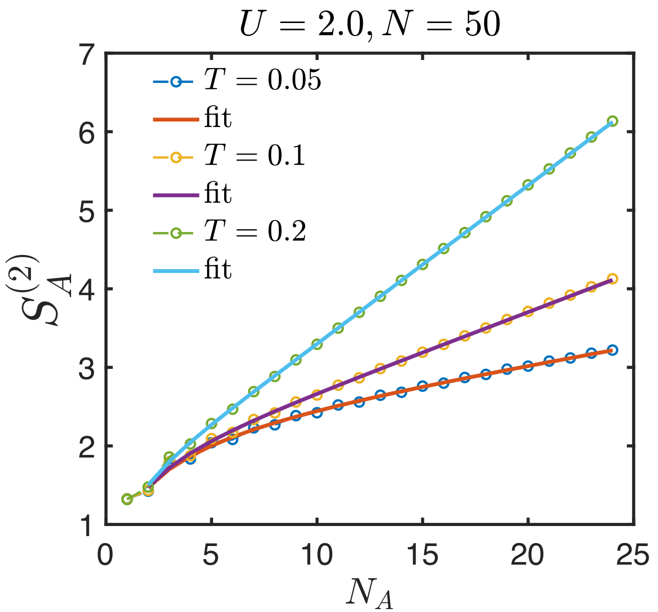
Comparison with QMC, $U \neq 0$ Broecker & Trebst, J. Stat. Mec. (2014)

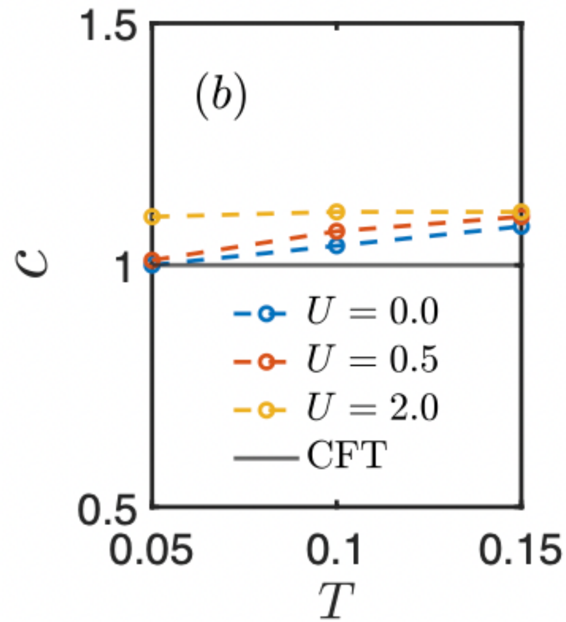


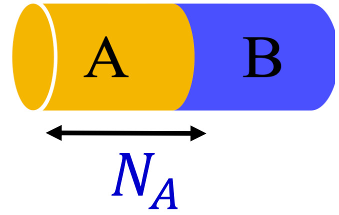
Comparison with QMC at intermediate T is quite good even with single-site DMFT + IPT approximation!

*DMFT cannot capture low-temperature 1D physics, charge gap at half filling, spin-charge separation and Luttinger liquid

1D Hubbard Model







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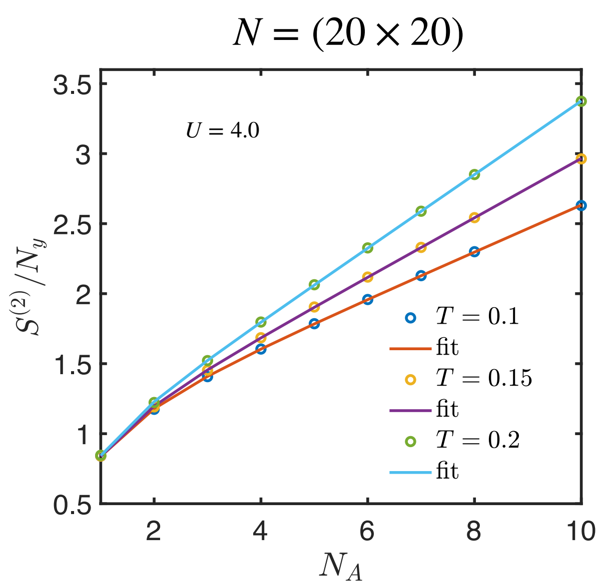
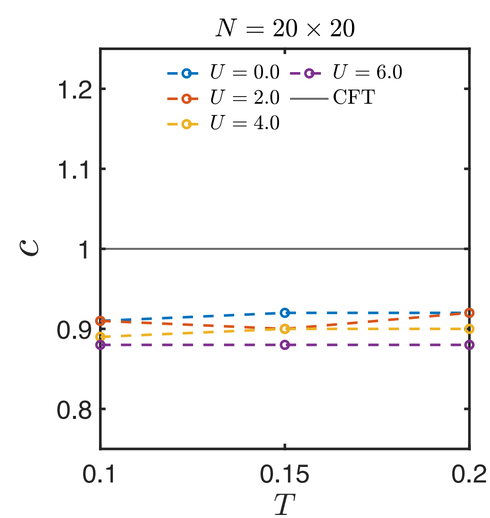
2D Hubbard Model





- 2D DMFT results well fitted by Widom crossover formula
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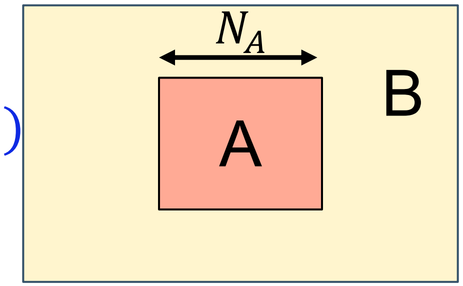
Measure of entanglement for a pure state $|\psi\rangle$



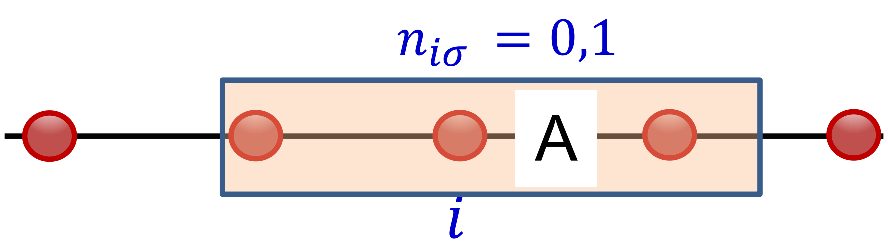
Reduced density matrix of a subsystem $\rho_A = Tr_B(|\psi\rangle\langle\psi|)$

n-th Renyi entropy $$S_A^{(n)} = \frac{1}{1-n} \ln Tr_A[\rho_A^n]$$

How do we compute entanglement entropy?

Hard to compute entanglement entropy.

Consider Hubbard model, $H = -t \sum_{i\sigma} \left(c_{i\sigma}^\dagger c_{i+1,\sigma} + h.c. \right) + U \sum_i n_{i\uparrow} n_{i\downarrow}$



N sites, one electron per site

$\sim \exp(N)$ states in Hilbert space basis

Many-body wave function is a complicated object,

$$|\psi\rangle = \sum_{\{n_{i\sigma}\}} C_{\{n_{i\sigma}\}} |n_{1\uparrow}, n_{1\downarrow}, n_{2\uparrow}, n_{2\downarrow}, \ldots\rangle$$

Need $\sim \exp(N)$ coefficients $C_{\{n_{i\sigma}\}}$

and then calculate $\rho_A = Tr_B(|\psi\rangle\langle\psi|)$