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Workshop on Synergies between Field Theory and Exact Computational Methods in Strongly Correlated Quantum Matter

24 - 29 July 2011

Impurity Entanglement in Spin Chains

E. Sorensen
McMaster University
Hamilton, Ontario
Canada

I. Affleck
University of British Columbia
Vancouver
Canada

N. Laflorencie
U Paris-Sud
Orsay
France

A. Deschner
McMaster University
Hamilton, Ontario
Canada

IMPURITY ENTANGLEMENT IN SPIN CHAINS

Erik Sorensen, McMaster University

With:
Ian Affleck (UBC)
Nicolas Laflorencie (Orsay/Toulouse)
Andreas Deschner

Trieste, July 26, 2011

$S(r, R) = -\mathrm{Tr}\rho_A \ln \rho_A$ von Neumann Entropy

(Renyi)

- Difficult to measure.

  Klich, Levitov, PRL 102, 100502 (2009)
  Song, Rachel, Le Hur, PRB 82, 012405 (2010)
  Song, Flindt, Rachel, Klich Le Hur, PRB 83, 161408(R) (2011)
  Song, Laflorencie, Rachel, Le Hur, PRB 83, 224410 (2011)

- Difficult for Numerics (Melko) easy for DMRG

- Area Law: Numerics Eisert, Cramer, Plenio, RMP 82, 277 (2010)

- Impurities

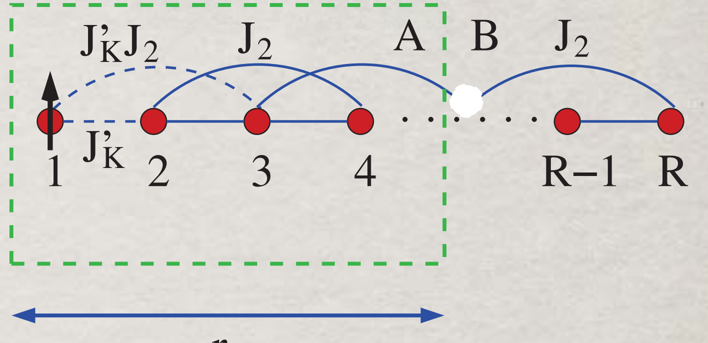
Outline

- Example Model
- Definition
- Gapless Systems: Kondo Impurities. Scaling, Screening Cloud.
- Intuitive Pictures: Impurity Valence Bonds (IVB) Single Particle Entanglement (SPE). Fixed Point Entanglement (FPE).
- Gapped Systems
- Boundary Fields (TFIM)

A SPIN CHAIN MODEL

Example Model

J1-J2 Spin Chain with Impurity



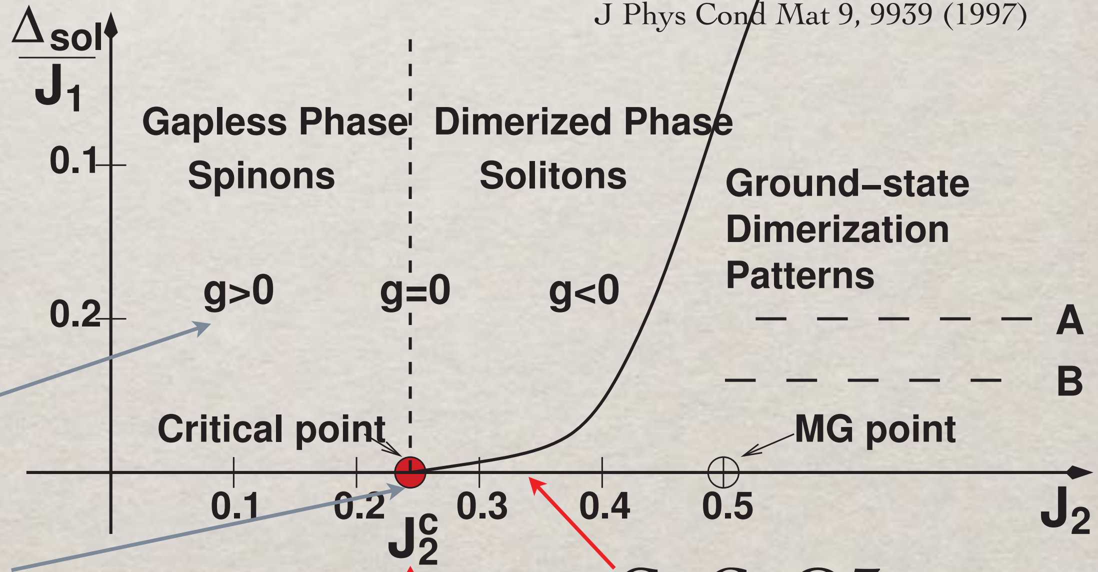
$$H = J'_K \left(\vec{S}_1 \cdot \vec{S}_2 + J_2 \vec{S}_1 \cdot \vec{S}_3 \right) + \sum_{r=2}^{R-1} \vec{S}_r \cdot \vec{S}_{r+1} + J_2 \sum_{r=2}^{R-2} \vec{S}_r \cdot \vec{S}_{r+2}$$

J2=0, Bethe Ansatz, Frahm, Zvyagin
J Phys Cond Mat 9, 9939 (1997)

- Impurity: Boundary or Spin Impurity J'_K
- For $J_2 \leq J_2^c$ directly related to the Kondo Model

S Eggert, I Affleck, PRB 46, 10866 (1992).
N. Laflorencie, ESS, I Affleck, JSTAT, P02007 (2008)

- Logarithmic corrections for $J_2 < J_2^c$



Log Corrections

No Log Corrections

CuGeO3

Cardy, Calabrese, JSTAT P06002 (2004)

S=1/2 spin chain with PBC: Critical Models

$$S^{PBC}(r,R) = \frac{c}{3}\ln\left[\frac{R}{\pi}\sin\left(\frac{\pi r}{R}\right)\right] + s_1$$

S=1/2 spin chain with OBC:

Non Universal Independent of BC

$$S_U(r,R) \simeq \frac{c}{6}\ln\left[\frac{2R}{\pi}\sin\left(\frac{\pi r}{R}\right)\right] + \ln g + \frac{s_1}{2}$$

Affleck, Ludwig PRL 67, 161 (1991)

Universal BC dependent (thermodynamic impurity entropy)

Impurity entanglement entropy should exhibit Universality

HOW TO DEFINE THE IMPURITY ENTANGLEMENT ?

Impurity Entanglement

The entanglement has both a uniform and an alternating part

$$S(r,R) = S_U(J'_K,r,R) + (-1)^r S_A(J'_K,r,R)$$

N. Laflorencie, ESS, M.-S. Chang, I Affleck, PRL 96, 100603 (2006).
P. Calabrese, J. Cardy, J. Stat. Mech. (2010) P04023
P. Calabrese, J. Stat. Mech. (2011) P01017

Then we can define the impurity entanglement as:

$$S_{imp} = S(\text{impurity}) - S(\text{no impurity})$$

$$S_{imp}(J'_K,r,R) \equiv S_U(J'_K,r,R) - S_U(1,r-1,R-1), \; r > 1.$$

The entanglement from a system with one site removed is subtracted ! (Also an alternating part).

Only Impurity, Single Site Impurity Entanglement

$$s_{\rm imp} \equiv S(l=1, L)$$

$$s_{\rm imp} = -\sum_{\pm} (\frac{1}{2} \pm m_{\rm imp}) \ln(\frac{1}{2} \pm m_{\rm imp}), \quad m_{\rm imp} = \langle S_1^z \rangle$$

Spin Boson Problem, NRG

Le Hur, PRL 98, 220401 (2007), Ann. Phys. 323, 2208

$$\mathcal{N} = \frac{\sum |\lambda_i| - 1}{2}$$

Eigenvalues of $\rho_{CA}^{T_A}$

Only Impurity, Negativity

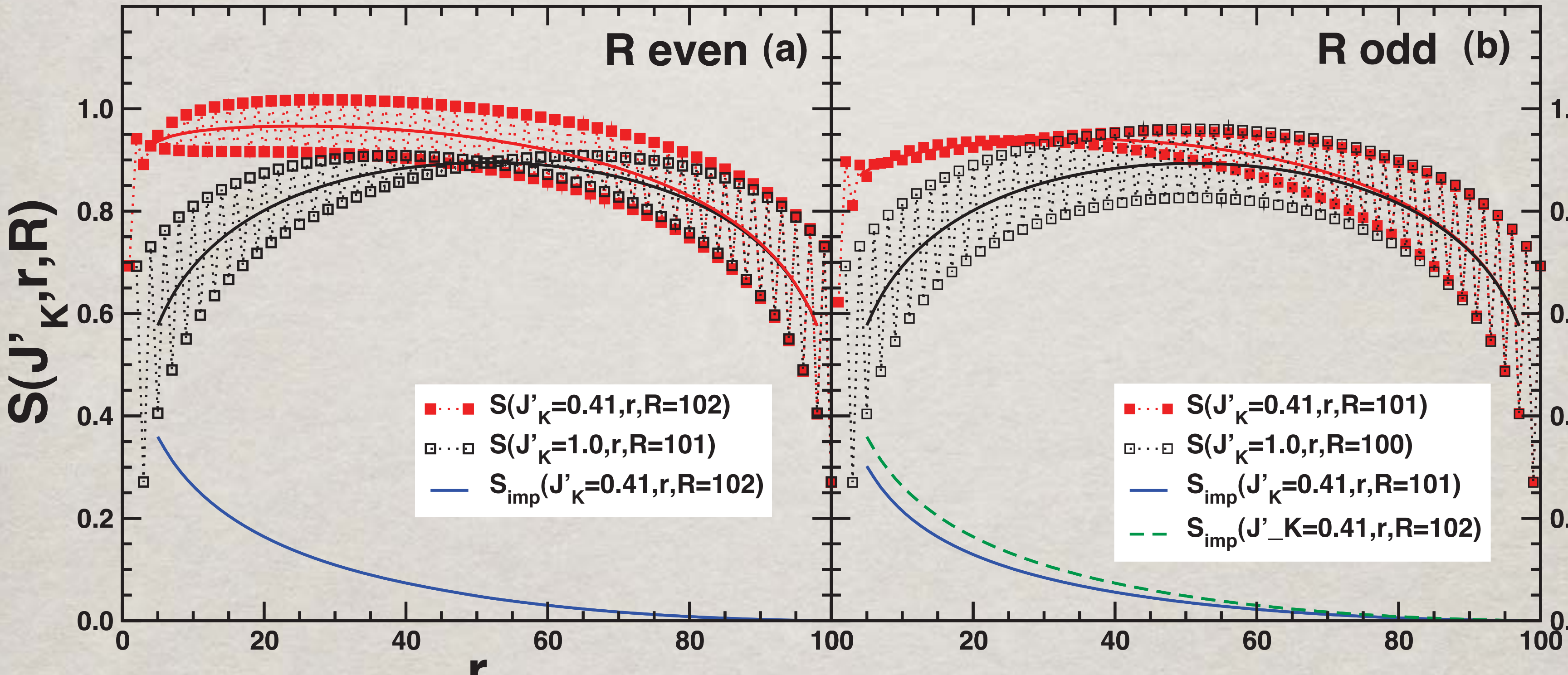
Sodano, Bose, Bayat, PRB 81 064429(2010), PRB 81 100412 (2010)

$$S_{imp}(J'_K, r, R) \equiv S_U(J'_K, r, R) - S_U(1, r-1, R-1), \;\; r > 1.$$

The entanglement from a system with one site removed is subtracted ! (Also an alternating part).

