Entanglement Entropy of Excited States in Disordered Interacting Finite 1D QD: Signs of Many-Body Delocalization?

Ground State
R. Berkovits, PRL 108 176803 (2012).

Excited State
(work in progress).

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Delocalization for a disordered interacting system

There has been a considerable amount of discussion in the literature on whether electron-electron interactions may enhance the localization length, motivated by the "2DMIT" (2D metal insulator transition) and 2 particle delocalization.

For spinless 1D systems it is clear that e-e interactions decrease the ground-state localization length (i.e., lead to stronger localization)

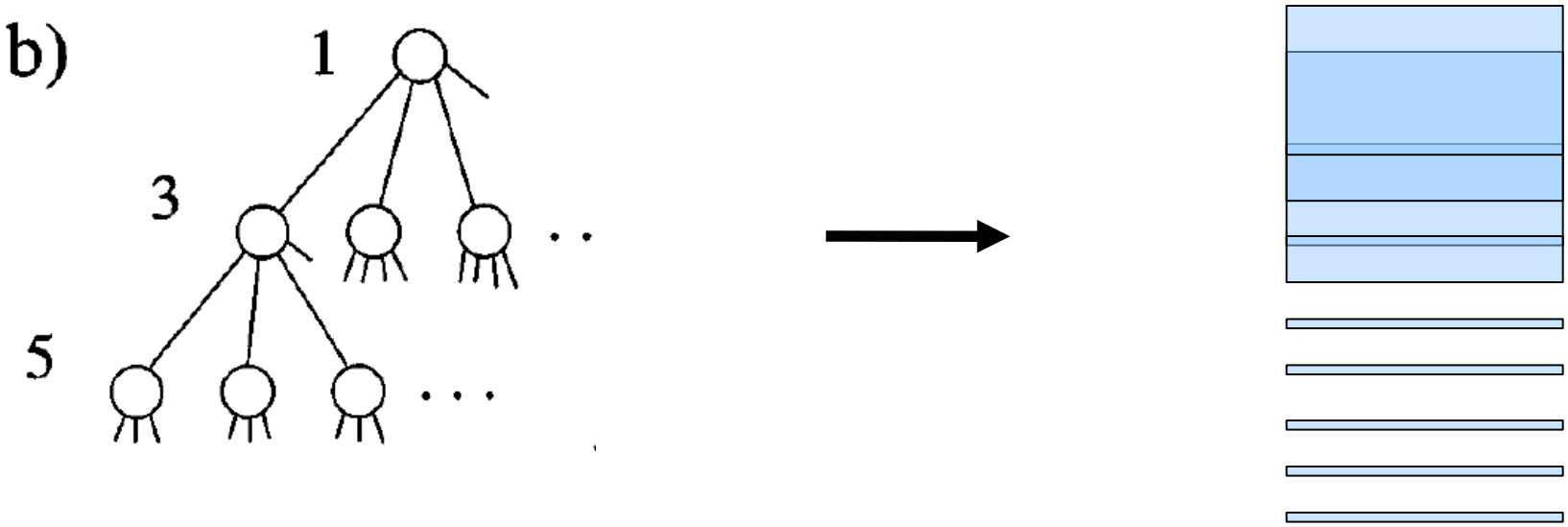
The ground state of a 1D disordered system is localized even in the presence of e-e interactions

What about the excited states?
Fock space localization

VOLUME 78, NUMBER 14 PHYSICAL REVIEW LETTERS 7 APRIL 1997

Quasiparticle Lifetime in a Finite System: A Nonperturbative Approach

Boris L. Altshuler,[1] Yuval Gefen,[2] Alex Kamenev,[2] and Leonid S. Levitov[3]



Sivan, Imry, Aronov, EPL 28,115 (1994)

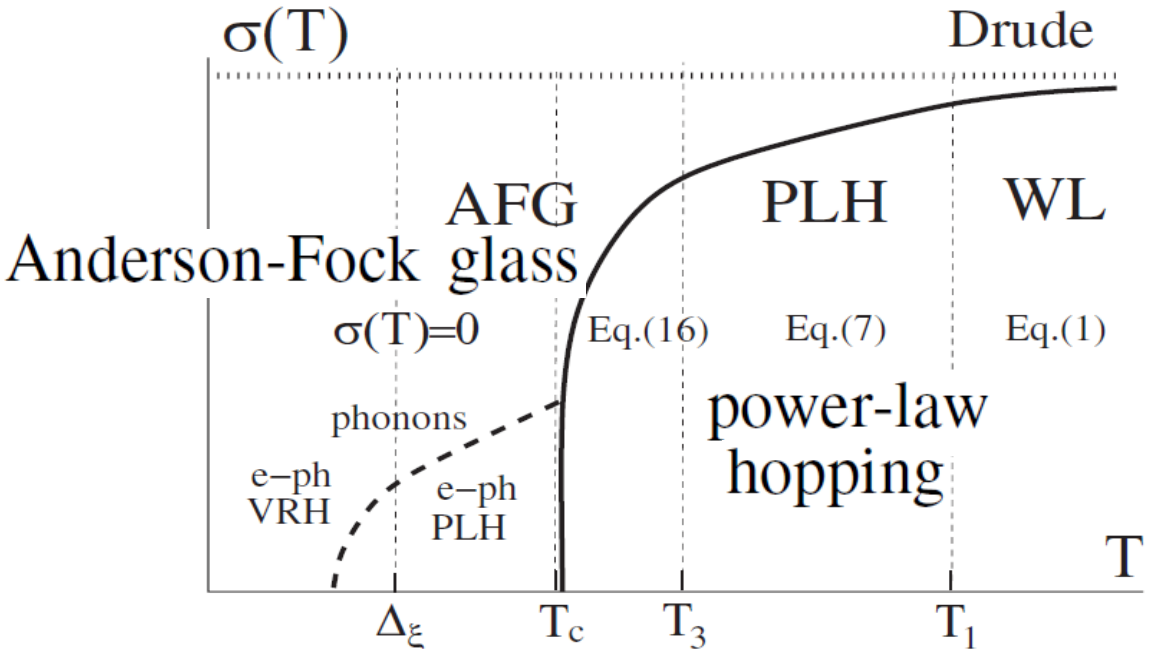
$\sigma(T) \propto \Gamma$ **Relevant to infinite systems?**

What about the excited states for infinite systems?

PRL **95,** 206603 (2005) PHYSICAL REVIEW LETTERS week ending 11 NOVEMBER 2005

Interacting Electrons in Disordered Wires: Anderson Localization and Low-*T* Transport

I. V. Gornyi,[1,*] A. D. Mirlin,[1,2,†] and D. G. Polyakov[1,*]



ELSEVIER

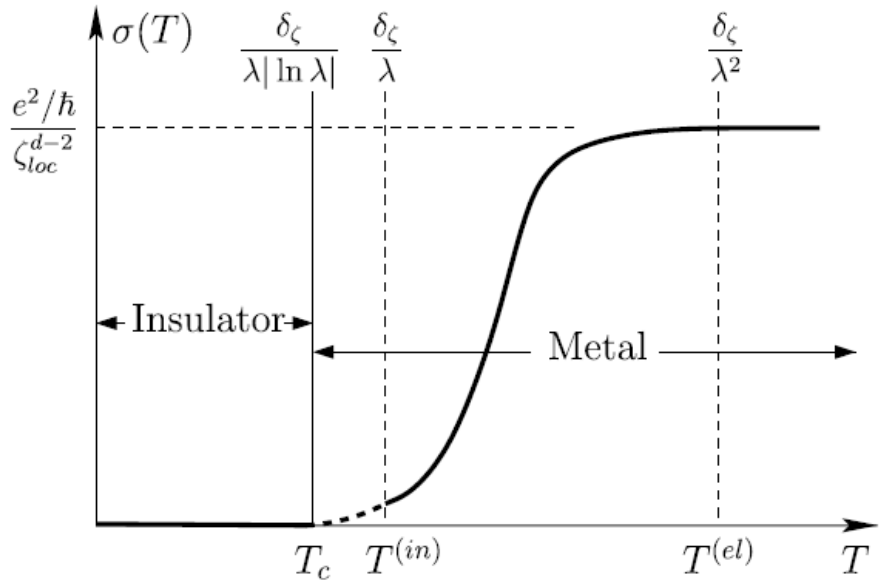
Annals of Physics 321 (2006) 1126–1205

PHYSICS

www.elsevier.com/locate/aop

Metal–insulator transition in a weakly interacting many-electron system with localized single-particle states

D.M. Basko [a,b,*], I.L. Aleiner [b], B.L. Altshuler [a,b,c]



Numerical Demonstration:

Conductance (especially for finite temperature) is computationally taxing.

