Title: Entanglement entropy and the Kondo screening cloud

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Abstract:

Quantum Impurity Entanglement Entropy

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with Erik Sorensen, Ming-Shyang Chang and Nicolas Laflorencie

Outline

- Review of Kondo effect- spin chain version
- Quantum Impurity Entanglement Entropy
- Q.I.E.E. in Kondo model

Kondo Effect & Screening Cloud

- a single impurity spin in a metal is described by the Kondo (or s-d) model:

$$H = \sum_{\vec{k}\sigma} \psi^{+}_{\vec{k}\sigma} \psi_{\vec{k}\sigma} \varepsilon_k + J \vec{S}_{imp} \bullet \vec{S}_{el}(r=0)$$

- here $\vec{S}_{imp}$ is the impurity spin operator (S=1/2) and $\vec{S}_{el}(\vec{r})$ is the electron spin density at position $\vec{r}$

• after expanding the electron field $\psi(\vec{r})$ in spherical harmonics, keeping only the s-wave, and linearizing the dispersion relation we obtain a relativistic quantum field theory, defined on a 1/2-line with the impurity at the origin:

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$$H = iv_F \int_0^\infty dx \left[\psi_L^+ \frac{d}{dx} \psi_L - \psi_R^+ \frac{d}{dx} \psi_R \right] + 2\pi v_F \lambda \vec{S}_{imp} \bullet \vec{S}_{el}(0)$$

- here λ is the dimensionless Kondo coupling, $J\nu$, where ν is the density of states
- $\psi_L(0)=\psi_R(0)$
- Kondo physics is fundamentally 1-dimensional

•further reduction is possible due to 1D spin-charge separation

$$H = H_c + H_s$$

$$H_s = (v/6\pi)\int_0^\infty dr\left[\vec{J}_L(r)\cdot\vec{J}_L(r) + \vec{J}_R(r)\cdot\vec{J}_R(r)\right] + v\lambda\vec{J}_L(0)\cdot\vec{S}$$

$$\vec{J}_L = \psi_L^+ \frac{\vec{\sigma}}{2}\psi_L$$

•the same low energy effective theory is obtained from S=1/2 Heisenberg antiferromagnetic spin chain with a weak link *at end of chain*

• J_K • J • J • J • J_K<<J=1

$$H = J_K \vec{S}_0 \cdot \vec{S}_1 + \sum_{j=1}^{R-1} \vec{S}_j \cdot \vec{S}_{j+1}$$

- Jordan-Wigner + bosonization gives same low energy theory
- (technicality: also add a 2nd neighbour coupling to eliminate bulk marginal operator)
- Spin chain version is useful for numerical work (DMRG) and for intuitive pictures

• to study the problem at low energies, we may apply the renormalization group, integrating out high energy Fourier modes of the electron operators, reducing the band-width, D:

$$\frac{d\lambda}{d\ln D} \approx -\lambda^2 + \bullet\bullet\bullet$$

$$\lambda_{eff}(D) \approx \frac{\lambda_0}{1-\lambda_0 \ln(D_0/D)} + \bullet\bullet\bullet$$

• effective coupling becomes O(1) at energy scale T_K:

$$T_K = D_0 \exp(-1/\lambda_0)$$

(D_0 is of order the Fermi energy)

• effective Hamiltonian has *wave-vector* cutoff:

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- strong coupling physics is easiest to understand in tight-binding model:

$$H = -t\sum_{j=0}^{\infty}(\psi_j^+\psi_{j+1} + \psi_{j+1}^+\psi_j) + J\vec{S}_{imp} \bullet \vec{S}_{el}(0)$$

• for J>>t, we simply find ground state of last term:
• 1 electron at j=0 forms spin singlet with impurity: $|\phi_0\rangle = (|\Uparrow\downarrow\rangle - |\Downarrow\uparrow\rangle)/\sqrt{2}$

• other electrons are free except that they must not go to j=0 since they would break the singlet

• effectively an infinite repulsion at j=0, corresponding to $\pi/2$ phase shift

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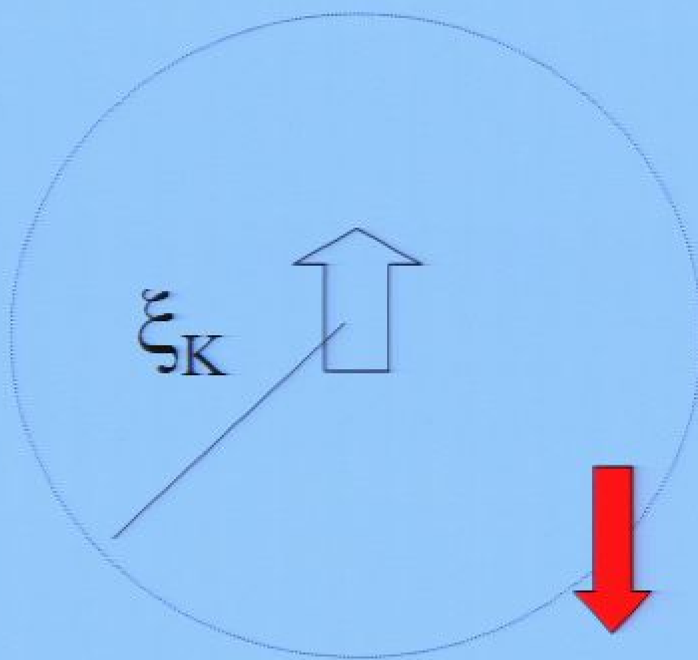
- for finite (small) λ_0, this description only holds at low energies and small $|k-k_F|$



- only long wavelength probes see simple $\pi/2$ phase

•Low energy ($E<<T_K$) effective Hamiltonian does not contain impurity operator, only conduction electrons (with $\pi/2$ phase shift)

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•Low energy/long distance properties can be calculated in perturbation theory in E/T_K and ξ_K/r – eg. $\chi_{imp} \rightarrow (1/4T_K)[1+cT/T_K+\ldots]$

We may equivalently use boundary condition to reflect right movers to negative r-axis

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Now it is clear that boundary perturbation, low energy remnant of Kondo interaction, is simply proportional to the energy density of spin sector of non-interacting system, *T* (0)

Quantum Impurity Entanglement Entropy

- Starting with ground state of system, trace over region B, to obtain reduced density matrix for region A, then calculate Neumann entropy