Note that : $S_{imp} \neq S(J'_K) - S(J'_K = 0)$

How does it work ?



$$S_U(r,R) \simeq \frac{c}{6}\ln\left[\frac{2R}{\pi}\sin\left(\frac{\pi r}{R}\right)\right] + \ln g + \frac{s_1}{2}$$

Cardy, Calabrese, JSTAT P06002 (2004)

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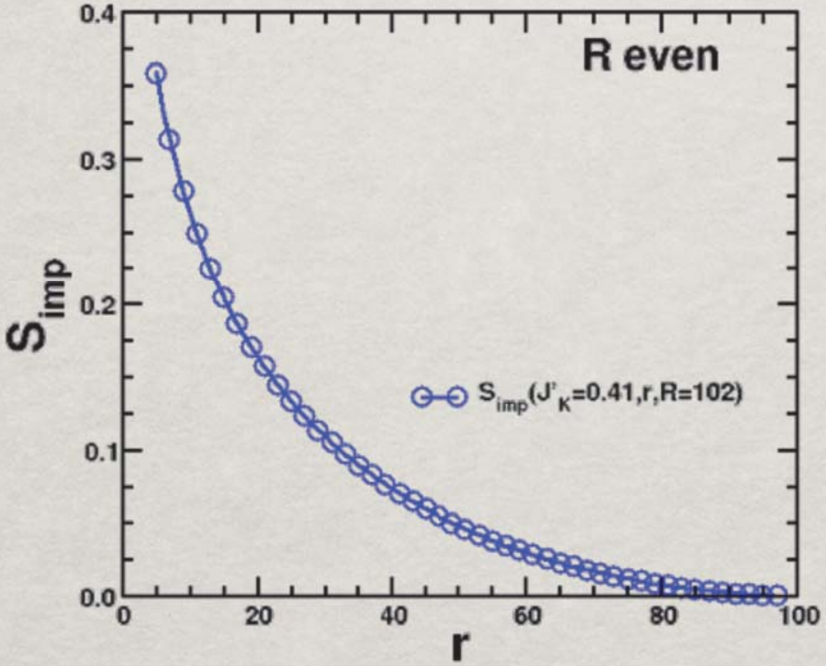

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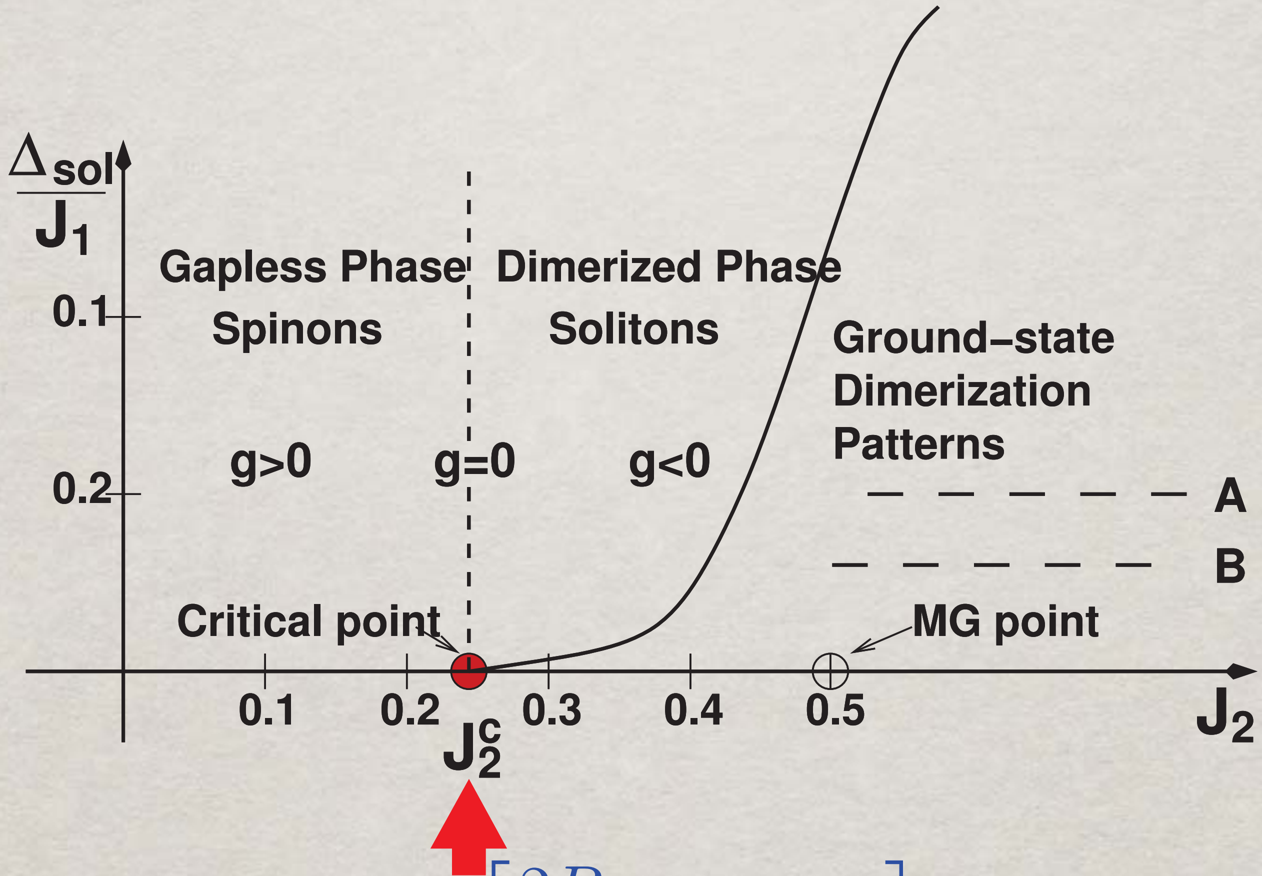
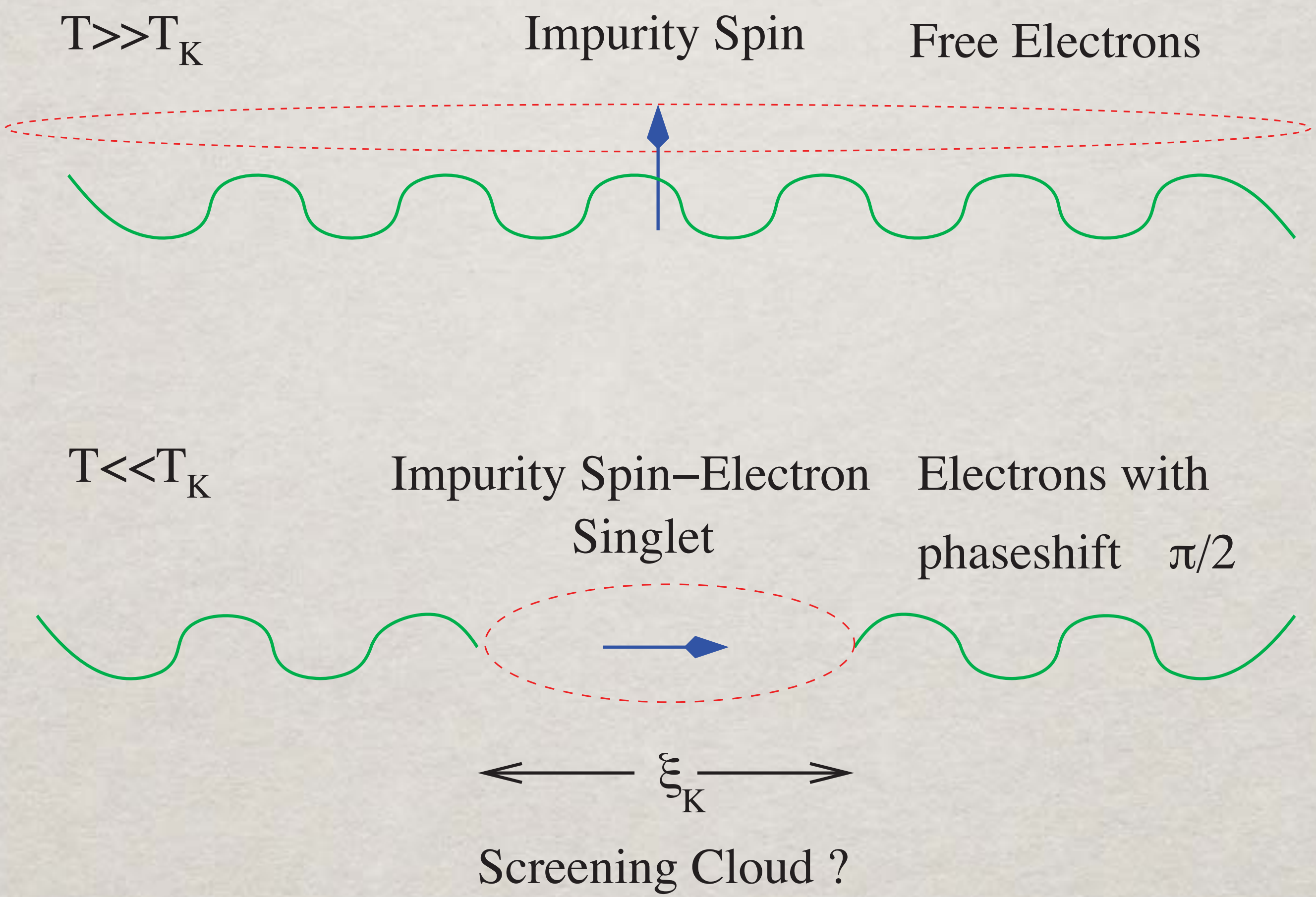


$$S_U(r,R) \simeq \frac{c}{6}\ln\left[\frac{2R}{\pi}\sin\left(\frac{\pi r}{R}\right)\right] + \ln g + \frac{s_1}{2}$$

Cardy, Calabrese, JSTAT P06002 (2004)

Kondo Physics



AF

$$H = J_K \mathbf{S}_{\rm imp} \cdot \psi_1^{\dagger\alpha} \frac{\sigma_\alpha^\beta}{2} \psi_1^\beta - t \sum_{i=1}^{L-1} \left(\psi_i^{\dagger\alpha} \psi_{i+1,\alpha} + \psi_{i+1}^{\dagger\alpha} \psi_{i,\alpha} \right)$$

$$\xi_K \sim \frac{e^{a/J'_K}}{\sqrt{J'_K}}$$

S Eggert, I Affleck, PRB 46, 10866 (1992).
N. Laflorencie, ESS, I Affleck, JSTAT, P02007 (2008)

In the spin sector: Same low energy effective Hamiltonian

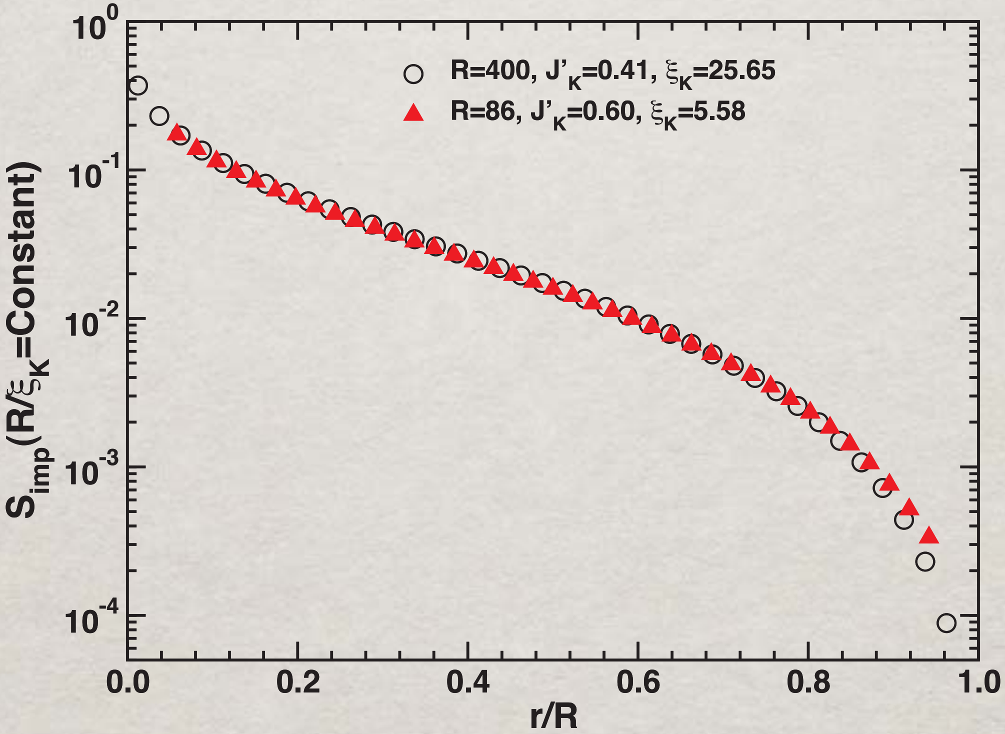
$$J_K \propto J'_K$$

$$H = J'_K \left(\vec{S}_1 \cdot \vec{S}_2 + J_2 \vec{S}_1 \cdot \vec{S}_3 \right) + \sum_{r=2}^{R-1} \vec{S}_r \cdot \vec{S}_{r+1} + J_2 \sum_{r=2}^{R-2} \vec{S}_r \cdot \vec{S}_{r+2}$$

$$S_U(r,R) \simeq \frac{c}{6} \ln \left[\frac{2R}{\pi} \sin\left(\frac{\pi r}{R} \right) \right] + \ln g + \frac{s_1}{2}$$

$$\ln g = \ln 2 \quad T >> T_K$$

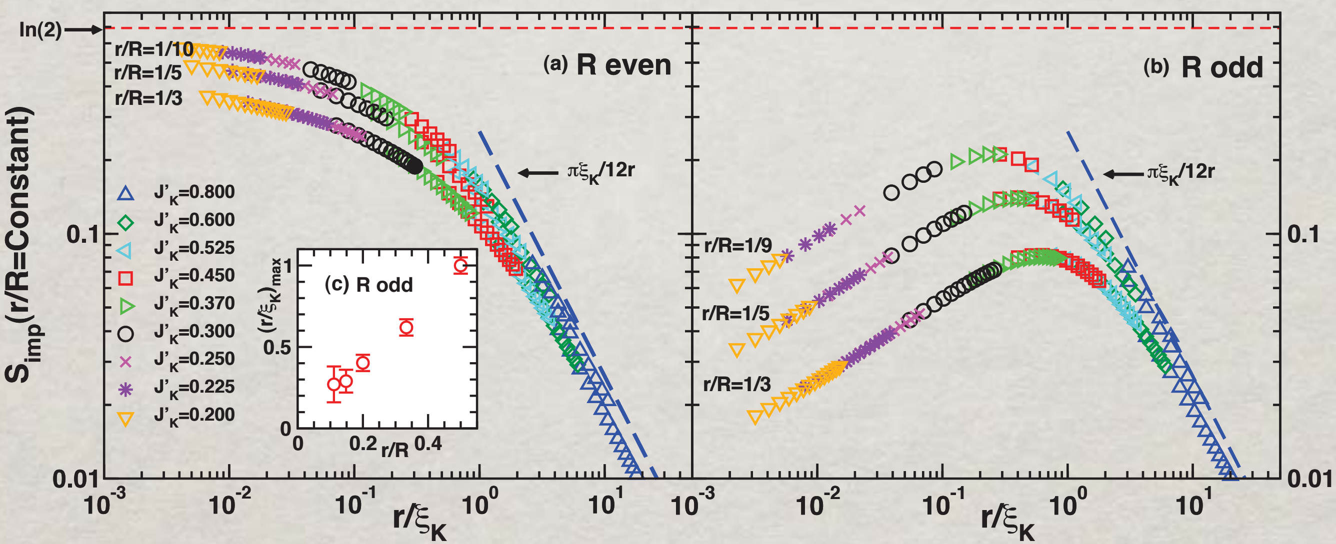
Universality, Scaling



$$S_{imp} \equiv S_{imp}(r/R, r/\xi_K)$$

ESS, M.-S. Chang, N. Laflorencie, I Affleck JSTAT L01001 (2007)