Level statistics is hard to interpret (requires extrapolation from small systems)

R. Berkovits and B. Shklovskii, J. Phys. CM 11, 779 (1999).
V. Oganesyan and D. A. Huse, PRB 75, 155111 (2007).

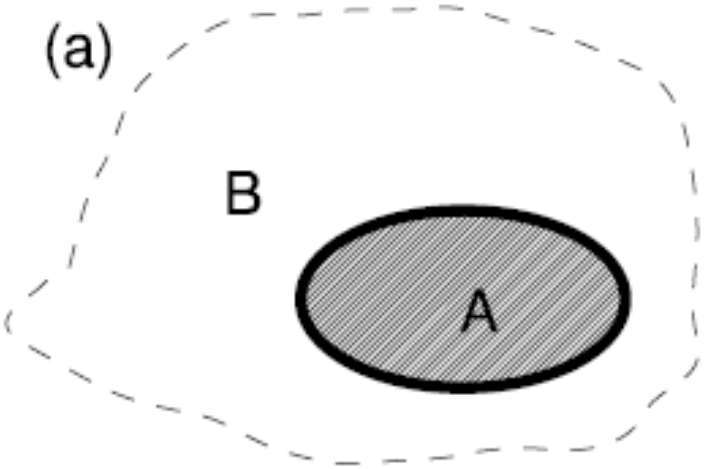
Renormalized hoppings (works for infinite temperature)

M. Cecile and G. Thomas, PRB 81 134202 (2010).

Entanglement Entropy (EE) may be the answer!

EE - Entanglement Entropy

System (a) Is in a pure state



Divide the system into two regions A and B. Any pure state:

$$|\Psi_{A,B}\rangle = \Sigma_{i,j}\alpha_{i,j}|\psi_{A,i}\rangle|\psi_{B,j}\rangle$$

Using the Schmidt decomposition

$$|\Psi_{A,B}\rangle = \Sigma_i \alpha_i |\phi_{A,i}\rangle |\phi_{B,i}\rangle$$

* two orthonormal basis $|\phi_{A,i}\rangle$ and $|\phi_{B,j}\rangle$
* $\alpha_i \geq 0$ and $\Sigma_i \alpha_i^2 = 1$

Reduced density matrix:

$$\hat{\rho}_{A/B} = \mathrm{Tr}_{B/A} |\Psi\rangle\langle\Psi|$$

$$\hat{\rho}_{A/B} = \Sigma_i \alpha_i^2 |\phi_{A/B,i}\rangle\langle\phi_{A/B,i}|$$

Definition of entanglement entropy

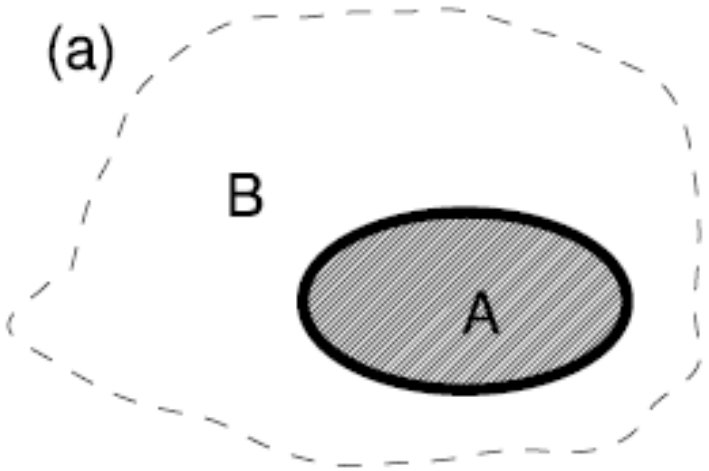
$$S_{A/B} = -\Sigma_i \alpha_i^2 \ln(\alpha_i^2)$$

i.e. the von Neuman (or Shannon in the context of Information theory) entropy of the reduced density matrix

$$\text{Obviously } S_A = S_B$$

Properties: additivity and convexity

Dependence of EE on dimension, shape and topology of the region A



The area law $S \propto L_A^{(d-1)}$

M. Srednicki, Phys. Rev. Lett., **71**, 666 (1993)

The EE is proportional to the surface area between A and B

Connections between EE and condensed matter physics

DMRG – Density Matrix Renormalization Group – an extremely accurate numerical method for the calculation of the ground state of a one-dimensional many-body system

QPT – Quantum Phase Transitions – EE exhibits a unique signature in its behavior at a QPT. This enables to identify and study the properties of QPT.

QPT and EE in one-dimensional systems

According to the area law $S \propto L_A^{(d-1)}$ **resulting in a constant EE for 1D systems**

Nevertheless for an infinite correlation length there are logarithmic corrections resulting in:

$$S_A \propto \frac{1}{3}\log(L_A) + C$$

while for systems with a finite correlation length (for example gapped systems):

$$S_A \propto \frac{1}{3}\log(\xi) + C'$$

Anderson Localization and EE

Metallic regime - extended states, infinite localization length and therefore we expect a logarithmic dependence of the EE for the ground state and a non suppressed EE for the excited states

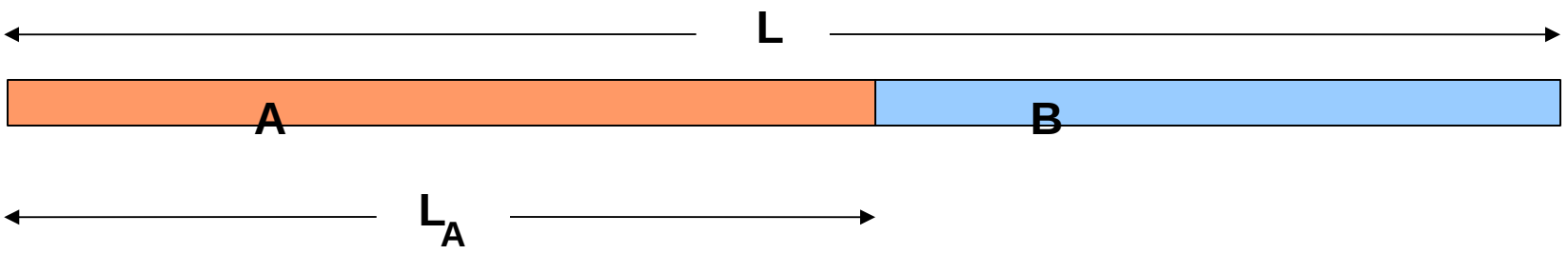
Localized regime – finite localization length (although there is no gap) and therefore we expect a constant EE both for the ground and excited states once the system size exceeds the localization length

A good way to identify the localization length for an interacting system

The one-dimensional Hamiltonian

$$H = \sum_{j=1}^{L} \epsilon_j \hat{c}_j^\dagger \hat{c}_j - t \sum_{j=1}^{L-1} (\hat{c}_j^\dagger \hat{c}_{j+1} + h.c.)$$

$$+ U \sum_{j=1}^{L-1} (\hat{c}_j^\dagger \hat{c}_j - \frac{1}{2})(\hat{c}_{j+1}^\dagger \hat{c}_{j+1} - \frac{1}{2}),$$



where the on-site energies are taken from the range [-W/2,W/2]

and the LL parameter g:

$$g(U) = \pi / [2 \cos^{-1}(-U/2)]$$

For the non-interacting case it is numerically known that the localization length depends on the width of the on-site energy distribution:

$$\xi(W, U = 0) \approx 105/W^2$$

Ro¨mer and Schreiber, PRL 78, 515 (1997).

While the influence of interaction was postulated to reduce the ground state localization length by:

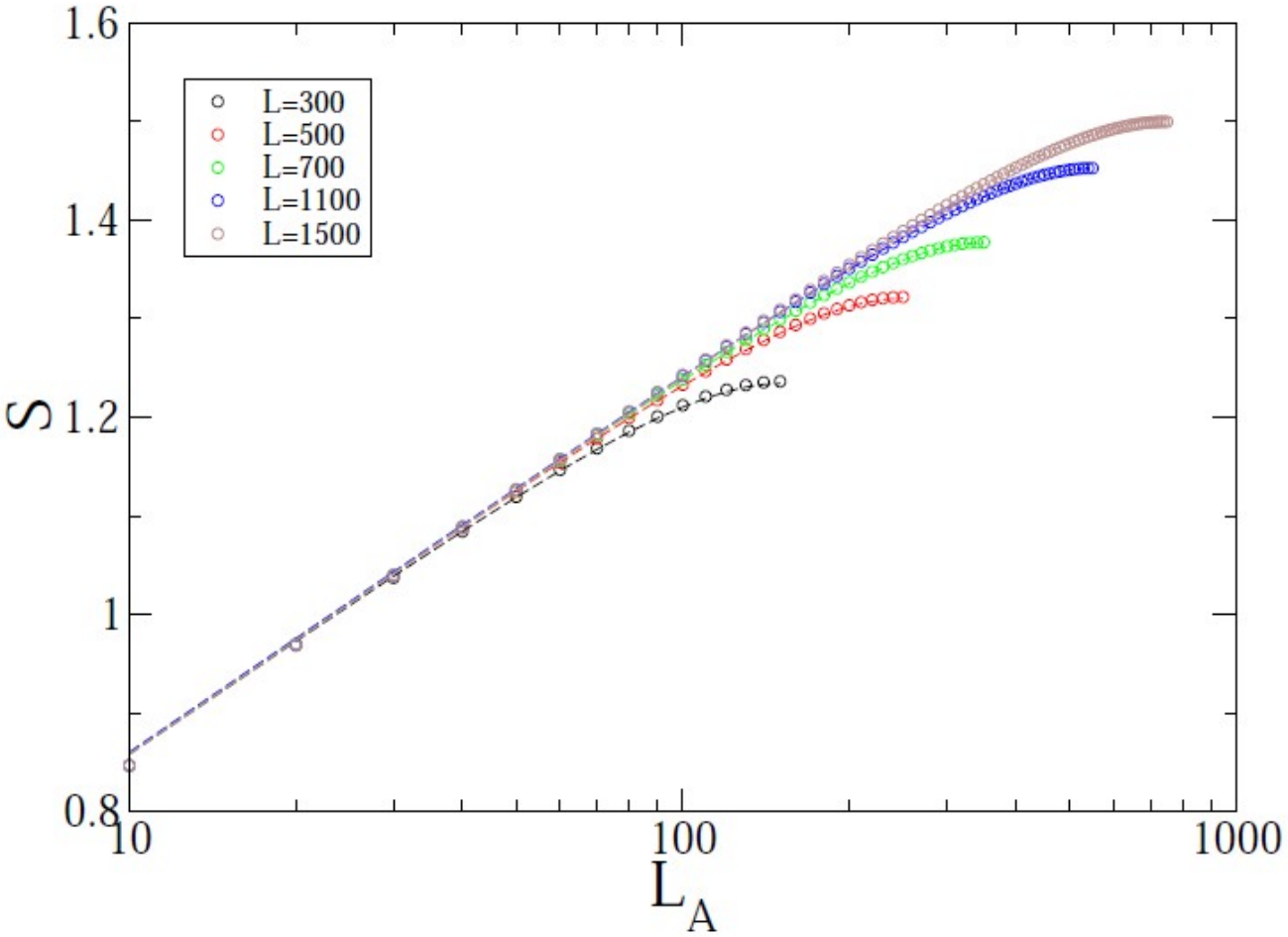
$$\xi(W, U) = (\xi(W, U = 0))^{1/(3-2g(U))}$$

Apel, J. Phys. C 15, 1973 (1982);
Giamarchi and Schulz PRB 37,325 (1988).

Ground state finite size effects (clean system)

$$S(L_A, L) = \frac{1}{6} \ln \left(\sin \left(\frac{\pi L_A}{L} \right) \right) + c$$

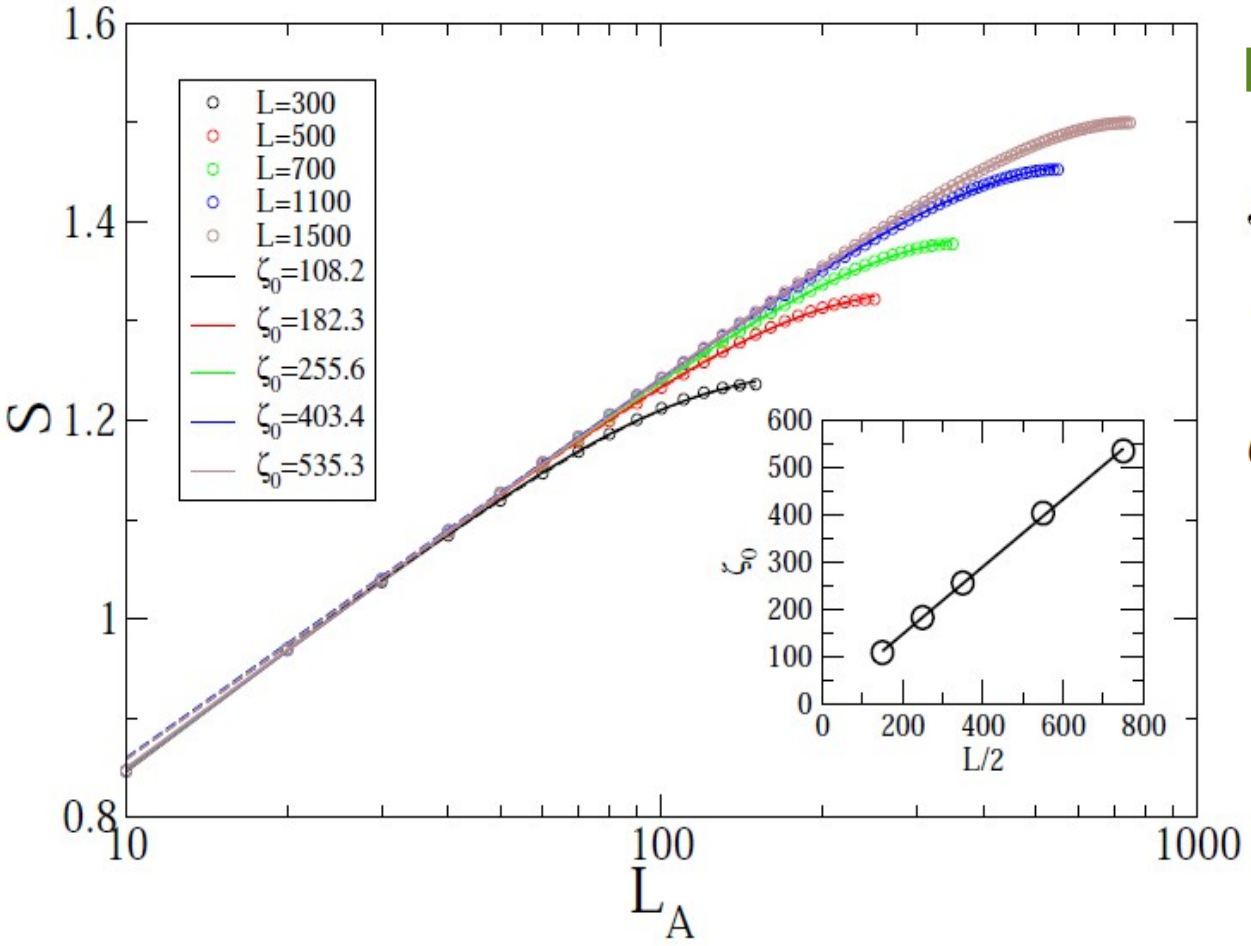
(Holzhey,Larsen,Wilczek,1994)



Finite size effects (disordered system)

$$S(L_A, \xi, L) = s(\xi) \ln\left(\mathrm{erf}\left(\frac{\mathrm{L_A}}{\zeta(\mathrm{L}, \xi)}\right)\right) + c$$