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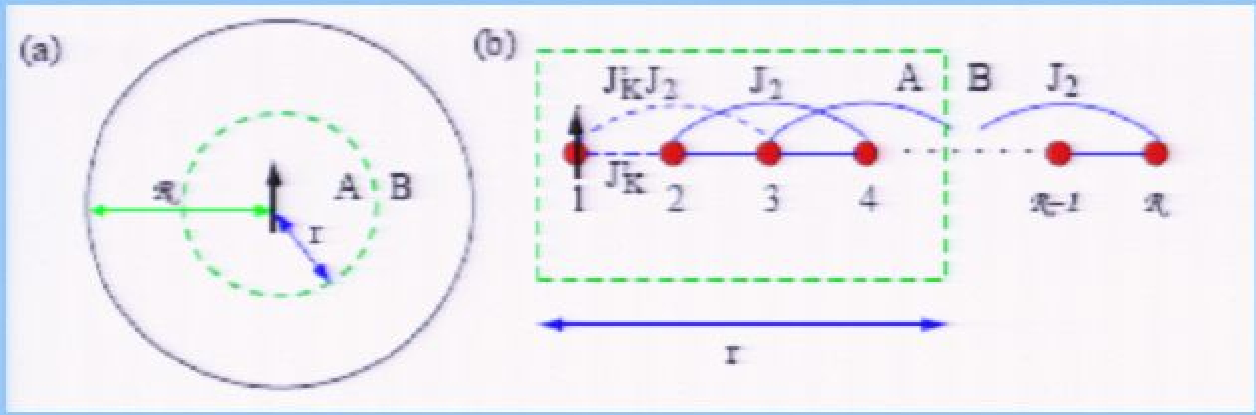
AB

$\psi=|\uparrow\uparrow>$ $\quad \rho_A = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ $\quad -\mathrm{tr}\, \rho_A \ln \rho_A = 0$

$\psi=(|\uparrow\downarrow>-|\downarrow\uparrow>)/\sqrt{2}$ $\quad \rho_A = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$ $\quad -\mathrm{tr}\, \rho_A \ln \rho_A = \ln 2$

We apply this to our system of spin impurity plus conduction electrons (or other spins) by defining region A to be a finite region Including impurity spin



•N.B. most of entanglement entropy *does not* come from impurity but essentially from boundary between regions A and B:

Quantum spin chain, D=(1+1), case:
$S_0 \rightarrow (1/6) \ln (r/a)$ (for $R=\infty$, $r>>1$)

D=(3+1) electron case:
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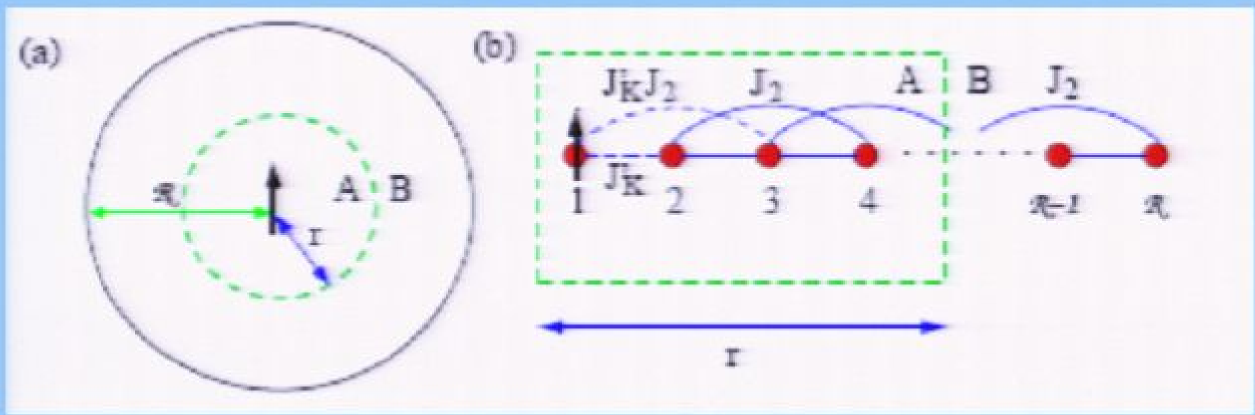

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- Analogous to the way *thermodynamic impurity entropy* is defined (and measured):
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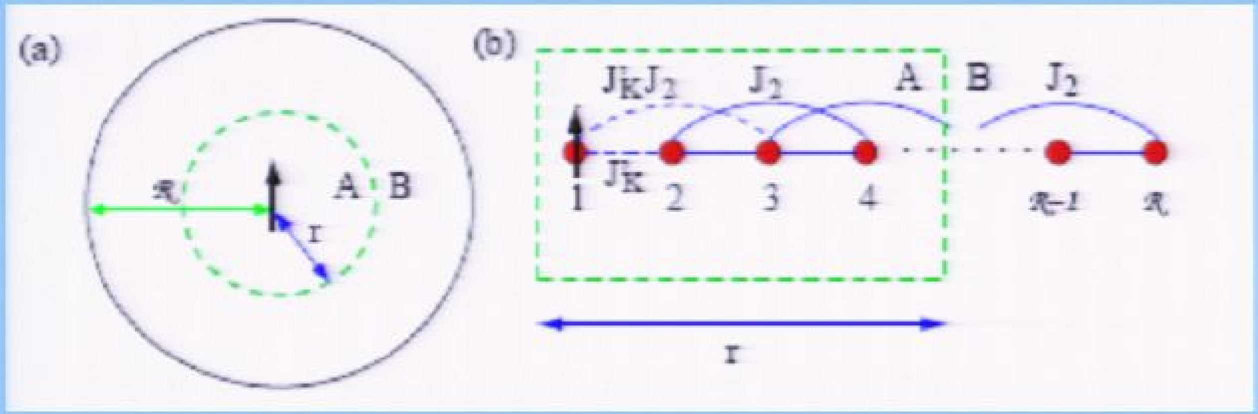