Universality, Scaling



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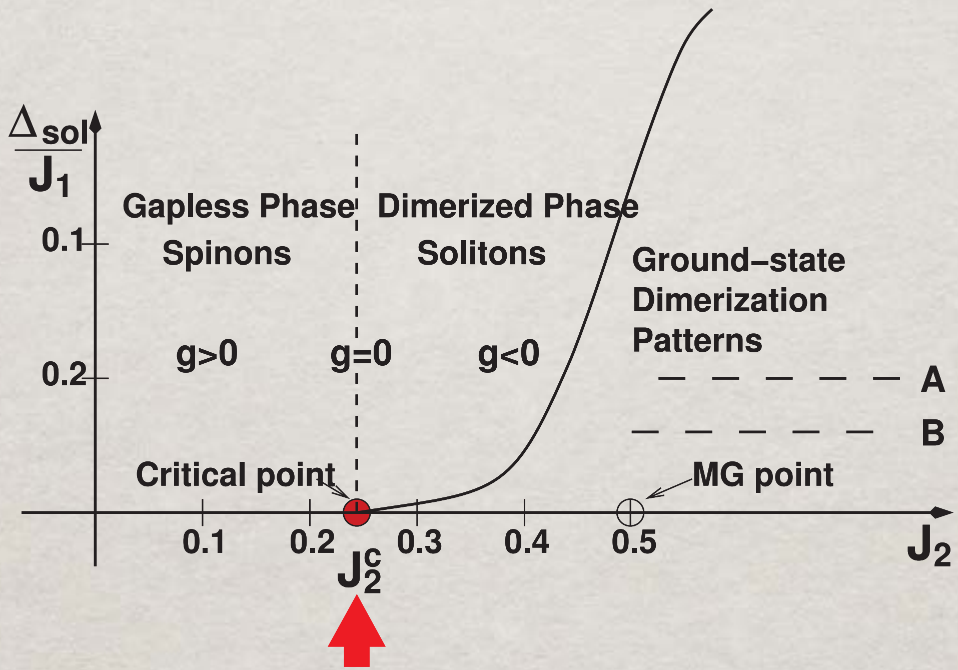

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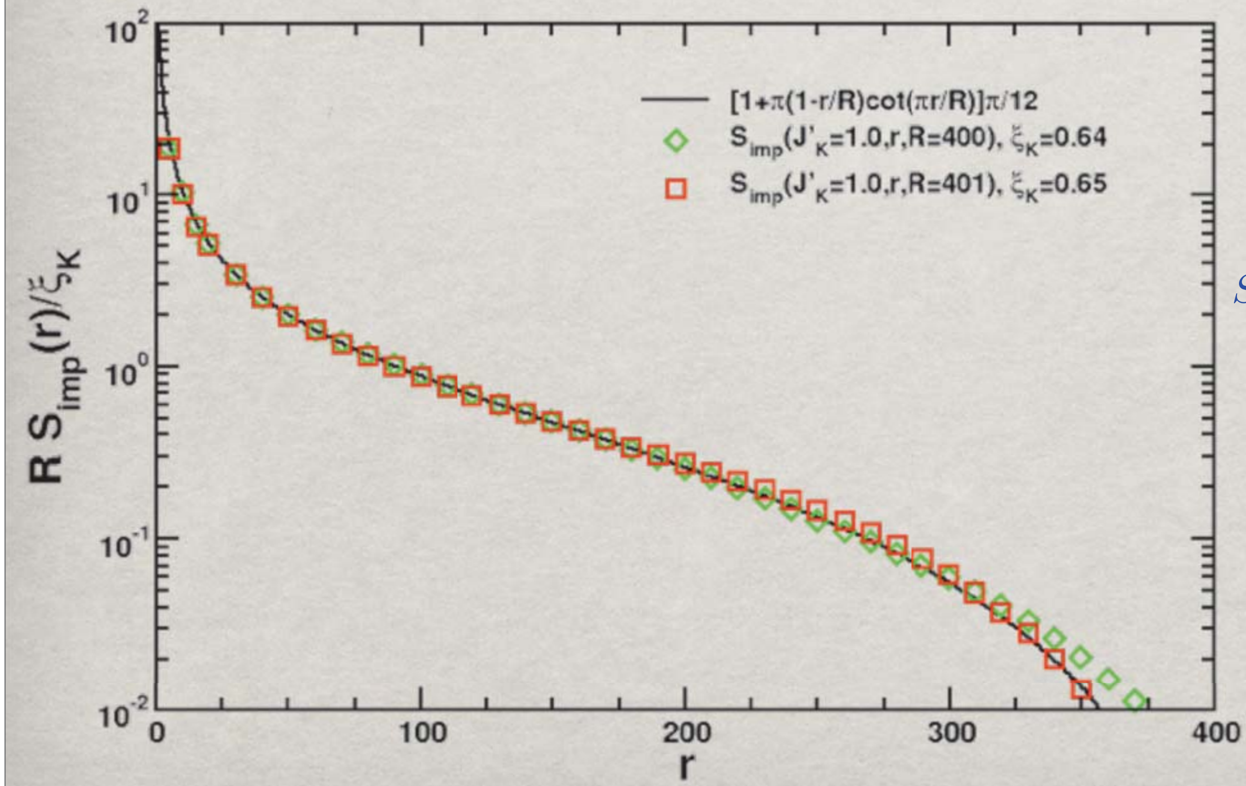
Fermi Liquid Theory

Free Hamiltonian density for left-moving spin bosons

Perturbation theory in: $H_{int} = -(\pi\xi_K)\mathcal{H}_{s,L}(0)$

$$S_{imp} = [\pi\xi_K/(12R)][1+\pi(1-r/R)\cot(\pi r/R)]$$



$$\rightarrow \boxed{\frac{\pi\xi_K}{12r}}$$

$$S_{imp}(T) = [\pi^2\xi_K T/(6v)]\coth(2\pi r T/v)$$

$$T, v/r \ll T_K$$

$$S_{imp}(T) \rightarrow c_{imp}(T) \quad rT \gg v$$

ESS, M.-S. Chang, N. Laflorencie, I Affleck JSTAT L01001 (2007)

Fermi Liquid Theory

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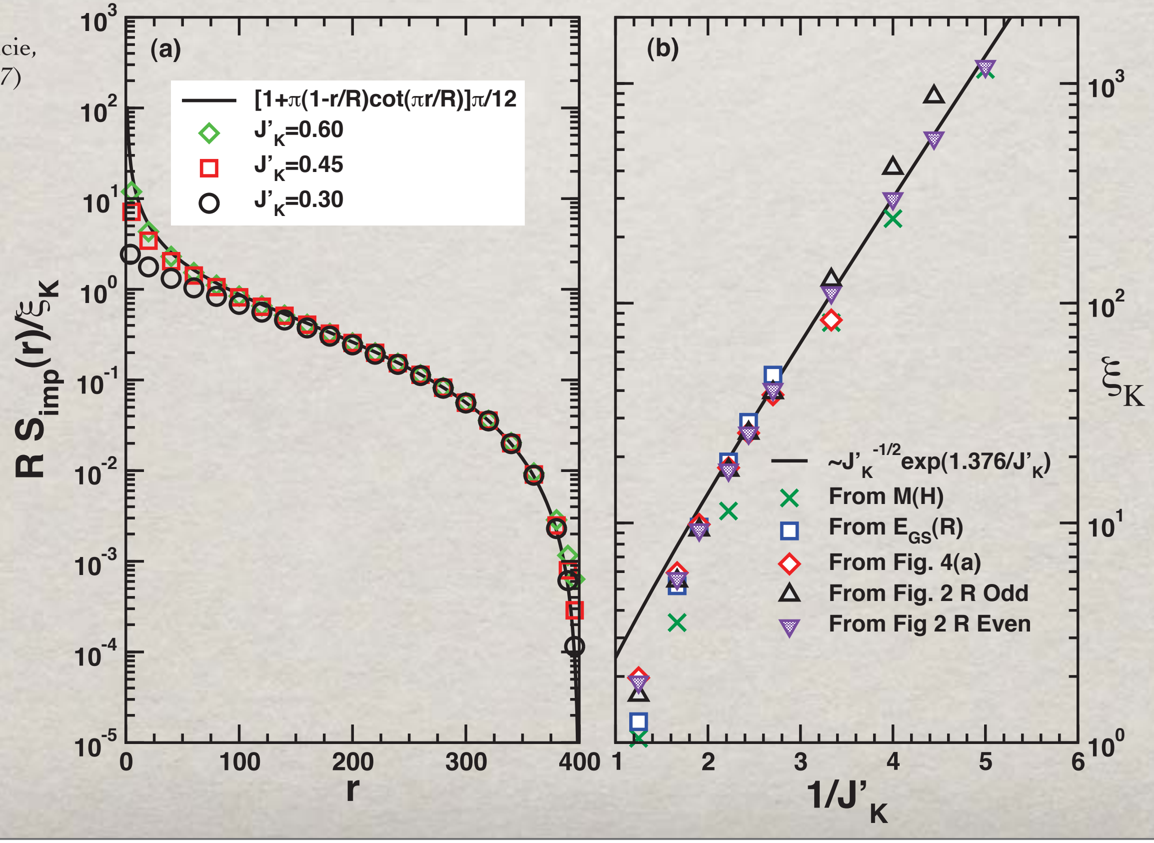
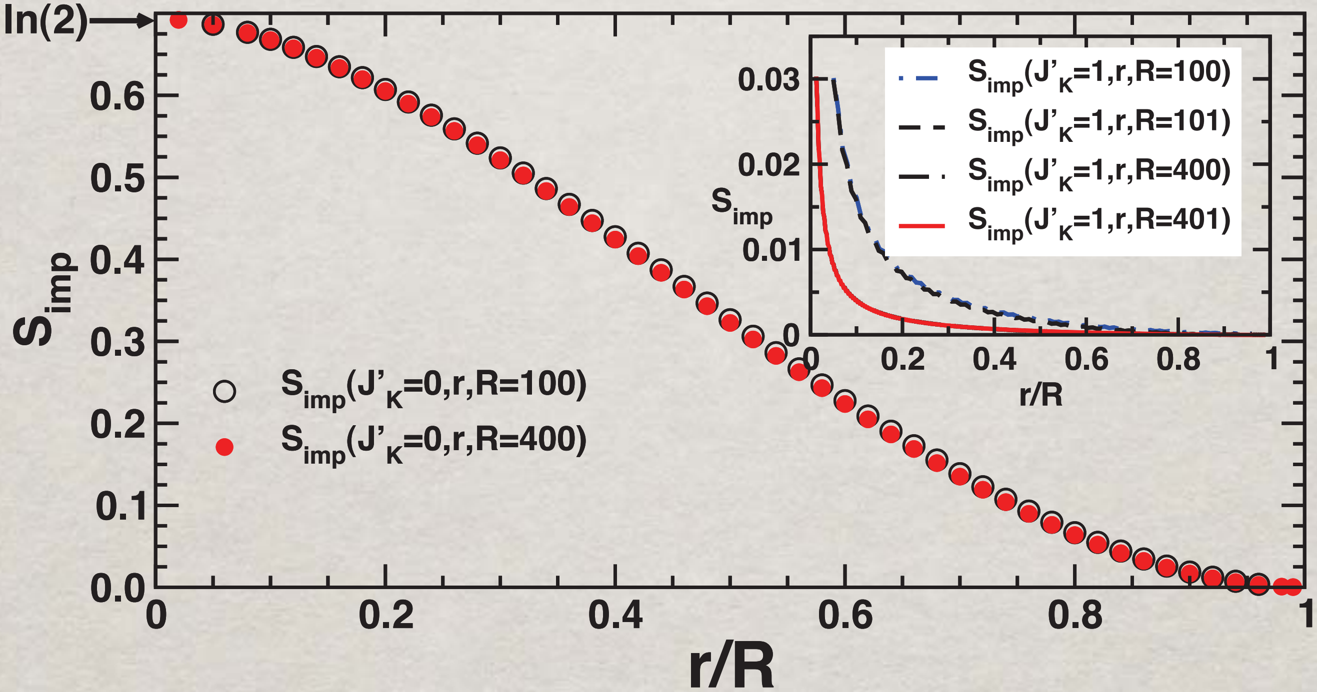


Fixed Point Entanglement

Let us take $J'_K \to 0$ (Weak Coupling Fixed point)