R. Berkovits, PRL 108 176803 (2012).

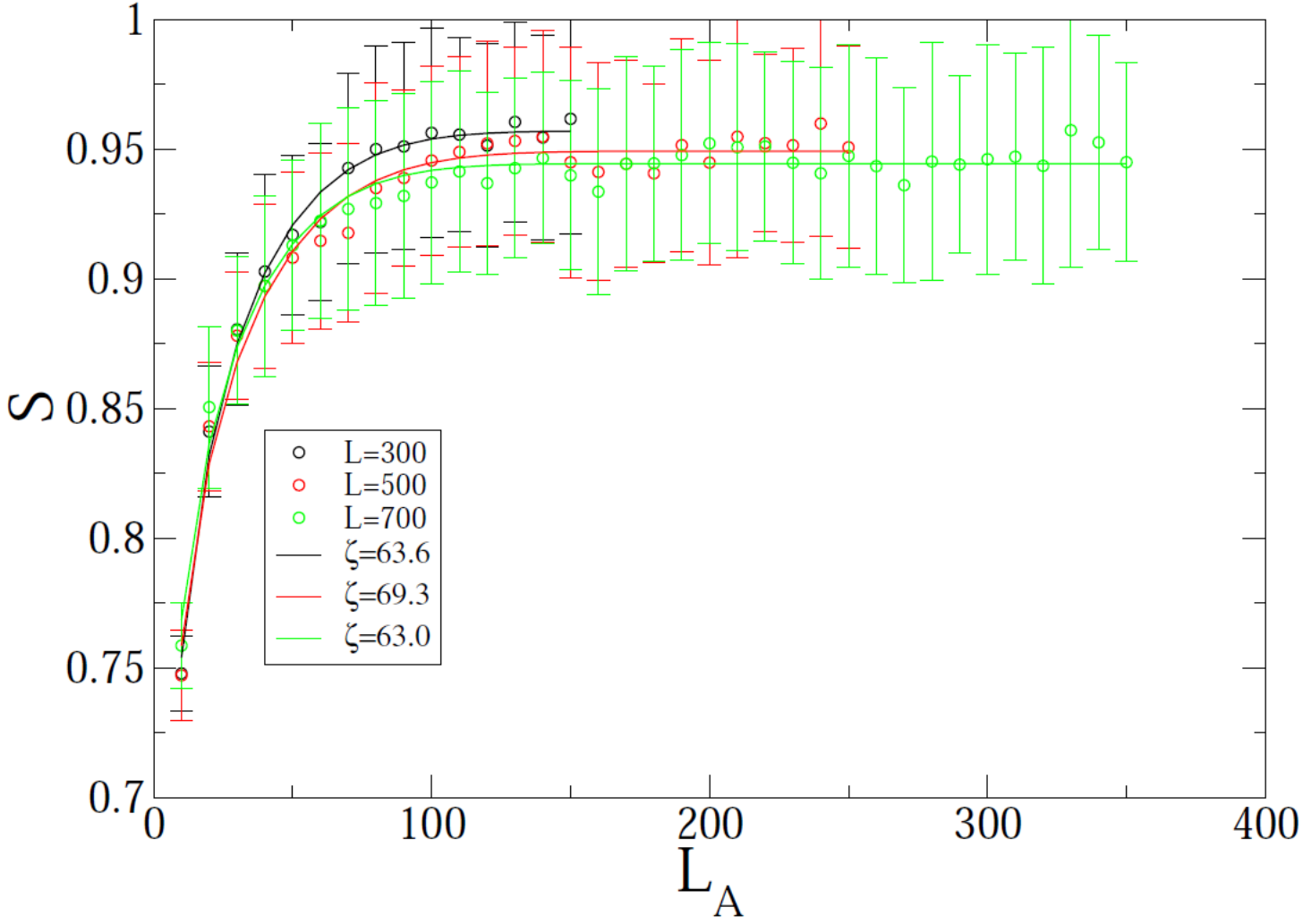


For a clean system

$$s(\xi \to \infty) \approx 1/6$$

$$\zeta_0(L) = \zeta(L, \infty)$$

$$\zeta_0 = 0.357L$$



$\xi = 57$

$\zeta \approx \xi$ for $L \gg \xi$

Interpolation of ζ

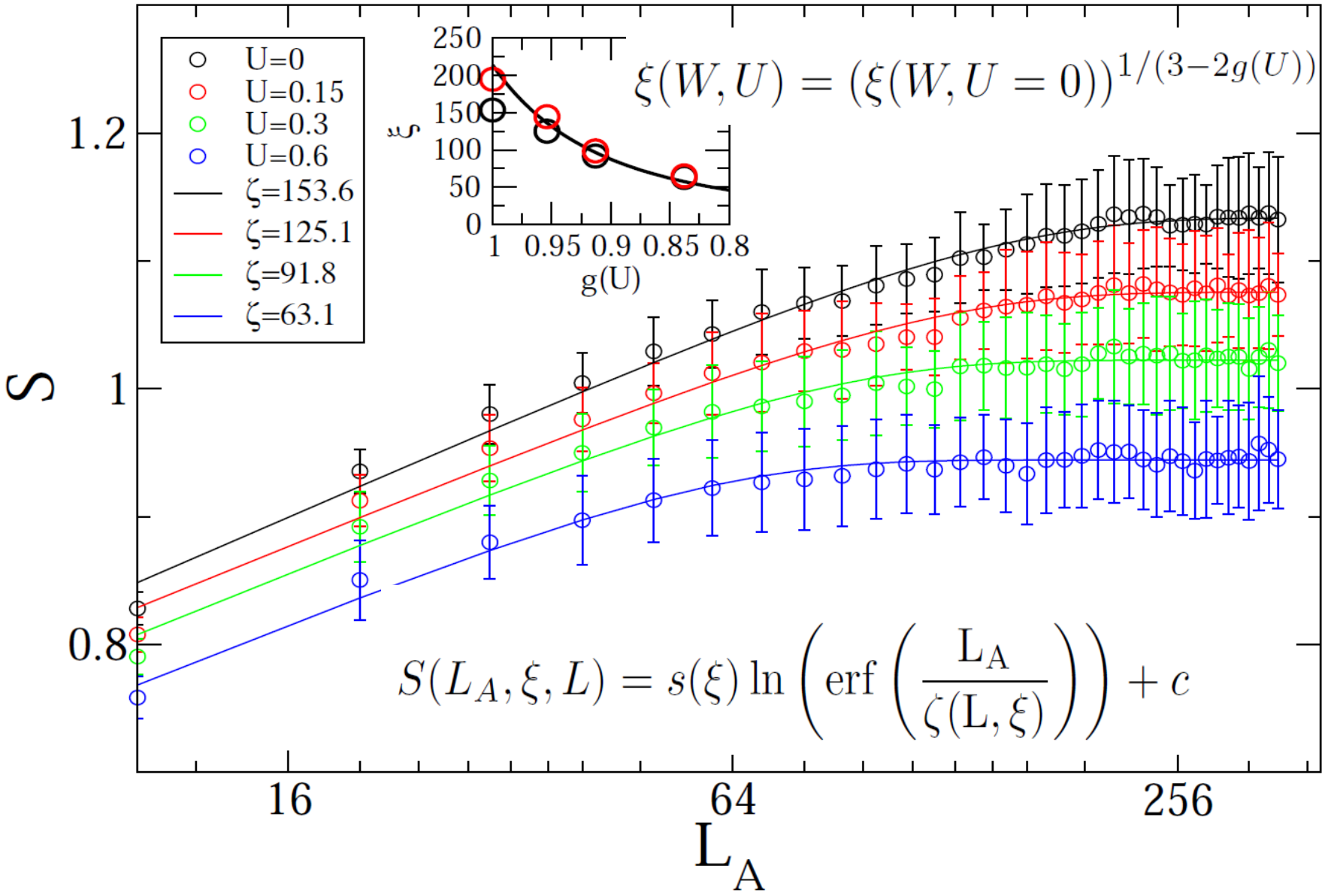
$$\zeta(L \gg \xi) \approx \xi$$

$$\zeta(L \ll \xi) = \zeta_0 = 0.357L$$

Interpolation between the two limits

$$\frac{1}{\zeta^2} = \frac{1}{\zeta_0^2} + \frac{1}{\xi^2}$$

Interacting systems



Entanglement entropy of excited states

Vincenzo Alba[1], Maurizio Fagotti[2] and Pasquale Calabrese[2]

Conversely, only little attention has been devoted to the entanglement properties of excited states (with the exception of a few papers [9]–[11]), although it is a very natural problem. Here we consider two topical spin chains [12] to address this issue. We first

No general understanding of the excited states EE is available even for a clean 1D non-interacting system

Two-Particle excited states EE

The study of two-particle excited states was very fruitful in understanding interaction induced (de)localization. (D. L. Shepelyansky 1994, Y. Imry 1995)

Simple enough to obtain some analytical results for the excited states EE

$$H = \sum_{j=1}^{N} \epsilon_j \hat{a}_j^\dagger \hat{a}_j - t \sum_{j=1}^{N} (e^{i\alpha} \hat{a}_j^\dagger \hat{a}_{j+1} + h.c.)$$