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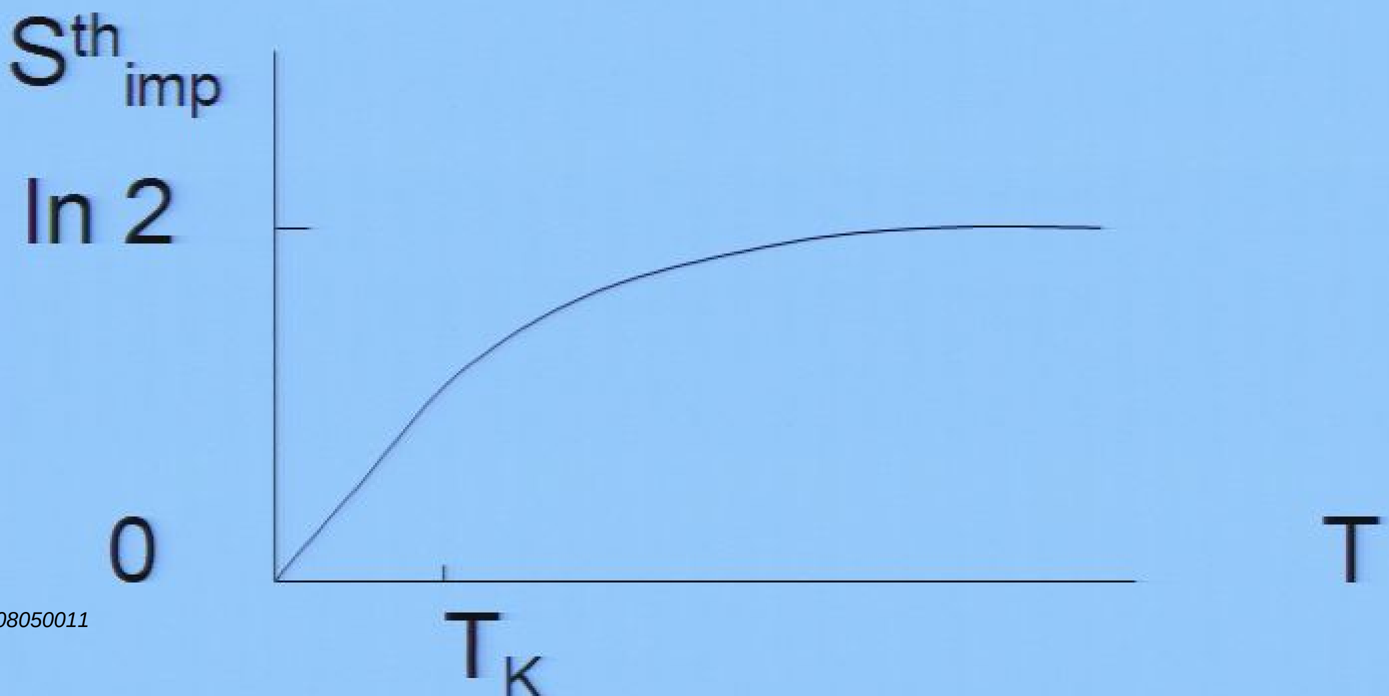
•Thermodynamic impurity entropy approaches ln 2 at $T \gg T_K$ since Kondo coupling is weak
•It approaches 0 at $T \ll T_K$ since impurity degree of freedom is eliminated by interaction with conduction electrons (spin singlet formed)



- This zero temperature thermodynamic impurity entropy is a useful way of classifying various renormalization group fixed points for boundary interactions in general (Affleck & Ludwig, 1991)
- It exhibits non-trivial values ($\neq \ln n$) for some boundary fixed points (such as 2-channel Kondo fixed point)

•We can find a simple analytic expression for S_{imp} when $r \gg \xi_K$ by doing lowest order perturbation theory in Fermi liquid interaction

$$H_s = (v/6\pi)\left[\int_{-\infty}^{\infty} dr\left[\vec{J}_L \cdot \vec{J}_L\right] - \pi\xi_K \vec{J}_L(0)\cdot\vec{J}_L(0)\right]$$