DMRG with spin inversion

$S^{fp}_{imp}(r/R)$

Fixed Point Entanglement

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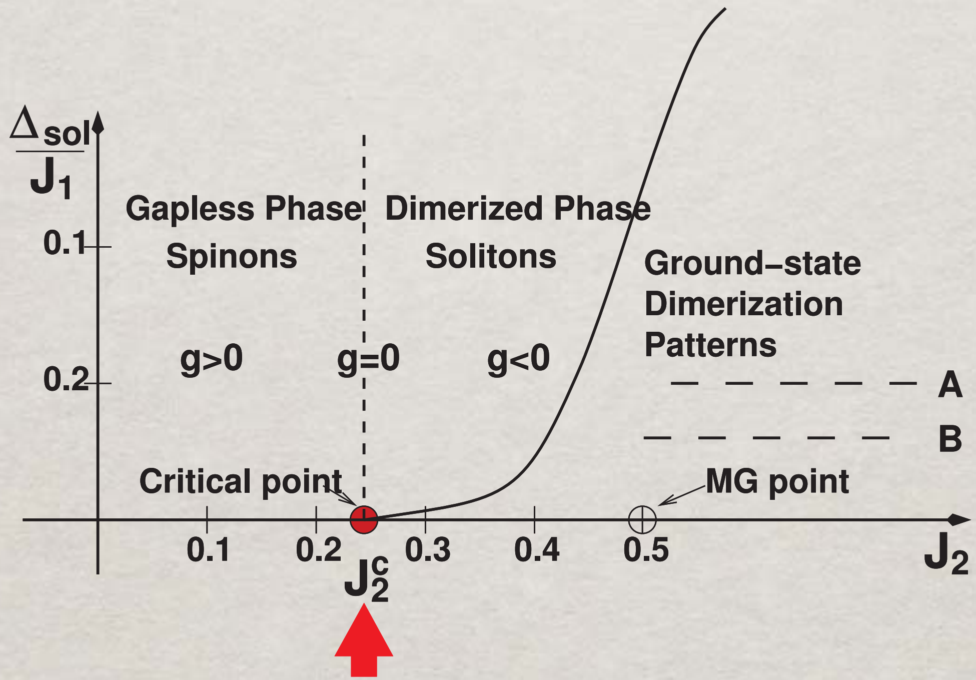


DMRG with spin inversion

$S^{fp}_{imp}(r/R)$

How can this be non-zero ?

Start with singlet ground-state

$$|\psi>= (1/\sqrt{2})[|\uparrow> |\Downarrow> -|\downarrow> |\Uparrow>]$$

The density matrix for the entire system:

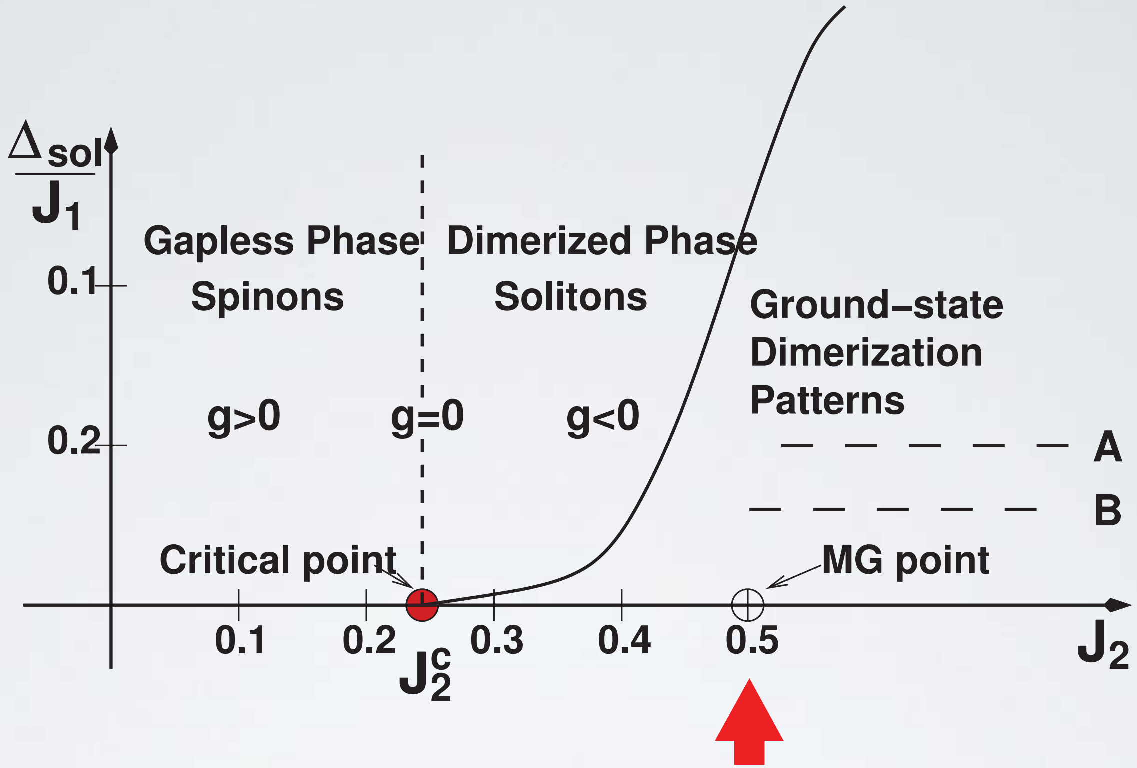
$$\rho_P \equiv |\psi >< \psi| = \frac{1}{2}\Big[|\uparrow><\uparrow|\otimes|\Downarrow><\Downarrow| + |\downarrow><\downarrow|\otimes|\Uparrow><\Uparrow|$$
$$-|\uparrow><\downarrow|\otimes|\Downarrow><\Uparrow| - |\downarrow><\uparrow|\otimes|\Uparrow><\Downarrow|\Big]$$

Do partial trace:

Defined on sites 2,3...R

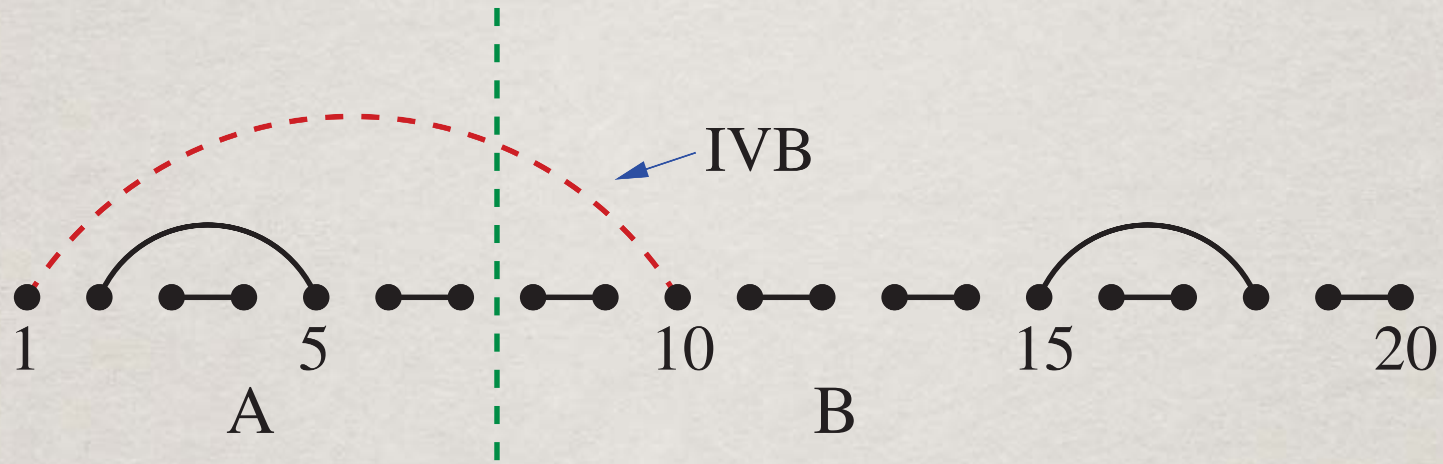
$$\rho = \frac{1}{2}\begin{pmatrix} \rho_{\Downarrow\Downarrow} & -\rho_{\Downarrow\Uparrow} \\ -\rho_{\Uparrow\Downarrow} & \rho_{\Uparrow\Uparrow} \end{pmatrix}.$$

CAN WE UNDERSTAND THIS ?



GAPPED SYSTEMS

Impurity Valence Bond



When a singlet (IVB) is cut by the boundary we get ln(2)

$$S_{imp} = (1-p)\ln 2$$

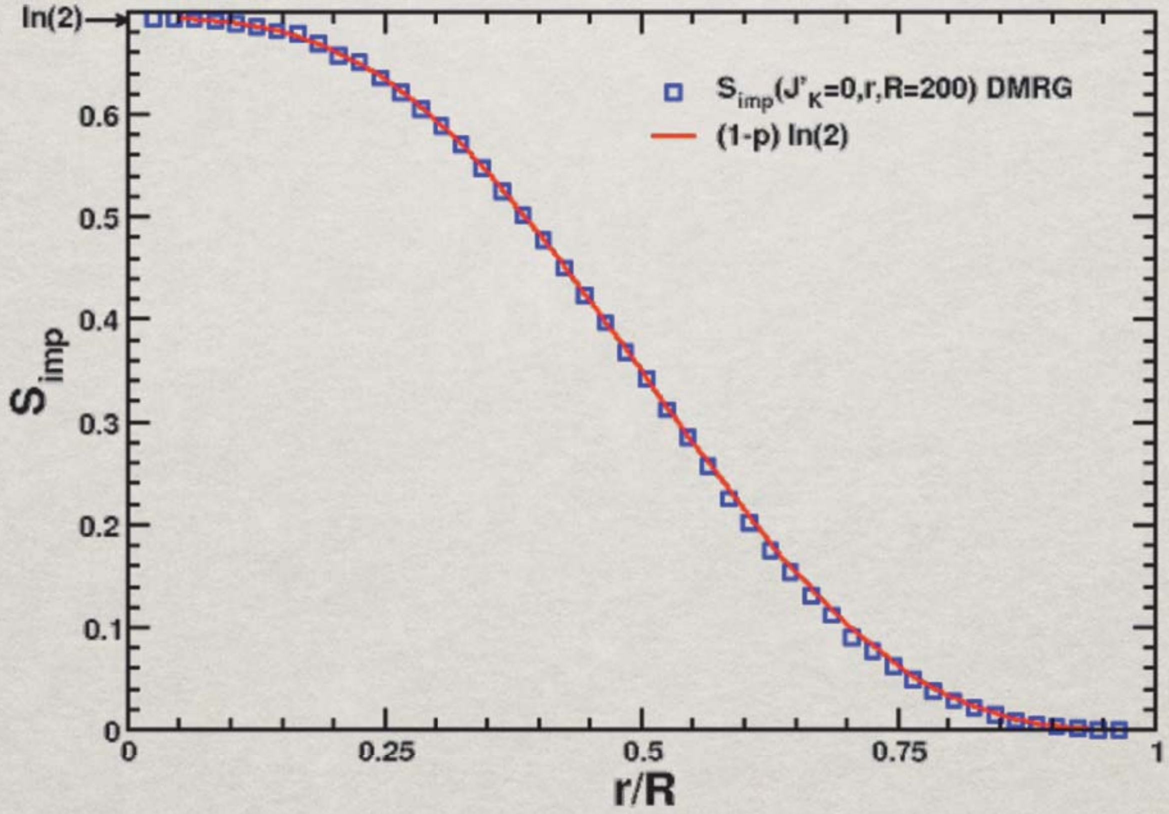
G. Refael, J. E. Moore, PRL 93, 260602 (2004).
ESS, M.-S. Chang, N. Laflorencie, I. Affleck, JSTAT L01001 (2007)

p is the probability that the IVB is in part A

$$p = \int_A |\Psi(x)|^2 dx, \quad \Psi(x) \sim \sin(\pi x/L)$$

Where $\Psi(x)$ is the wavefunction with a single Soliton (L odd)