$|k_1, k_2\rangle$ **Two-particle state**

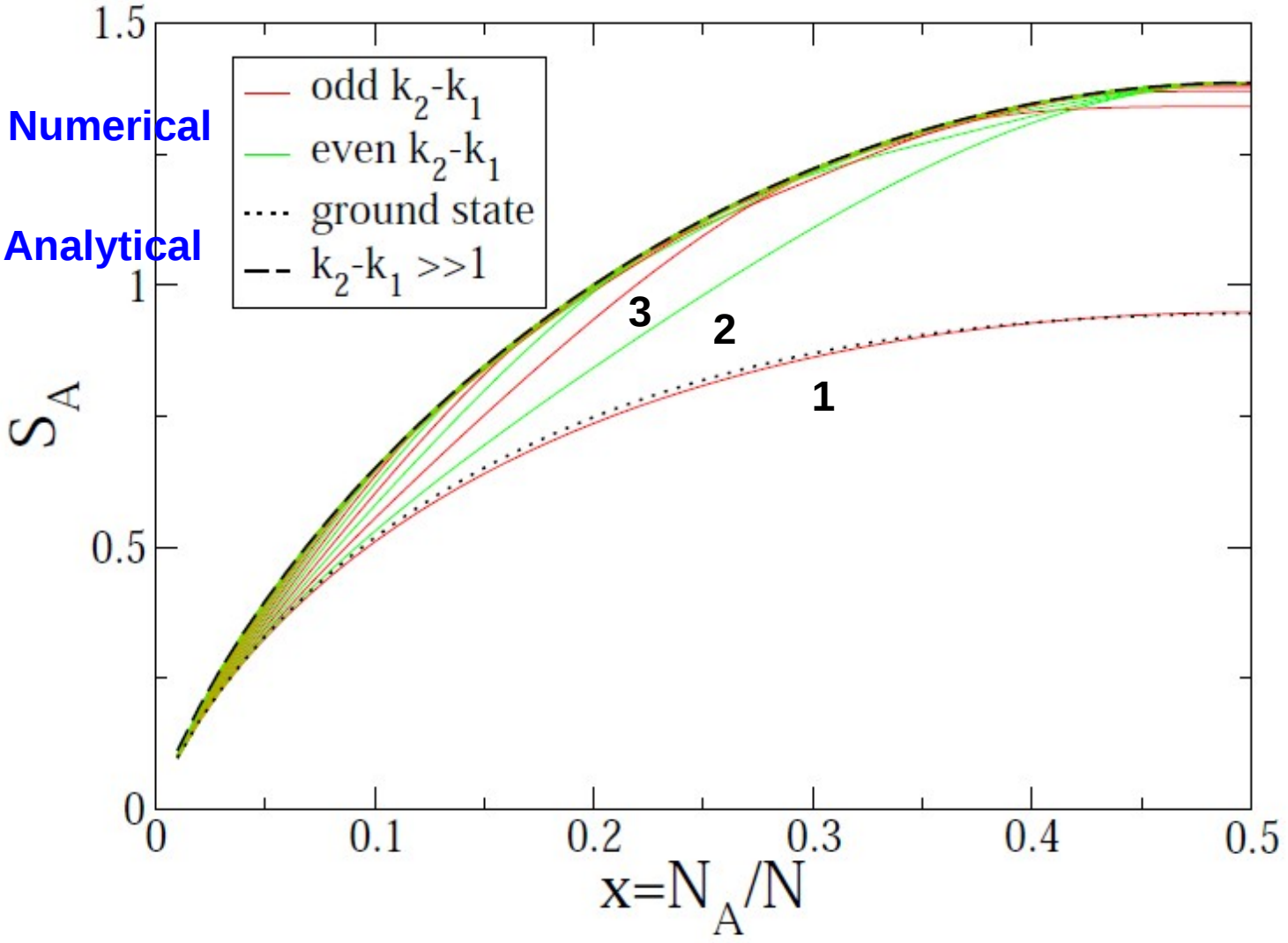
EE $S_A(k_2 - k_1 \gg 1) = -2(1-x)\ln(1-x) - 2x\ln(x)$

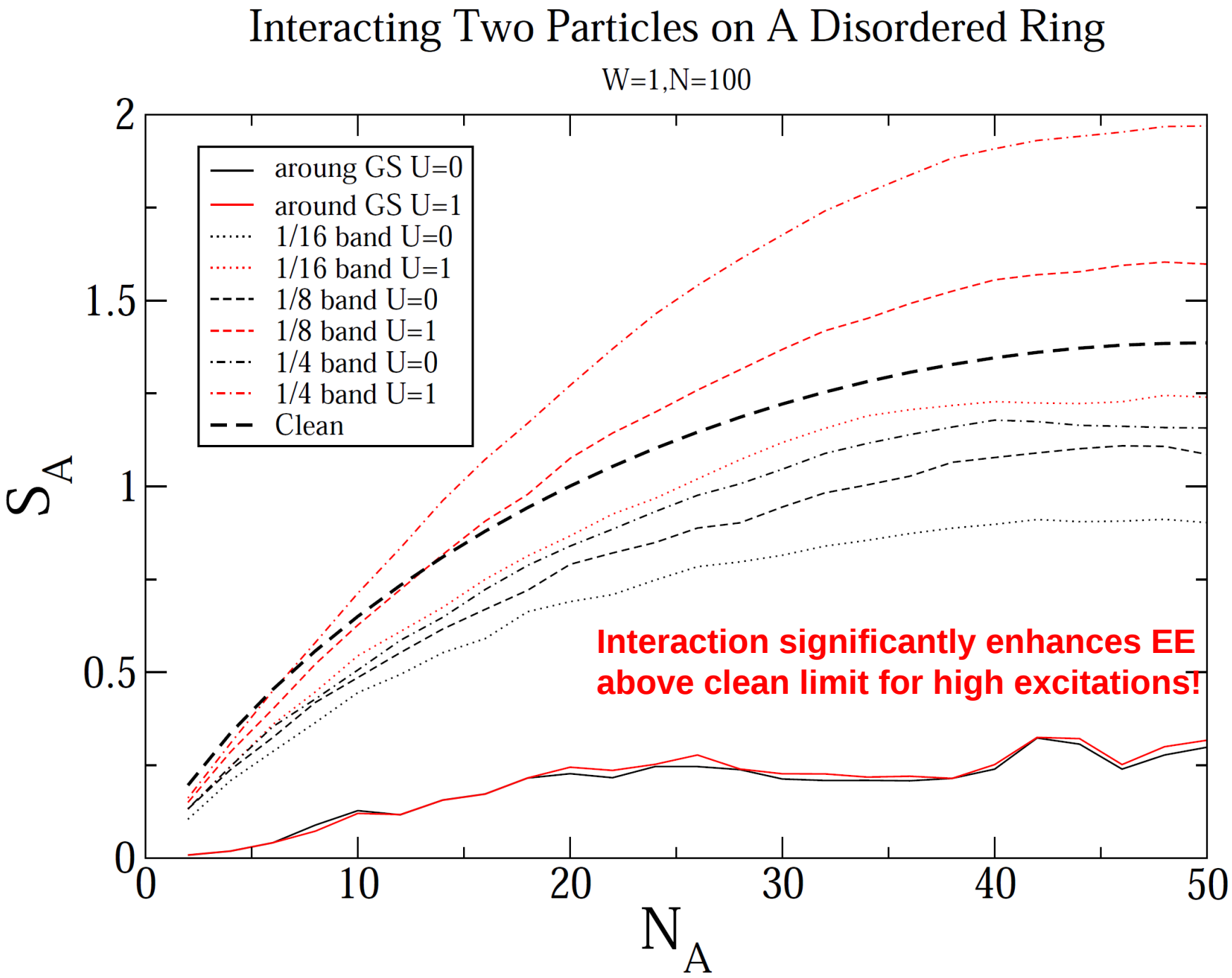
where $x = N_A/N$

Clean Ring N=1000

Numerical

Analytical



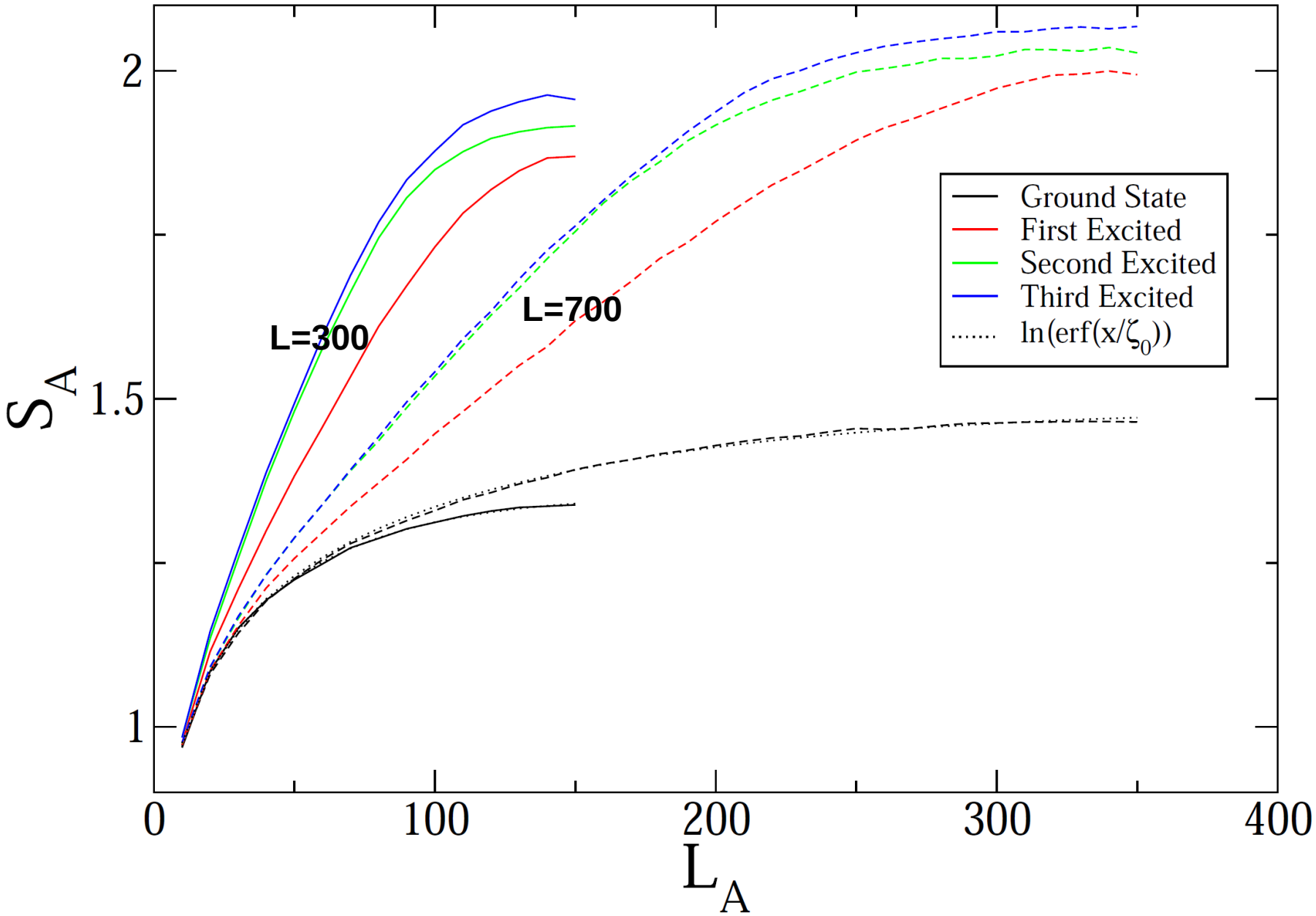

Interacting Two Particles on A Disordered Ring
W=1,N=100
aroung GS U=0
around GS U=1
1/16 band U=0
1/16 band U=1
1/8 band U=0
1/8 band U=1
1/4 band U=0
1/4 band U=1
Clean
Interaction significantly enhances EE
above clean limit for high excitations!
S_A
N_A
0
0.5
1
1.5
2
0
10
20
30
40
50