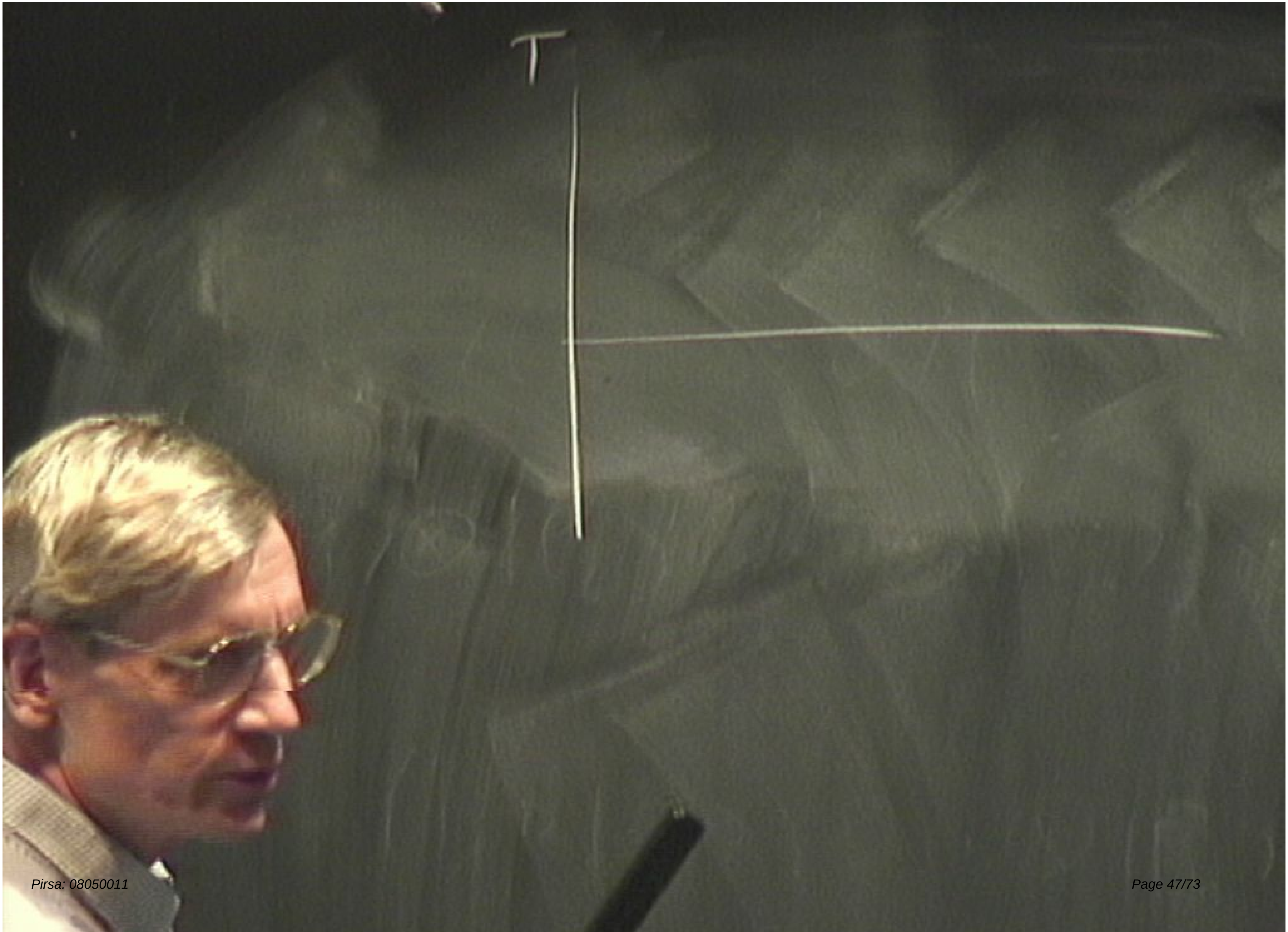
•Will give $S_{imp} \propto \xi_K/r$

•Following Holzey-Wilczek and Cardy-Calabrese S is obtained from partition function Z_n on n-sheeted Riemann surface with sheets joined along cut from 0 to r, using replica trick ($n \rightarrow 1$)

i.e. Z_n (A) is partition function for n-sheeted Riemann surface with sheets sewn together on region A

$$tr\,\rho_A^n \equiv \frac{Z_n(A)}{Z^n} = \sum_i \lambda_i^n$$

$$S_A = -\lim_{n\to 1}\frac{\partial}{\partial n} tr\,\rho_A^n$$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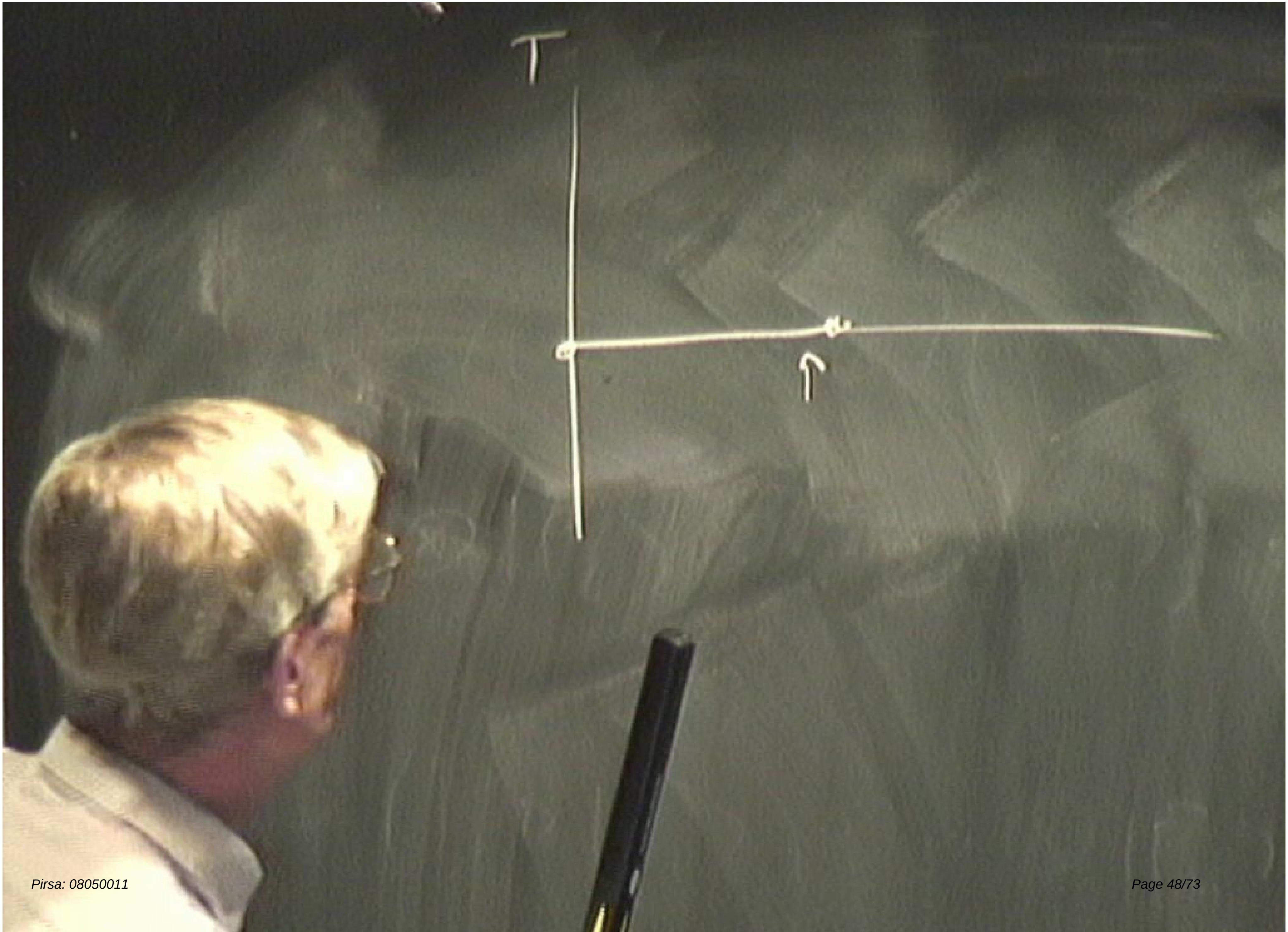
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- C&C argued that Z_n is given by 2-point function of peculiar operators Φ_n ,Φ_{-n} on C
- An intermediate step in their argument involved showing that $<T(z)>$ on R_n is the same as $< \Phi_n (0)\Phi_{-n}(r)T(z)>$ on C
- Very fortunately, our perturbation is precisely T so C&C have kindly calculated 1st order perturbation theory for us!
- Perturbation to Z_n gives: $S_{imp} = \pi\xi_K/(12r)$
- Agrees with DMRG data