IVB Entanglement



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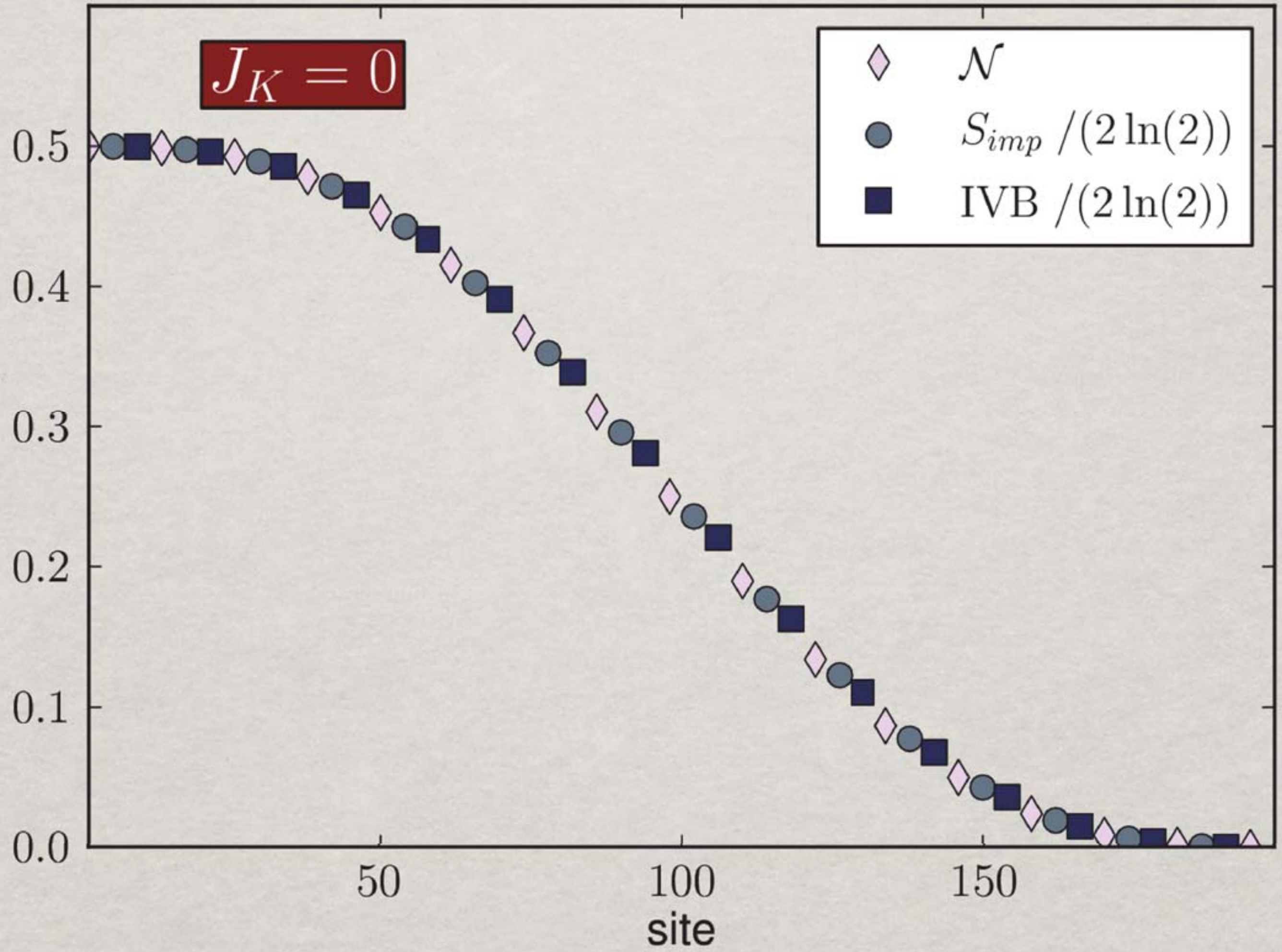
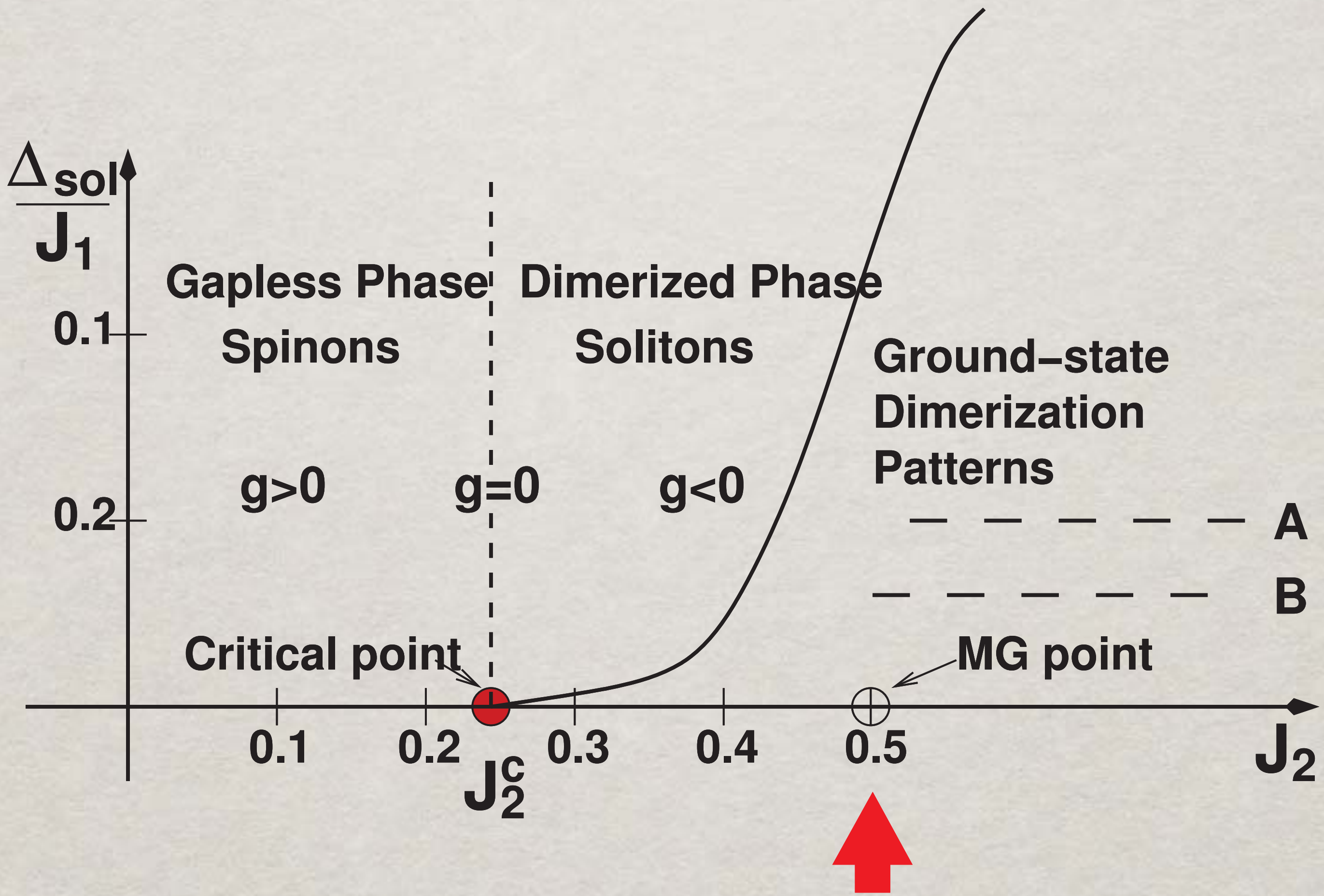
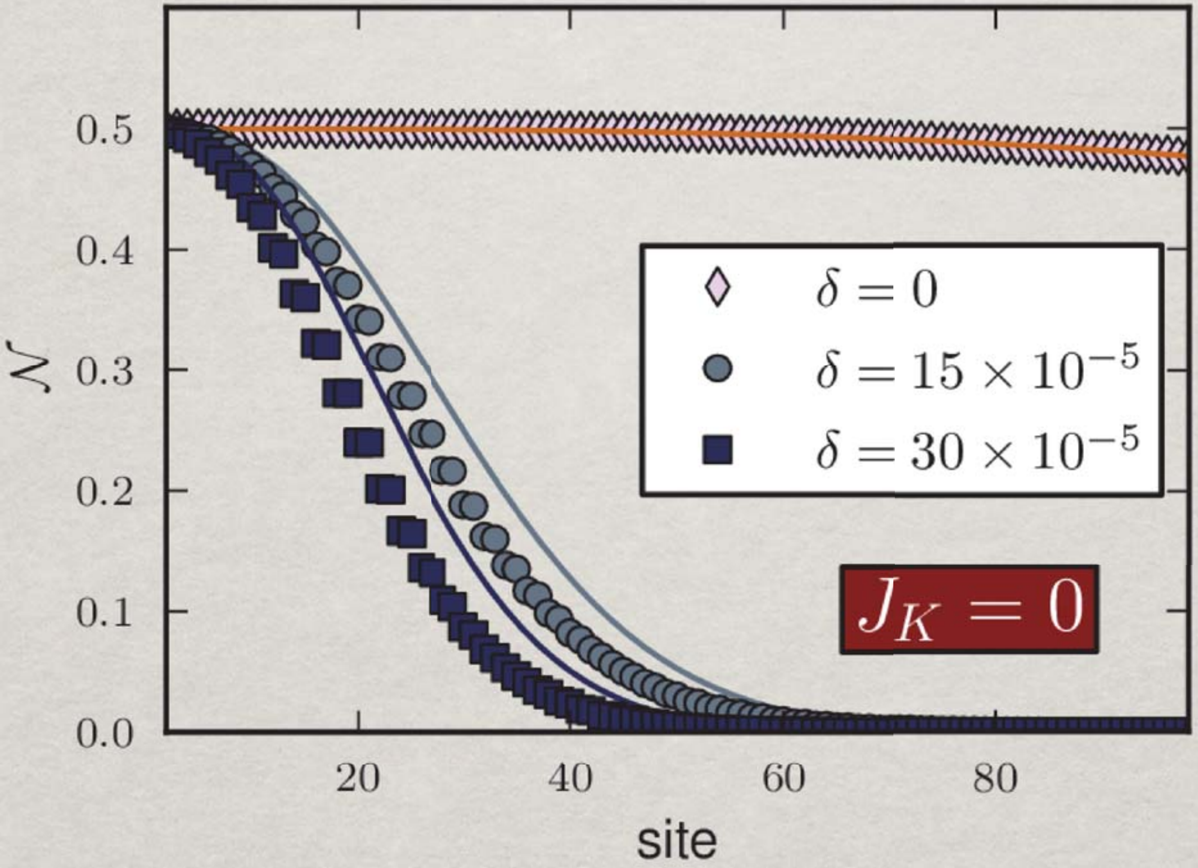


IVB Entanglement



Non-zero Dimerization



Single Particle Entanglement

Consider tight binding model with a single particle

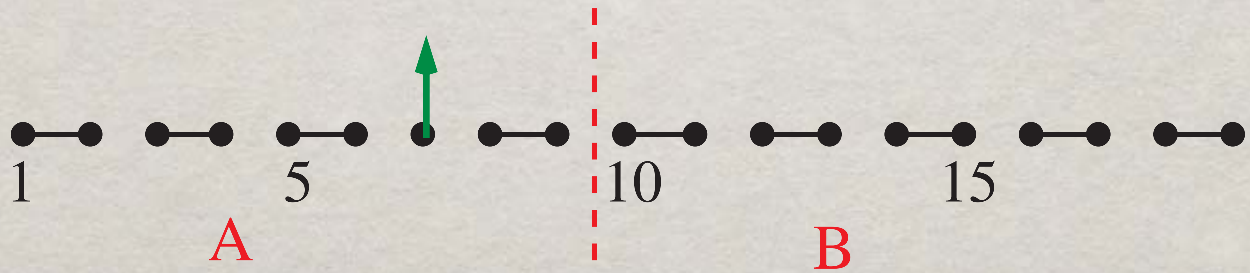
$$\rho_A = p|1\rangle\langle 1| + (1-p)|0\rangle\langle 0|$$

Where $|1\rangle$ is the state with the particle in A

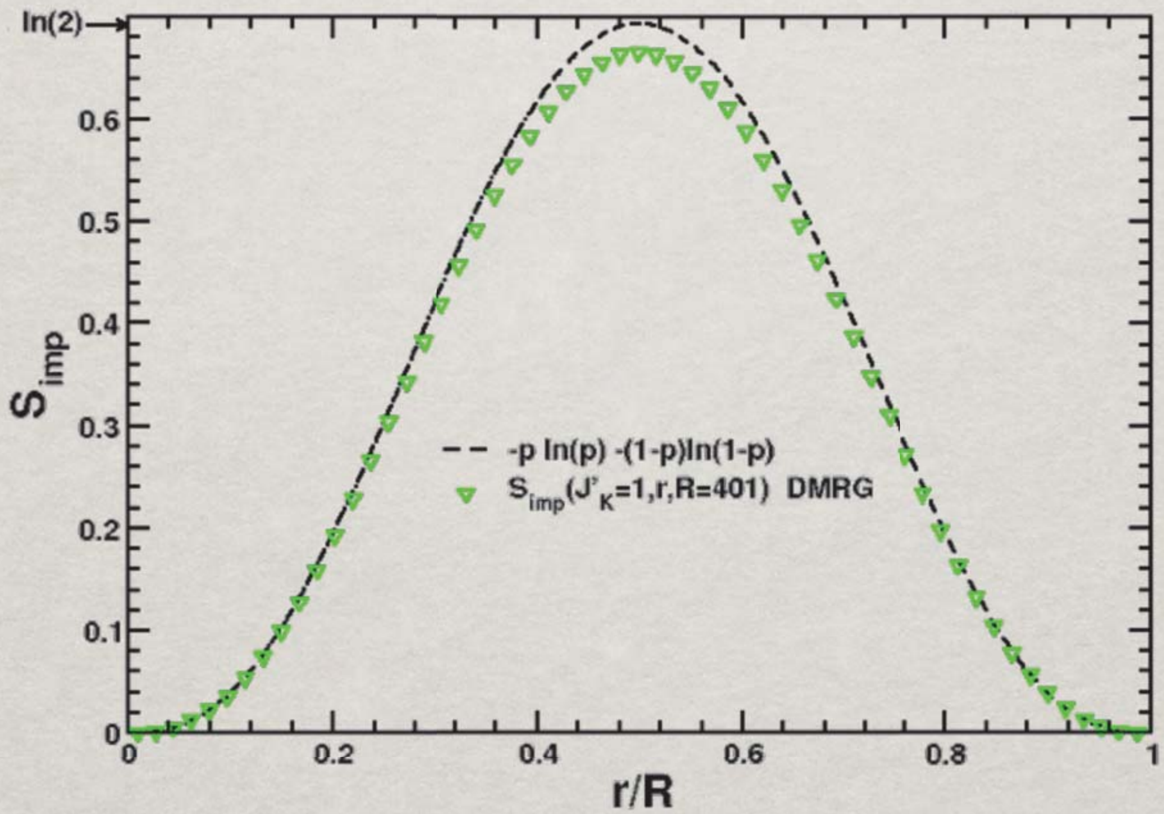
Then we get:

$$S_{\text{SPE}} = -p\ln p - (1-p)\ln(1-p)$$

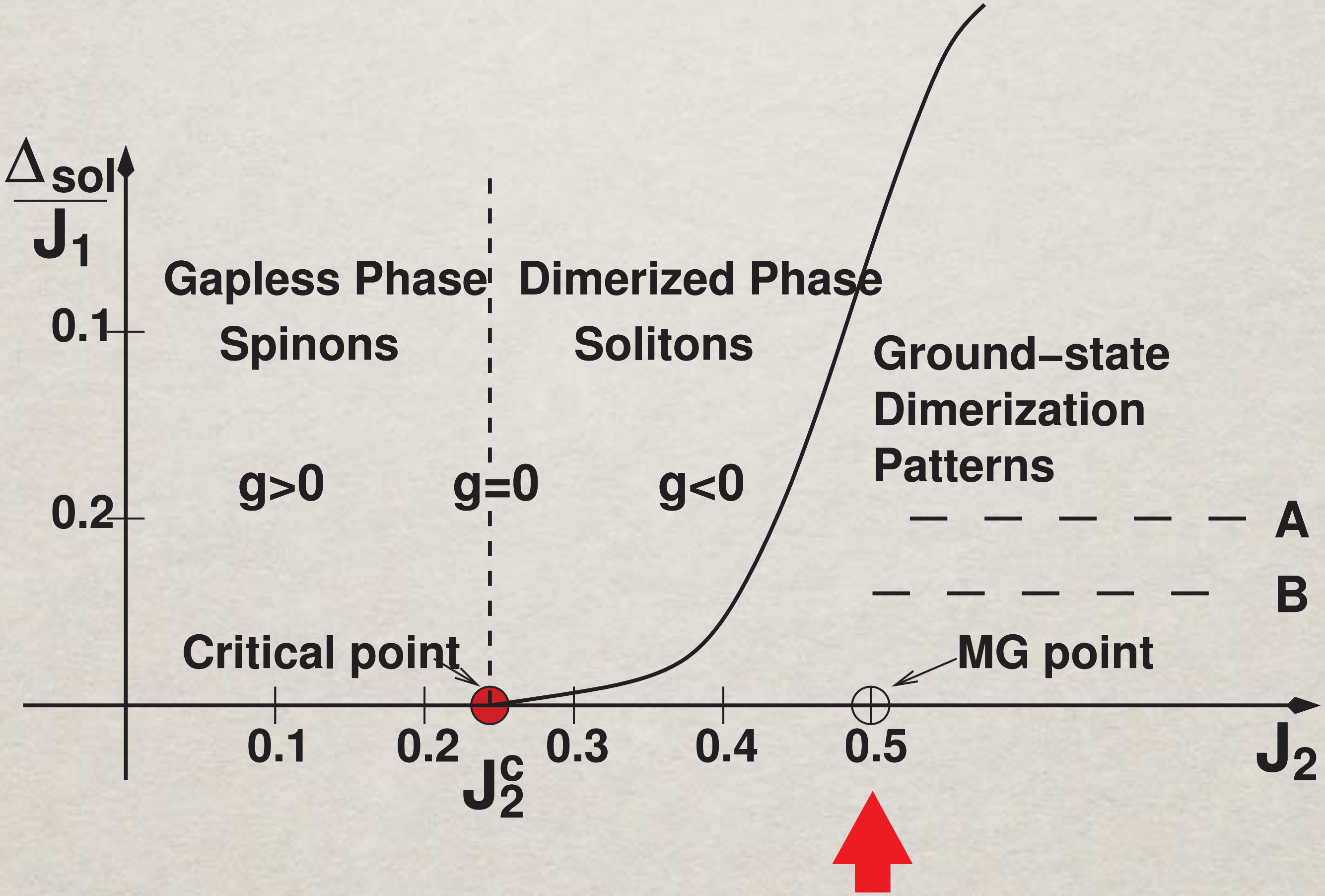
For R odd and $J'_K = 1$ a soliton is present we use this:



Single Particle Entanglement

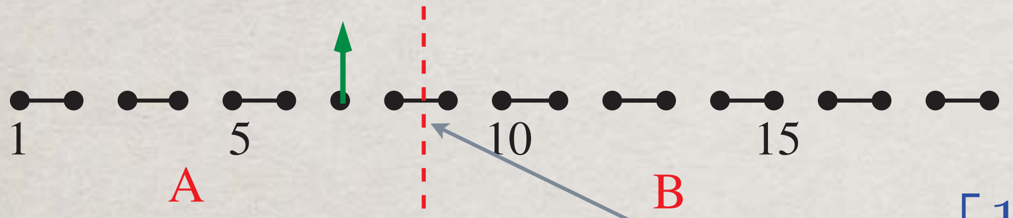


Single Particle Entanglement



Single Particle Entanglement

For the *total* entanglement there's an additional term:



L odd and $J'_K = 1$

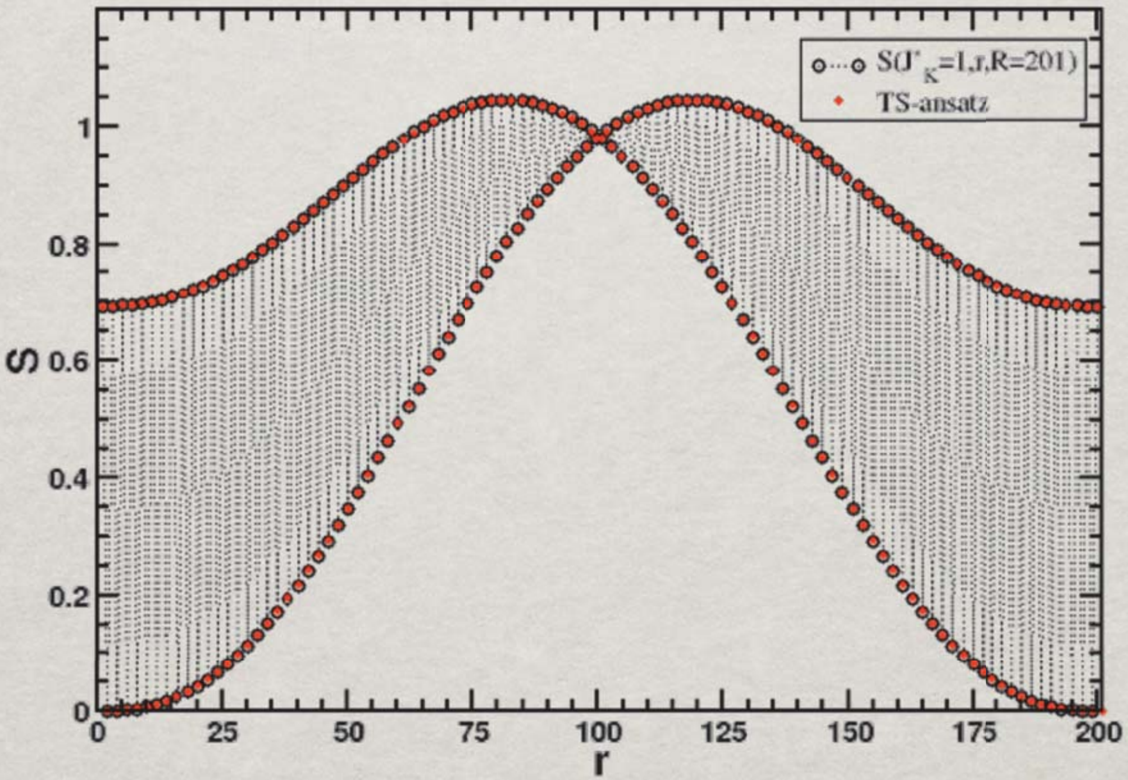
$$\Delta S = \left[\frac{1}{2} + (-1)^r (p - \frac{1}{2})\right] \ln(2)$$

$$J'_K = 1$$

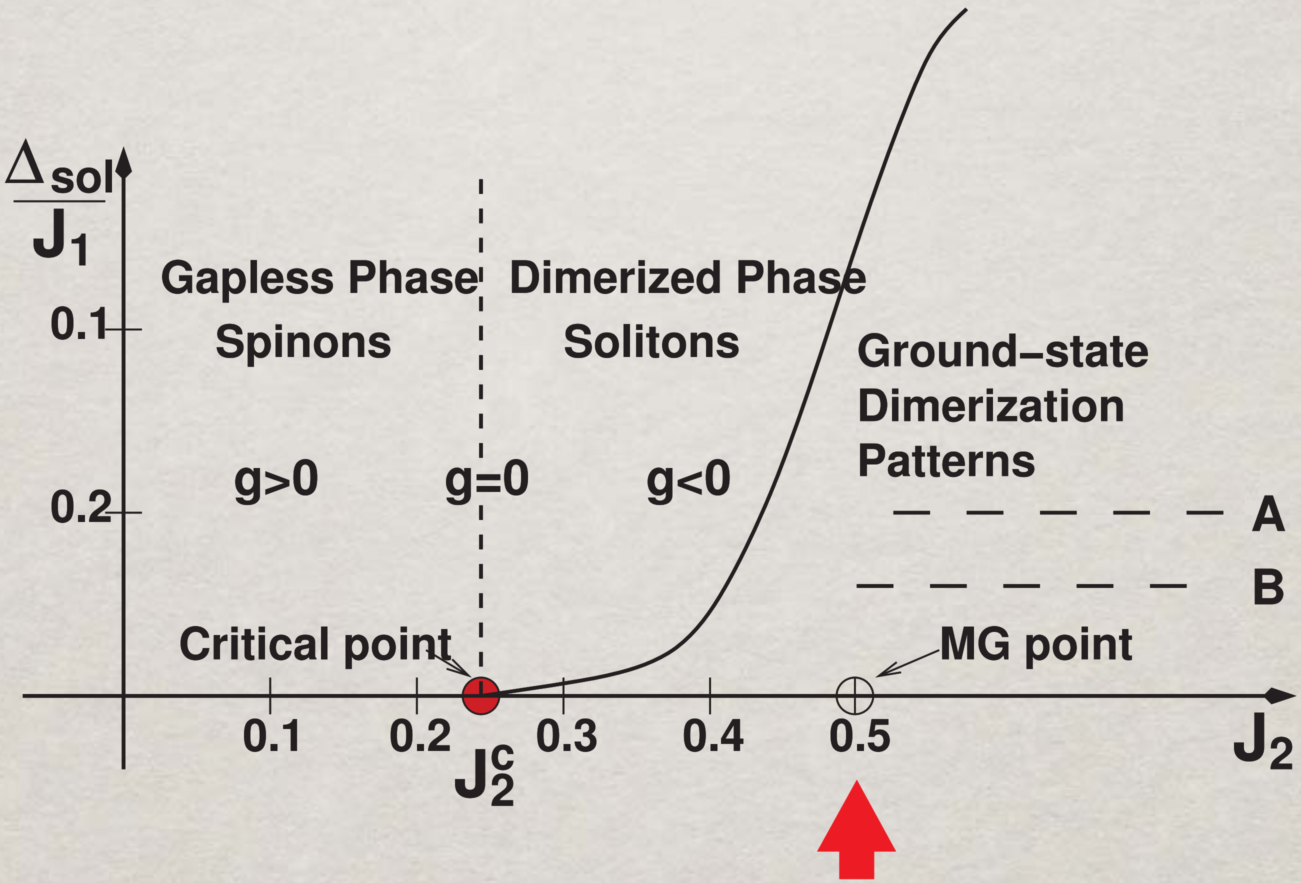
For L odd and $J'_K = 1$ a soliton is present we then get:

$$\begin{aligned} S &= S_{\mathrm{SPE}} + \Delta S \\ &= p \ln p - (1-p)\ln(1-p) + \left[\frac{1}{2} + (-1)^r (p - \frac{1}{2})\right] \ln(2) \end{aligned}$$

Total Entanglement



Total Entanglement



Soliton Ansatz at J2=J/2

Thin soliton state: $|n\rangle \equiv |\overbrace{- \;\ldots\; -}^{n} \uparrow - \;\ldots\; -\rangle$

Orthogonal TS-ansatz

Variational Ansatz: $|\Psi^{\Uparrow}_{TS}\rangle \simeq \sum_{n=0}^{N_d} \psi^{sol}_n |n\rangle$

$$|\Psi^{\Uparrow}_{TS}\rangle = \sum_{i,j=0}^{3} C_{i,j} |\psi_i\rangle |\phi_j$$