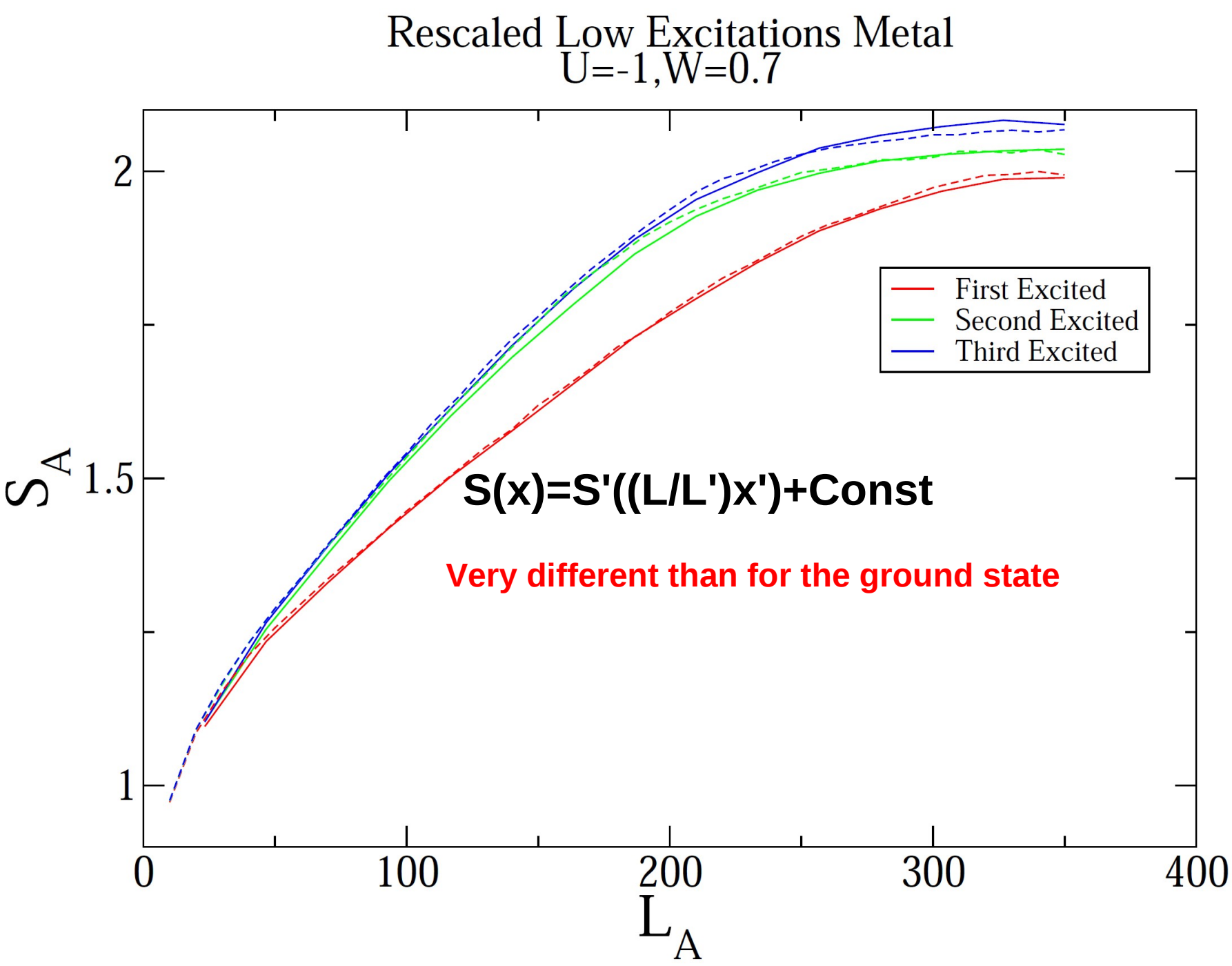
How should the many particle delocalization influence the EE?

EE of excitations below the critical energy (temperature): Similar behavior to the localized ground state, i.e., saturate at ξ.

EE of Excitations above the critical energy: should not saturate. A smoking gun would be no decrease as the system size is enhanced.

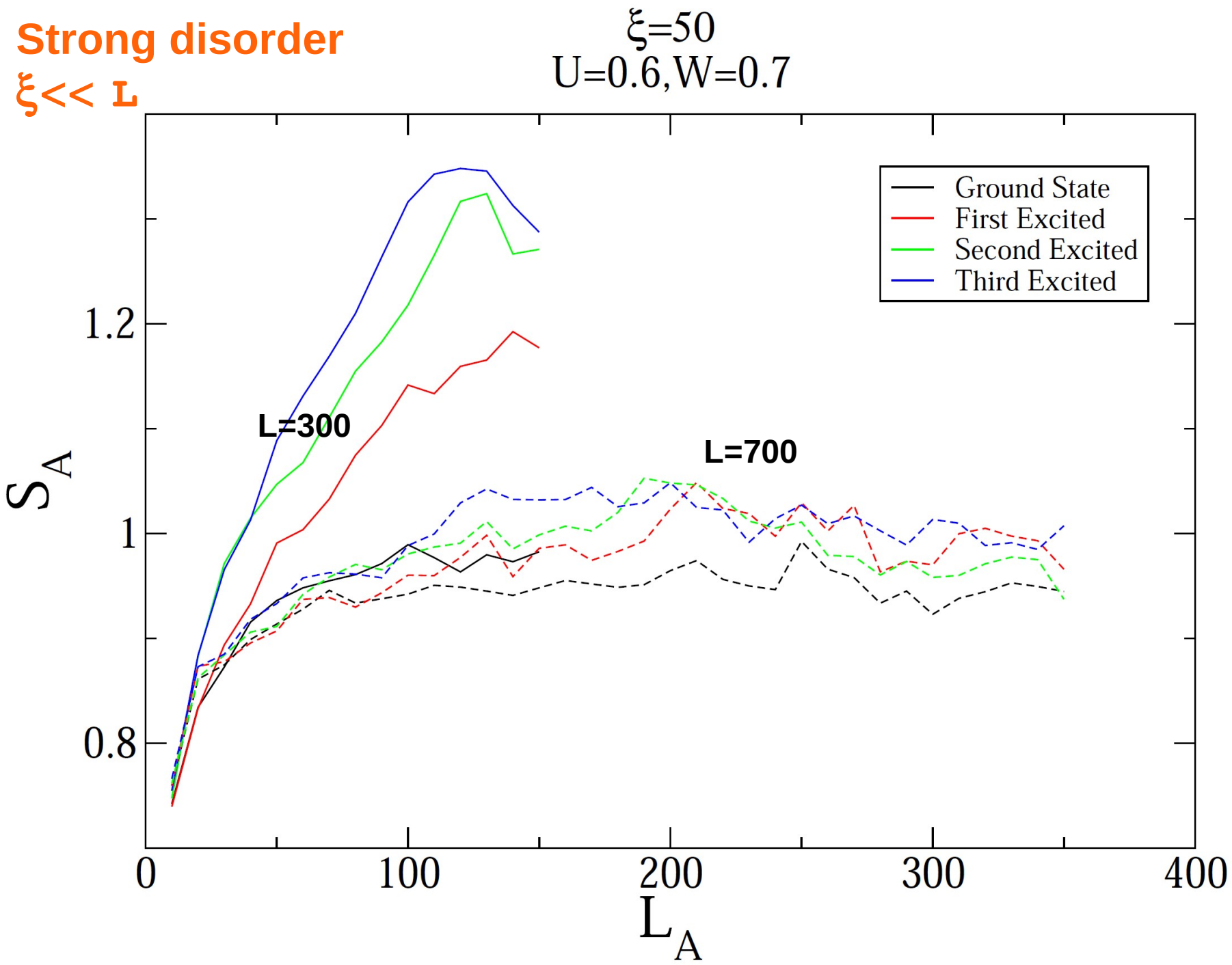
Location of critical energy should shift with interaction (note that the ground state localization also depends on the interaction strength).