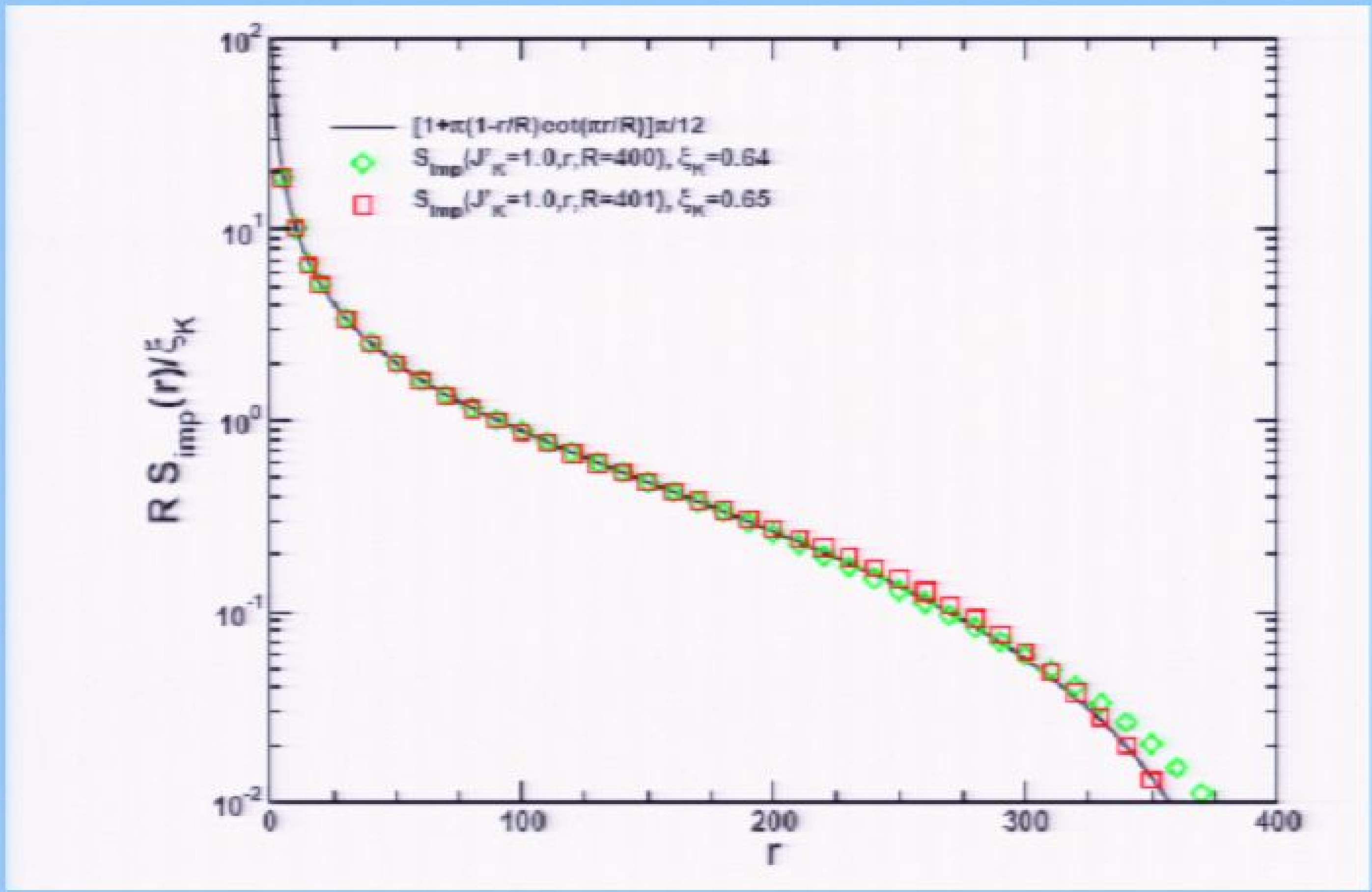
- We can easily obtain $<\Phi_n(0)\Phi_{-n}(r)T(z)>$ at finite R (i.e. on a cylinder) by a standard conformal transformation
- This gives S_{imp} for any r/R when $\xi_K << r$

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

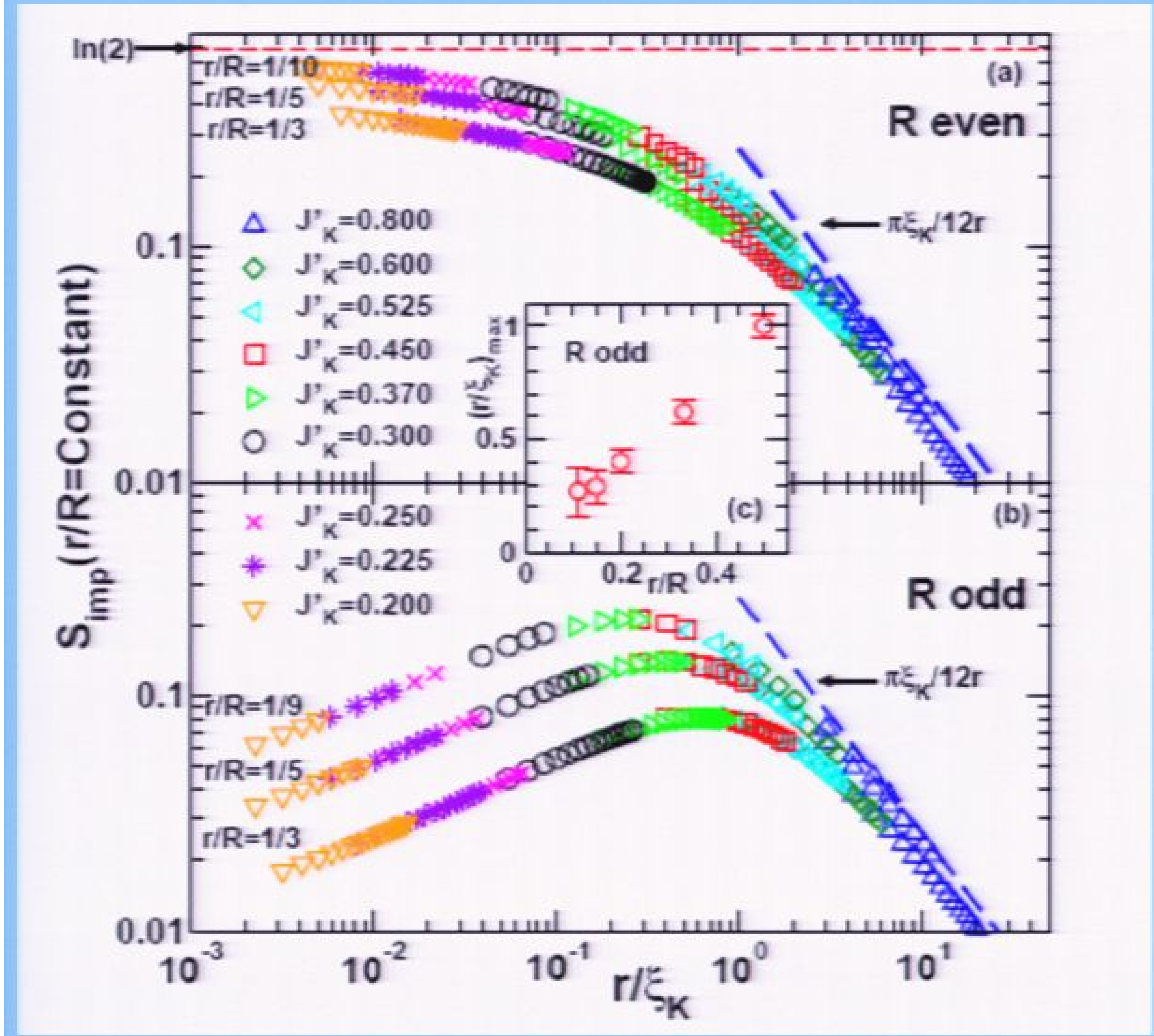
- We calculated S_{imp} (r,R,J_K) using Density Matrix Renormalization Group (DMRG) numerical method
- This is a method for building up a spin chain by sequentially adding pairs of sites near the middle, truncating the Hilbert Space at each step to a manageable size (few hundred)
- Optimum truncation scheme is based on *Density Matrix*