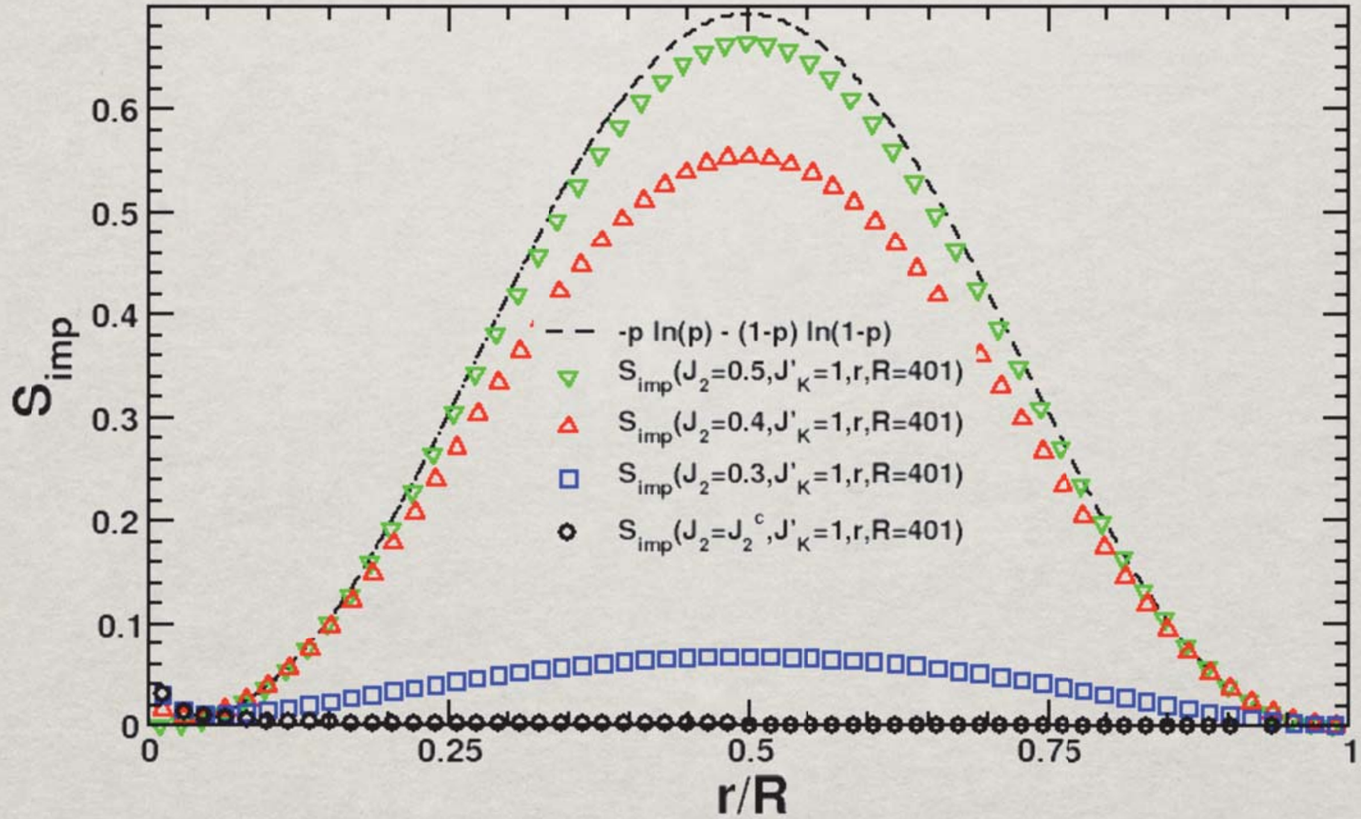
R odd $J'_K = 1$

$$|\psi_1\rangle = \sum_{n=0}^{\frac{r-1}{2}} \psi^{sol}_n |\overbrace{- \;\ldots\; -}^{n} \uparrow - \;\ldots\; -\rangle \quad |\phi_1\rangle = |\overbrace{- - - \;\ldots\; - - -}^{\frac{R-r}{2}}\rangle$$

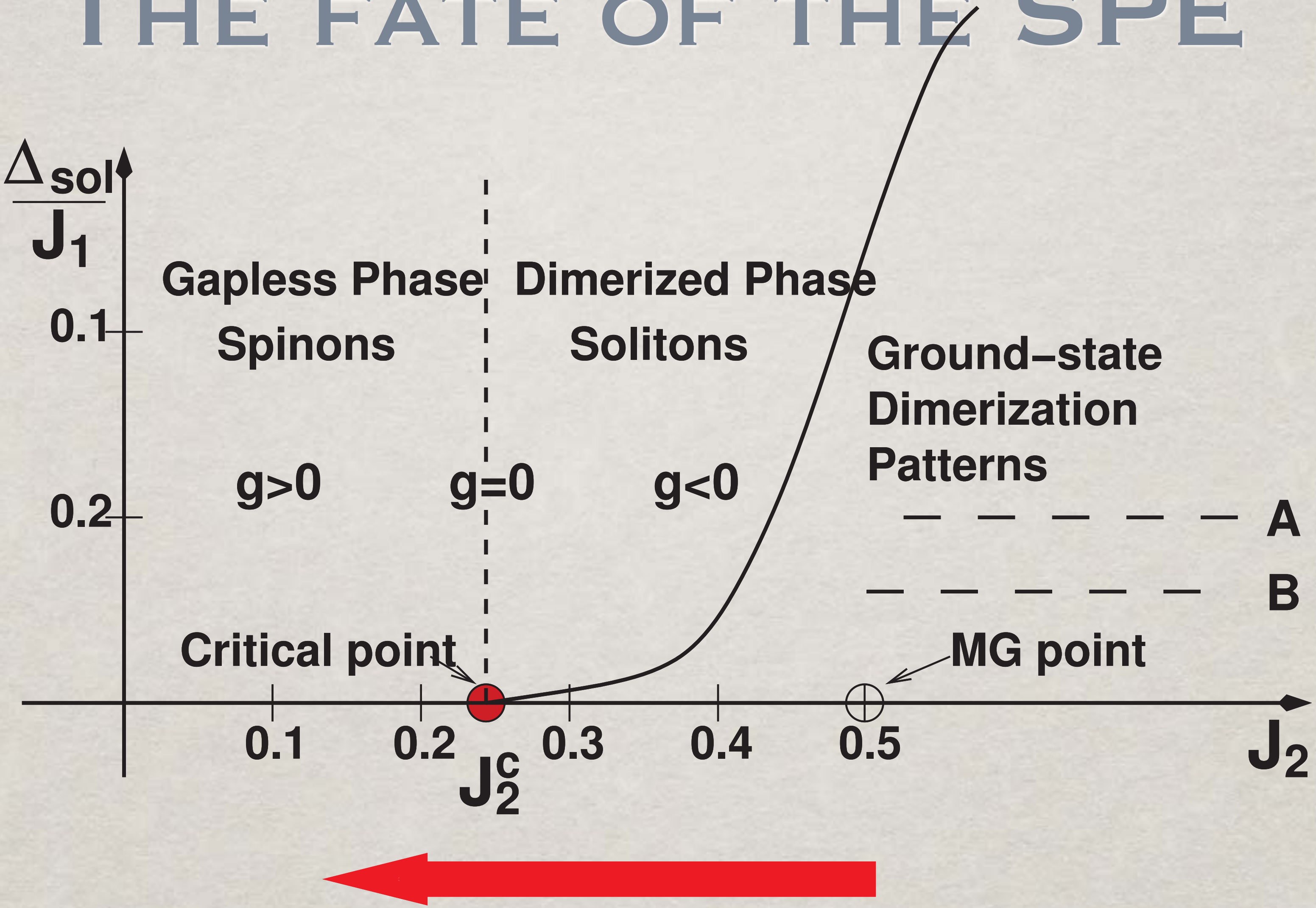
$$|\psi_2\rangle = |\overbrace{- - - \;\ldots\; - - -}^{\frac{r-1}{2}} \uparrow\rangle |\phi_2\rangle = \sum_{n=0}^{\frac{R-r}{2}-1} \psi^{sol}_{\frac{r+1}{2}+n} |\downarrow \overbrace{- \;\ldots\; -}^{n} \uparrow - \;\ldots\; -\rangle$$

$$|\psi_3\rangle = |\overbrace{- - - \;\ldots\; - - -}^{\frac{r-1}{2}} \downarrow\rangle |\phi_3\rangle = \sum_{n=0}^{\frac{R-r}{2}-1} \psi^{sol}_{\frac{r+1}{2}+n} |\uparrow \overbrace{- \;\ldots\; -}^{n} \uparrow - \;\ldots\; -\rangle$$