DMRG Low Excitations Metal
U=-1,W=0.7
L=300
L=700
Ground State
First Excited
Second Excited
Third Excited
ln(erf(x/ζ0))
S_A
L_A
1
1.5
2
0
100
200
300
400


Rescaled Low Excitations Metal
U=-1,W=0.7
First Excited
Second Excited
Third Excited
S(x)=S'((L/L')x')+Const
Very different than for the ground state
S_A
L_A
1
1.5
2
0
100
200
300
400

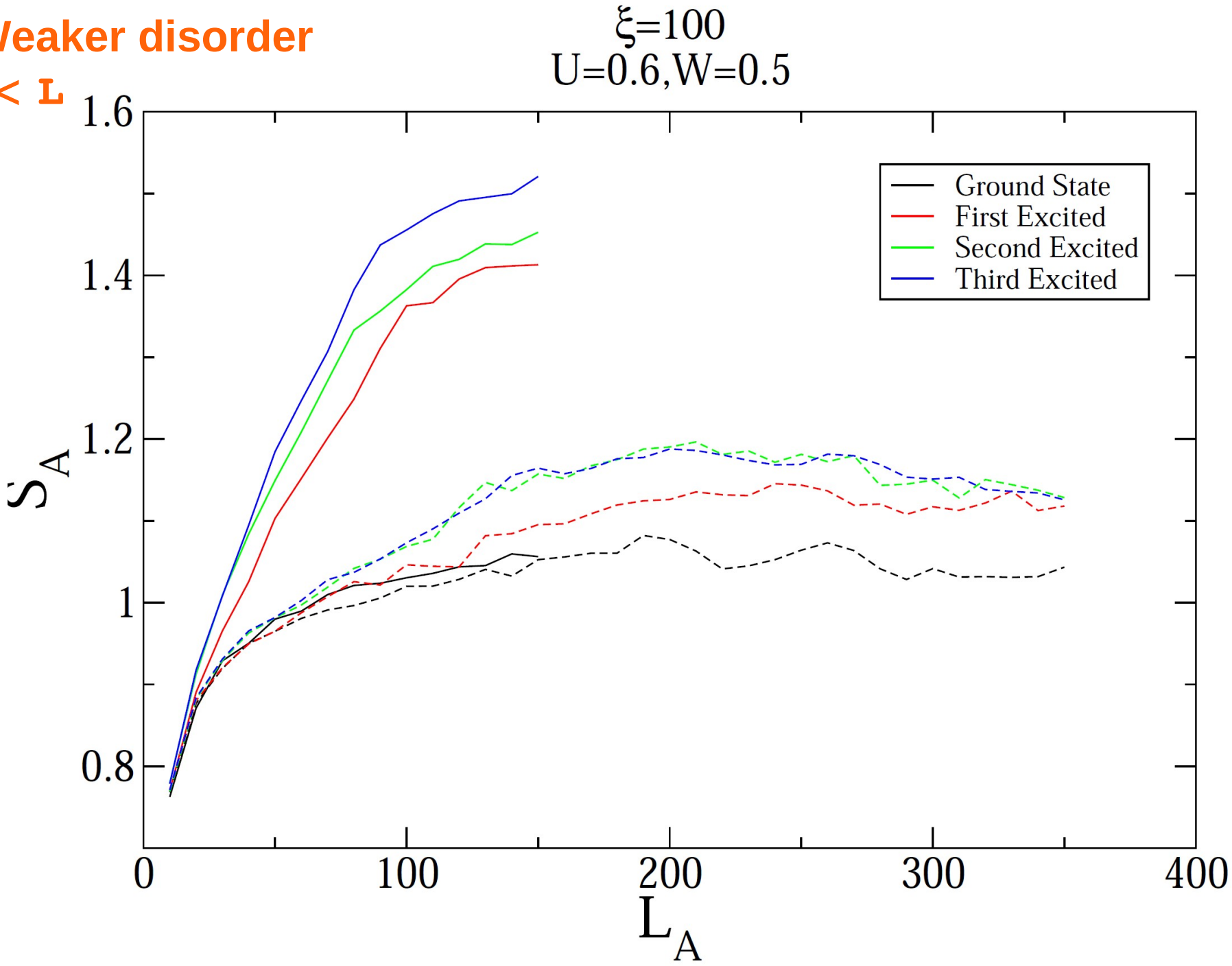
Strong disorder

ξ<< L



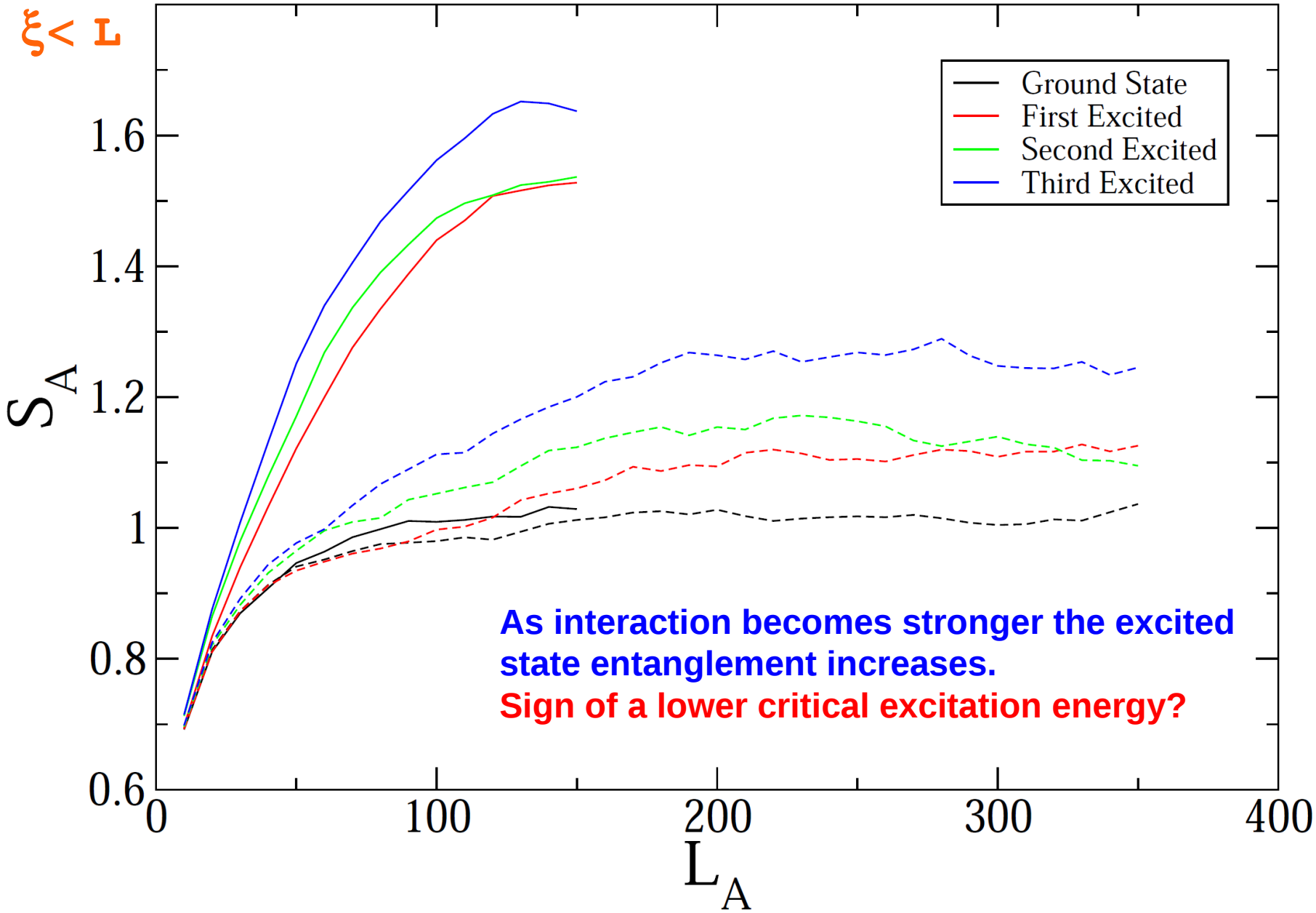
Weaker disorder

$\xi < L$



Same localization length
larger interaction
$\xi < L$

ξ=100
U=1.8,W=0.15



As interaction becomes stronger the excited state entanglement increases.
Sign of a lower critical excitation energy?

Summary

- Entanglement entropy behavior depends on the correlation length of the system.
- Thus, EE could be used to identify different phases of a system and identify quantum phase transitions such as the Anderson localization transition.
- Furthermore, EE could be used to calculate the correlation (localization) length.
- Excited states EE show glimpses of many-electron metal-insulator transition.