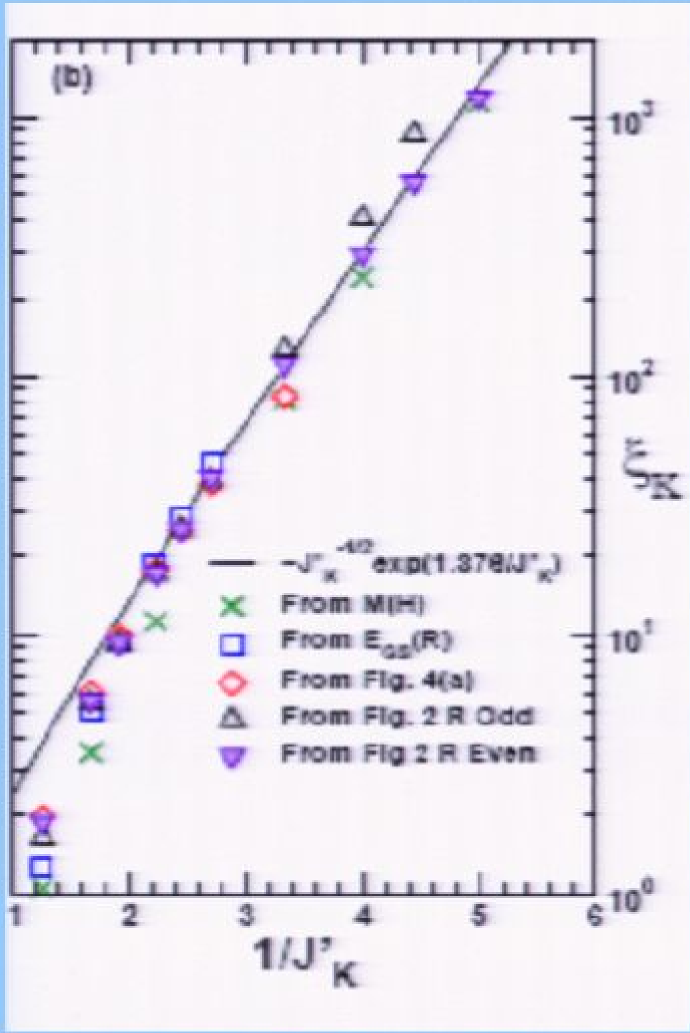
- Optimum set of states to keep in A are those with largest eigenvalues of ρ_A (S.R. White)
- Has become a highly accurate method of choice for finding ground states of D=(1+1) quantum systems
- A byproduct is determination of ρ_A (and S_A)

•For $r >> \xi_K$, perturbative calculation agrees well with DMRG



- We found, numerically, that $S_{imp}(r,R,J_K/J)$ is a universal scaling function of r/R, r/ξ_K
- Thermodynamic impurity entropy, and many other physical quantities in Kondo model are also universal scaling functions
- Basically follows from renormalizability of Kondo model, in limit $\lambda \to 0$
- Our results indicate that impurity entanglement entropy is another such universal scaling function (with zero anomalous dimension)