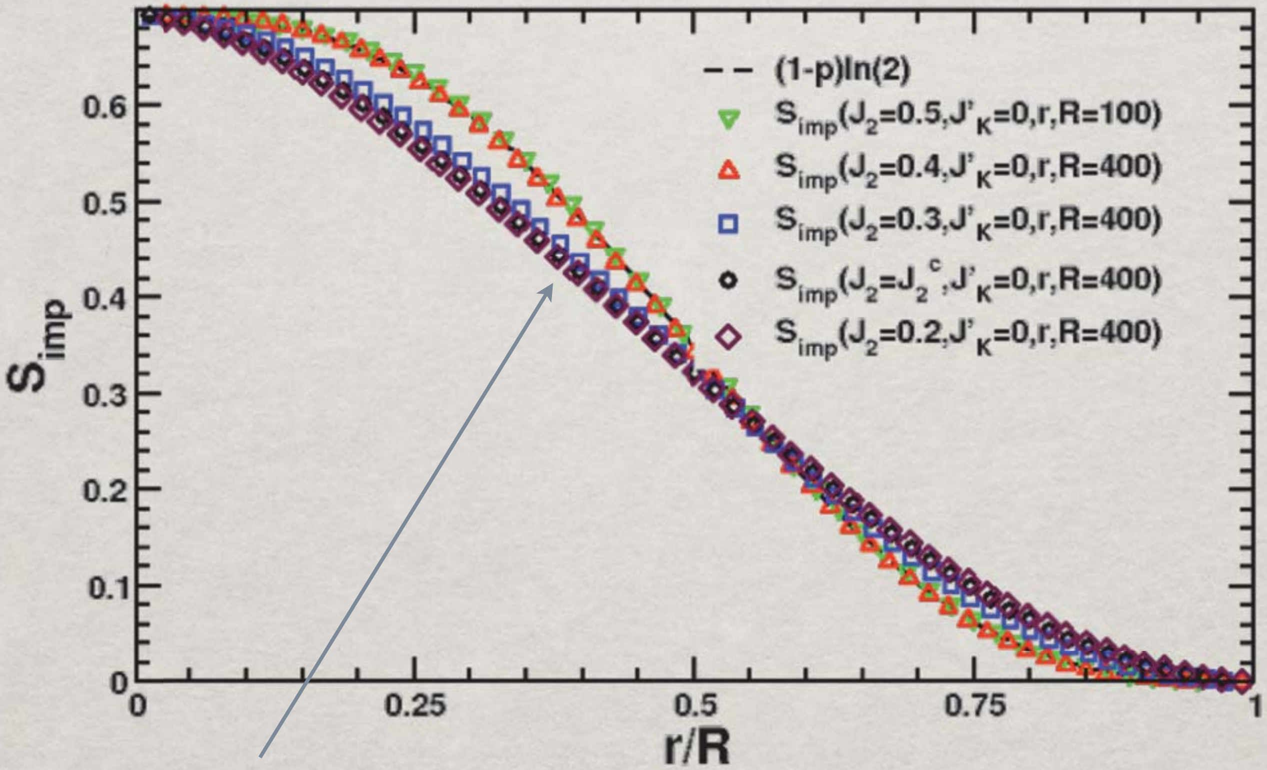
The fate of the SPE



The fate of the SPE

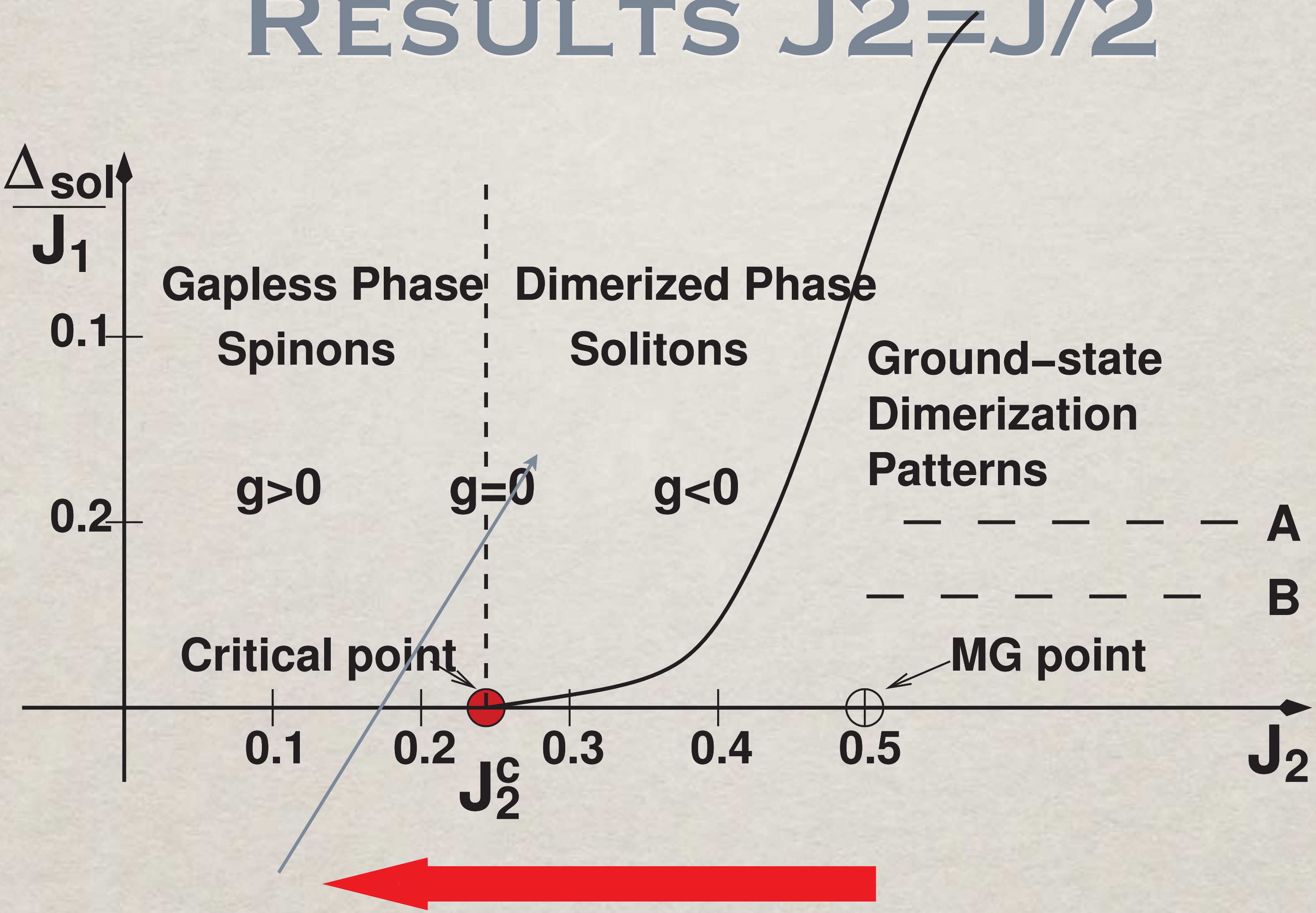


Almost Exact Results J2=J/2



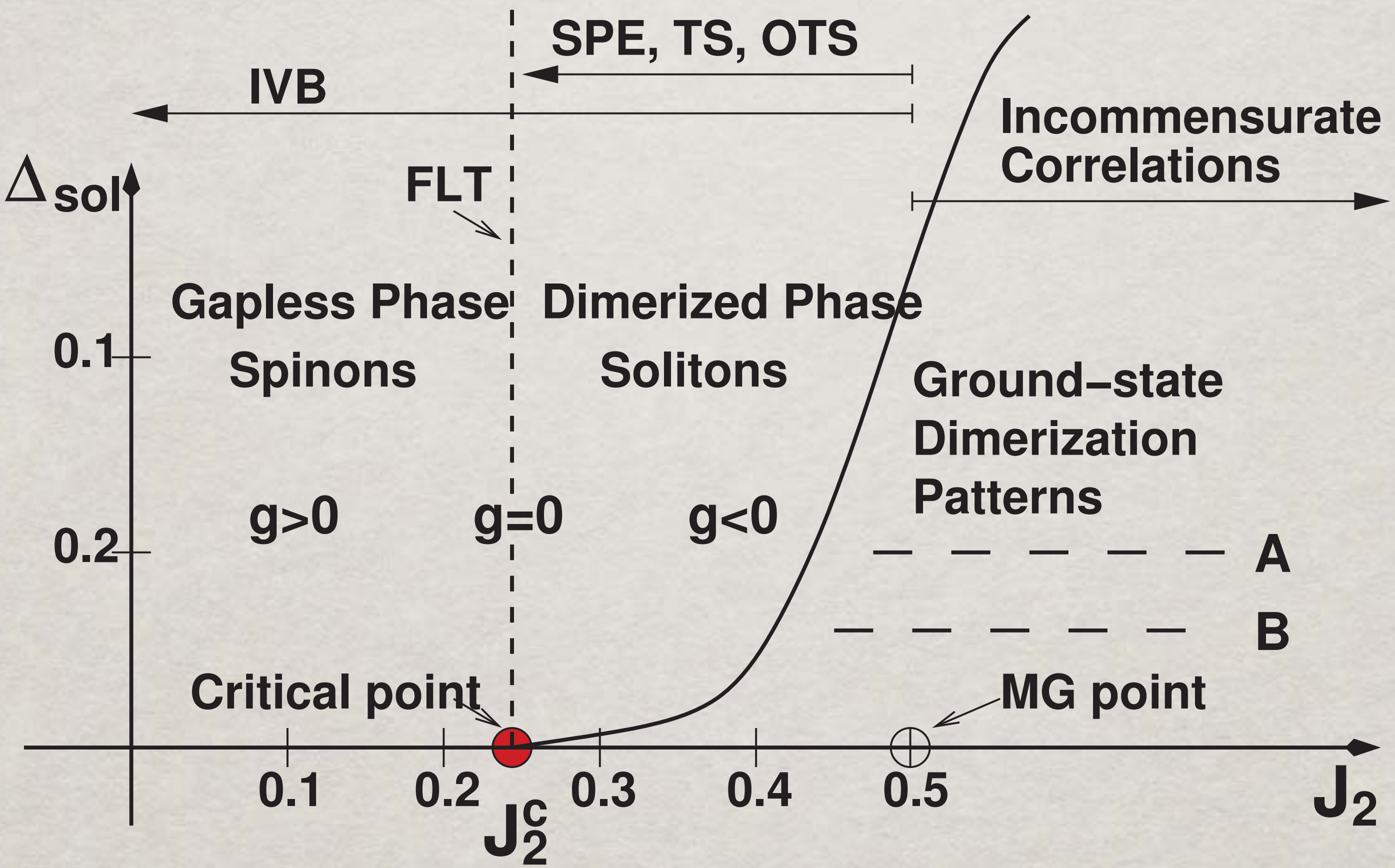
Universal at critical point. Analytical expression !?

Almost Exact Results J2=J/2



Universal at critical point. Analytical expression !?

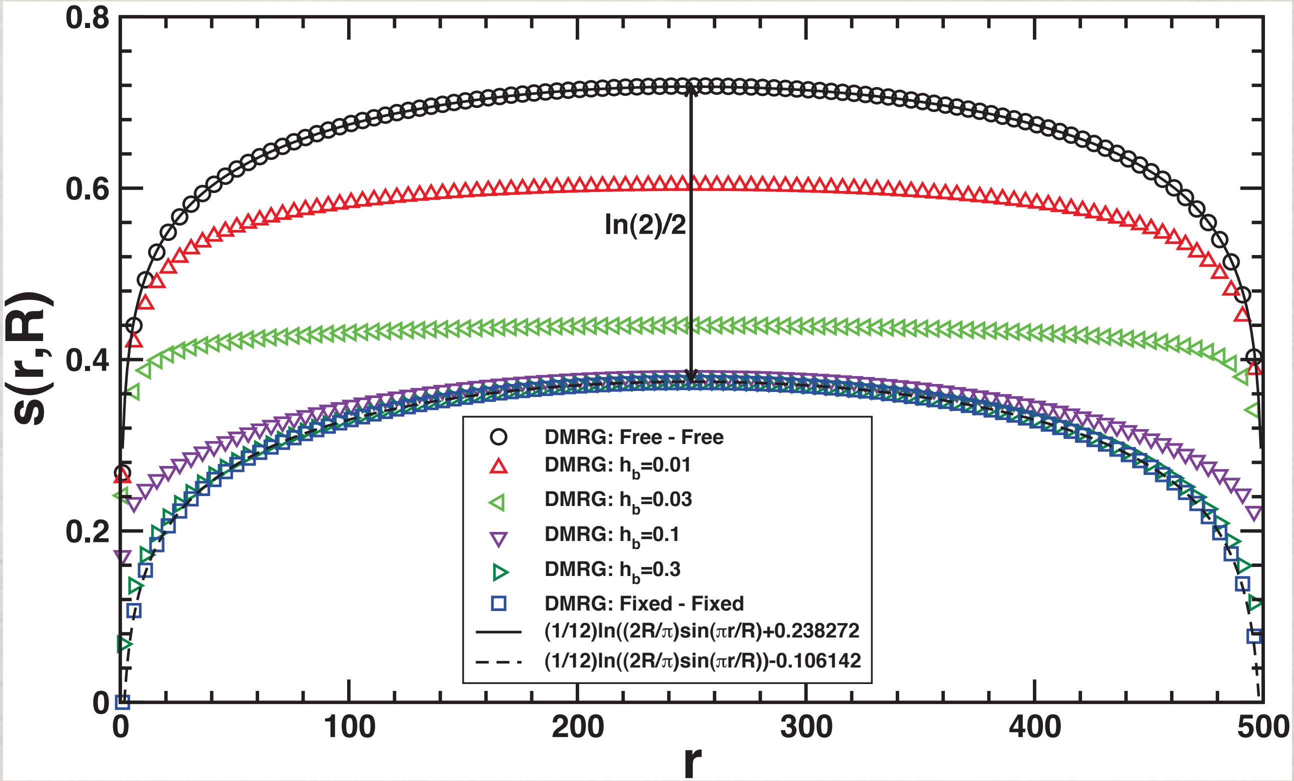
Intuitive Picture



OTHER IMPURITY ENTANGLEMENT

Boundary Fields

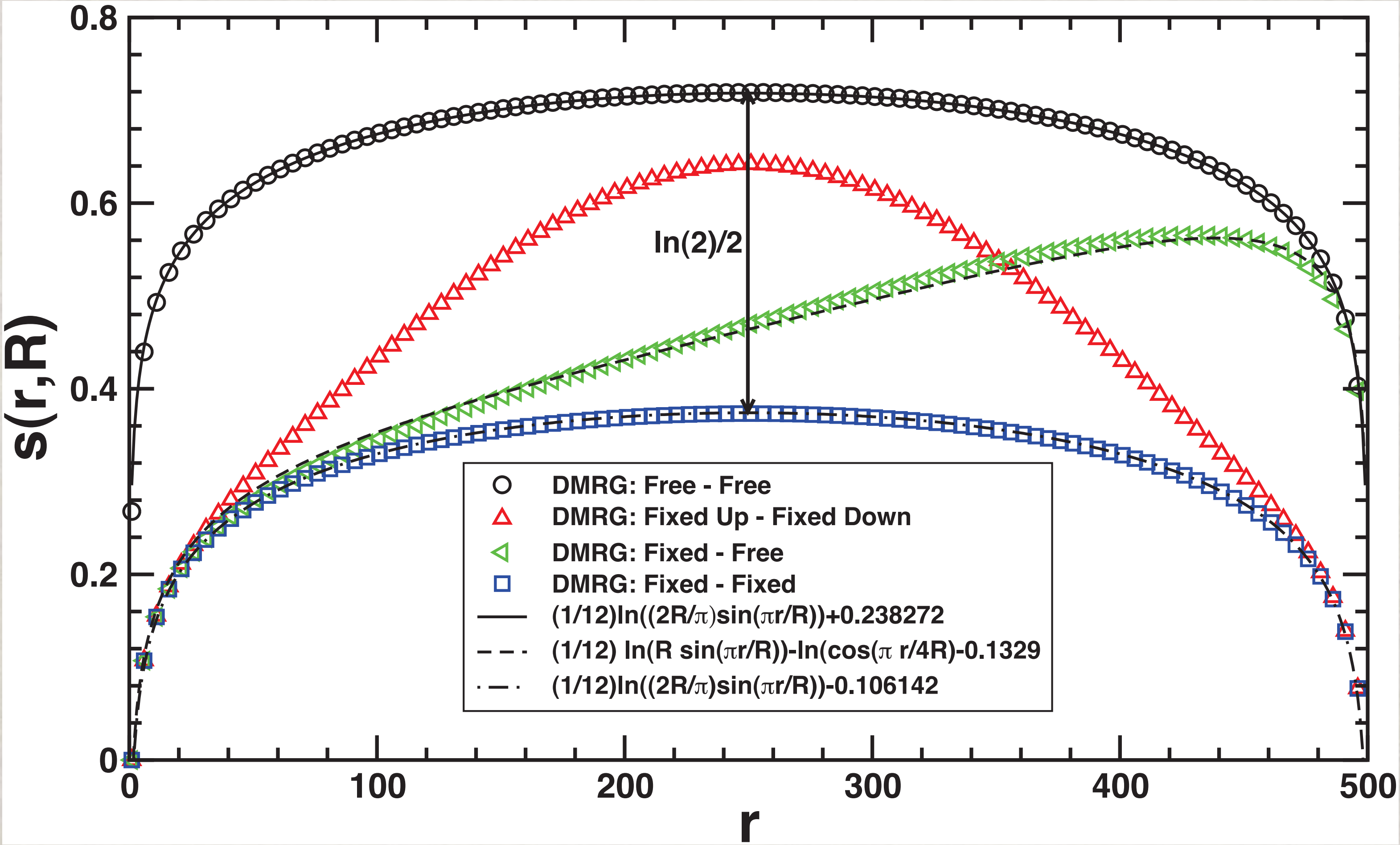
Critical TFIM



Zhou, Barthel, Fjaerestad, Schollwock, PRA 84 050305

g=1 free, $g=1/\sqrt{2}$ fixed

Boundary Fields



THANKS

ArXiv:1107.2907
J. Phys A, 42, 504009(2009)
JSTAT, P02007 (2008)
JSTAT, P08003 (2007)
JSTAT, L01001 (2007)
PRL 96, 100603 (2006)