Density Matrix Renormalization Group (DMRG)

PHYSICAL REVIEW B VOLUME 48, NUMBER 14 1 OCTOBER 1993-II

Density-matrix algorithms for quantum renormalization groups

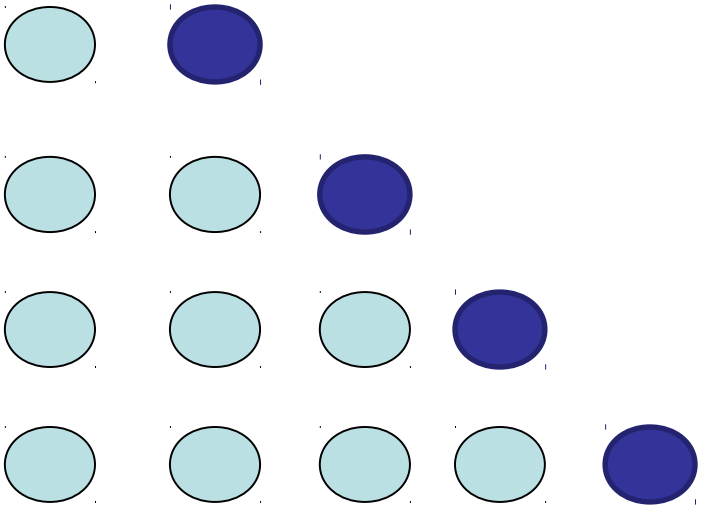
Steven R. White

REVIEWS OF MODERN PHYSICS, VOLUME 77, JANUARY 2005

The density-matrix renormalization group

U. Schollwöck

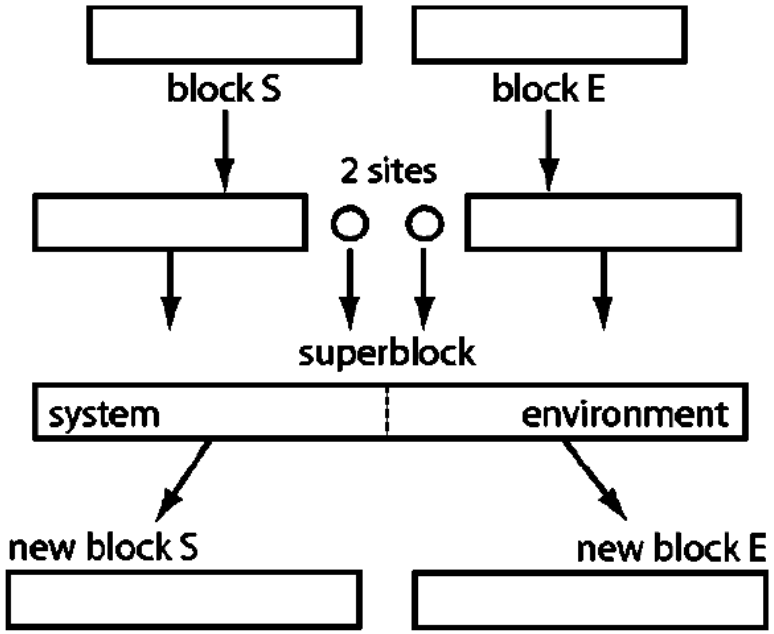
Numerical Renormalization Group (NRG)



1. Add an additional site
2. Retain only the m states with the lowest energy

Works perfectly for impurity problems (Kondo)

Fails miserably for extended systems (Luttinger Liquids)



Infinite size DMRG

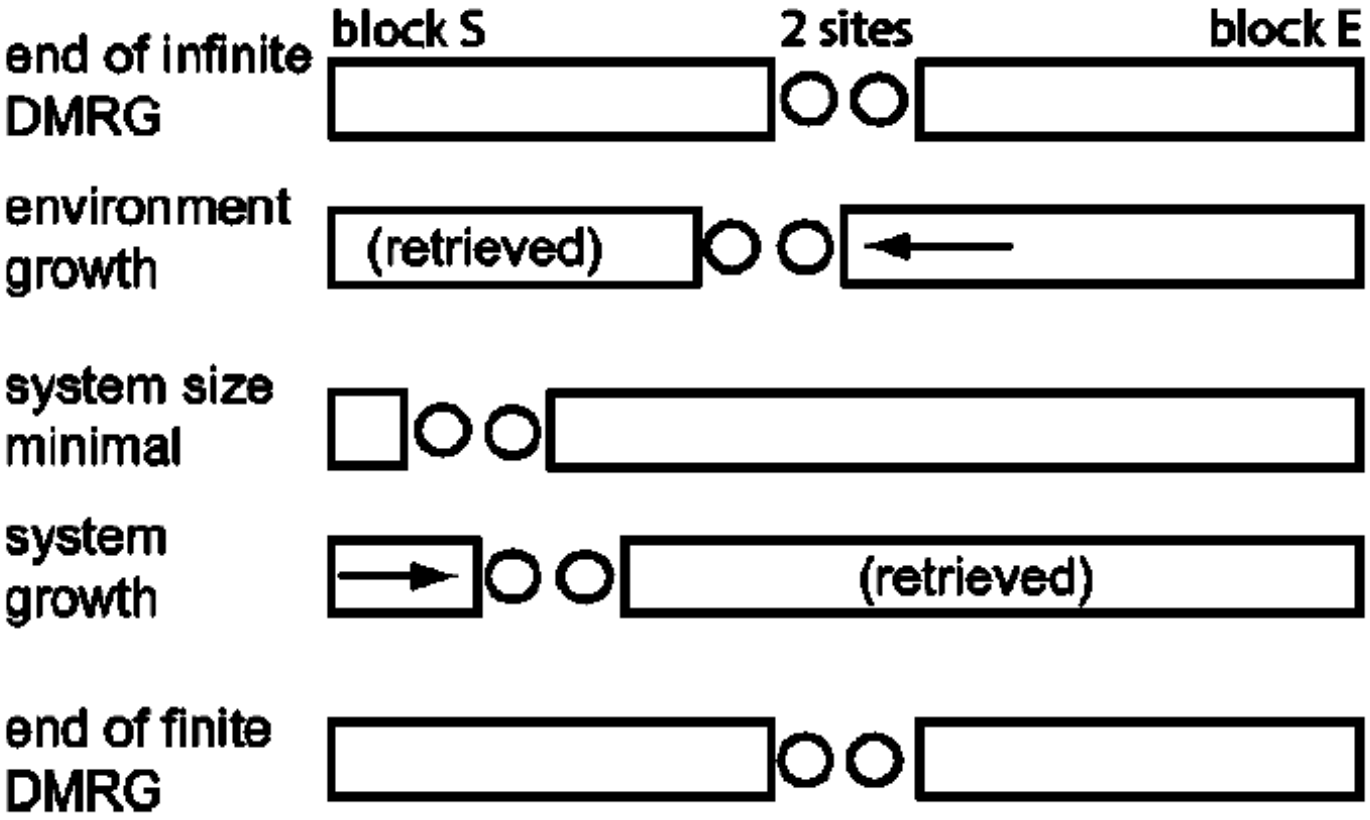
1. Add an additional site to the system and environment
1. Form the density matrix for the system
3. Retain only the m states with the highest density matrix eigenvalues

$$\lambda_i = \alpha_i^2$$

TABLE II. Infinite system density-matrix algorithm for a 1D system.

1. Make four initial blocks, each consisting of a single site, representing the initial four site system. Set up matrices representing the block Hamiltonian and other operators.
2. Form the Hamiltonian matrix (in sparse form) for the superblock.
3. Using the Davidson or Lanczos method, diagonalize the superblock Hamiltonian to find the target state $\psi(i_1, i_2, i_3, i_4)$. ψ is usually the ground state. Expectation values of various operators can be measured at this point using ψ.
4. Form the reduced density matrix for the two-block system 1-2, using $\rho(i_1, i_2; i_1', i_2') = \sum_{i_3, i_4} \psi(i_1, i_2, i_3, i_4)\psi(i_1', i_2', i_3, i_4)$.
5. Diagonalize ρ to find a set of eigenvalues w_α and eigenvectors $u^\alpha_{i_1, i_2}$. Discard all but the largest m eigenvalues and associated eigenvectors.
6. Form matrix representations of operators (such as H) for the two-block system 1-2 from operators for each separate block [cf. Eq. (4)].
7. Form a new block 1 by changing basis to the u^α and truncating to m states using $H^{1'} = OH^{12}O^\dagger$, etc. If blocks 1 and 2 have m_1 and m_2 states, then O is an $m \times m_1 m_2$ matrix, with matrix elements $O(\alpha; i_1, i_2) = u^\alpha_{i_1, i_2}$, $\alpha = 1, \ldots, m$.
8. Replace old block 1 with new block 1.
9. Replace old block 4 with the reflection of new block 1.
10. Go to step 2.

Finite size DMRG



Iteration improve dramatically the accuracy

At each point in the DMRG iteration on has all the ingredients to calculate the EE