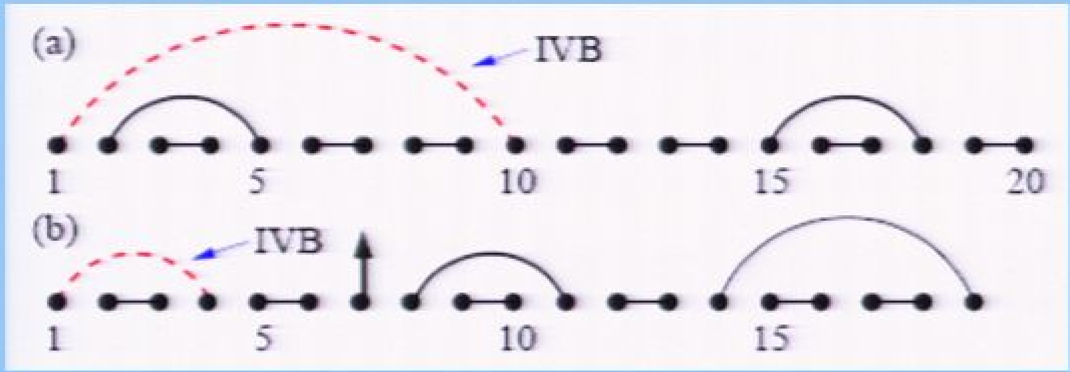




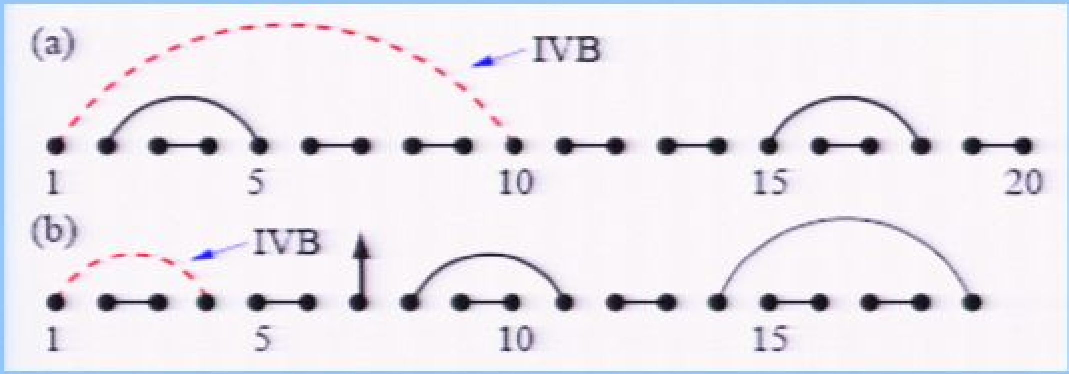
- $S_{imp}(r/R, r/\xi_K)$ scales, with expected ξ_K
- S_{imp} is different for R even/odd
- Large r/ξ_K limit the same, given by CFT

- Cross-over of S_{imp} from ln 2 at short distances to 0 at long distances confirmed for R even
- For R odd, behavior looks much more complicated but at $R \to \infty$ we get same result
- This confirms that change, $\Delta S^{ent}_{imp} = \Delta S^{th}_{imp} = -\ln 2$ between 2 fixed points
- A formal argument was given for this general result by Cardy and Calabrese
- This confirms it in a particular lattice model

Intuitive Picture for S_{imp} $(r/R, r/\xi_K)$



- impurity may be "Kondo screened", by an impurity valence bond (IVB) to some other spin
- *Heuristically* S_{imp} is ln 2 times probability of the IVB being present and stretching into region B (>r)



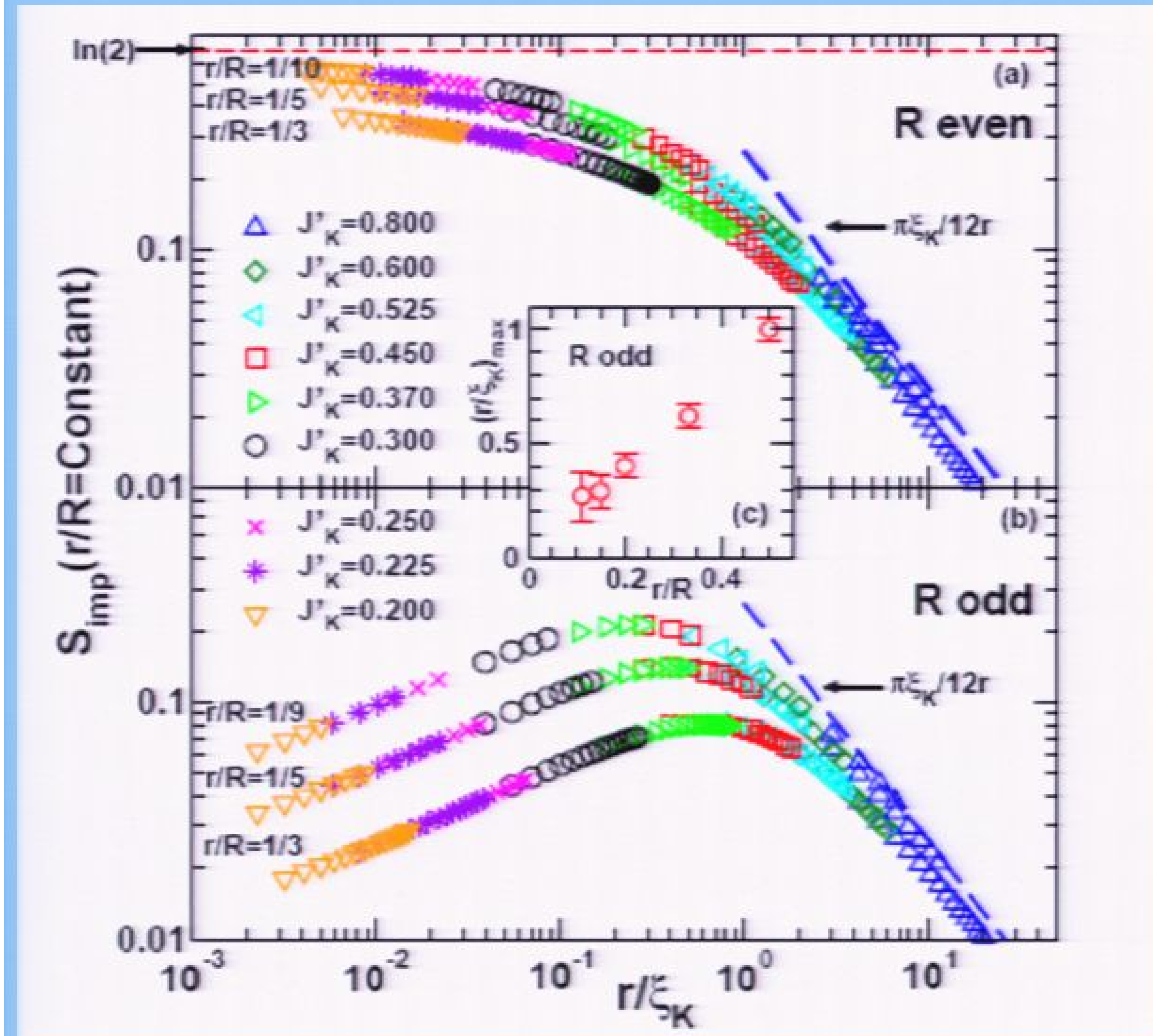
- Typical length of IVB is ξ_K so, for R even, S_{imp} decreases monotonically on scale ξ_K
- For R odd, there may be no IVB since there is an unpaired spin somewhere in chain
- Unpaired spin is impurity for λ=0: S_{imp}=0
- With decreasing ξ_K, (i.e. increasing λ) probability of having an IVB increases but its length (when it exists) decreases

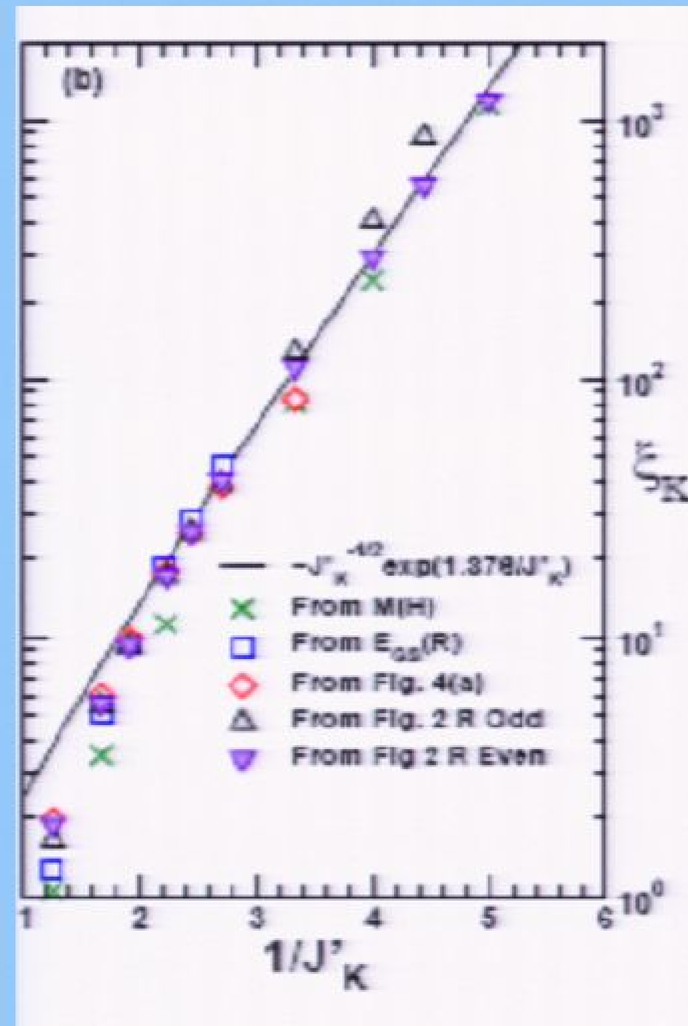
•R/ξ_K controls strength of effective Kondo interaction (strong for $\xi_K<R$)

•Prob (IVB) versus average length of IVB trade off to produce a maximum in S_{imp} at $R\sim\xi_K$ (agrees well with DMRG data)

Conclusions

- Impurity entanglement entropy is a useful probe for quantum impurity problems
- S_{imp} a universal scaling function of r/ξ_K , r/R
- $\Delta S=\Delta(\ln g)=-\ln 2$ from $r<<\xi_K$ to $r>>\xi_K$
- S_{imp} is given by simple analytical expression for $\xi_K<<r$





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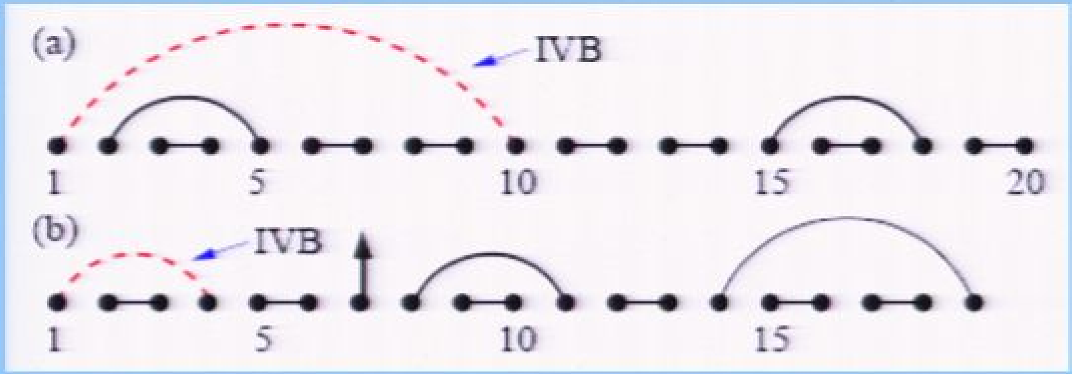

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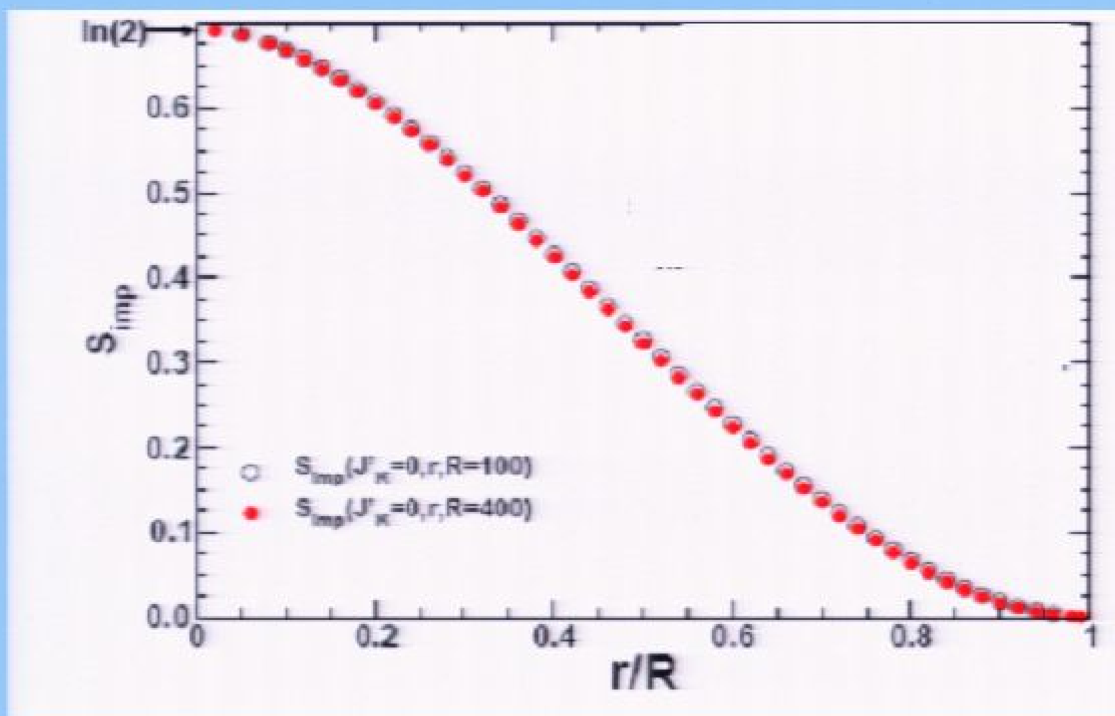
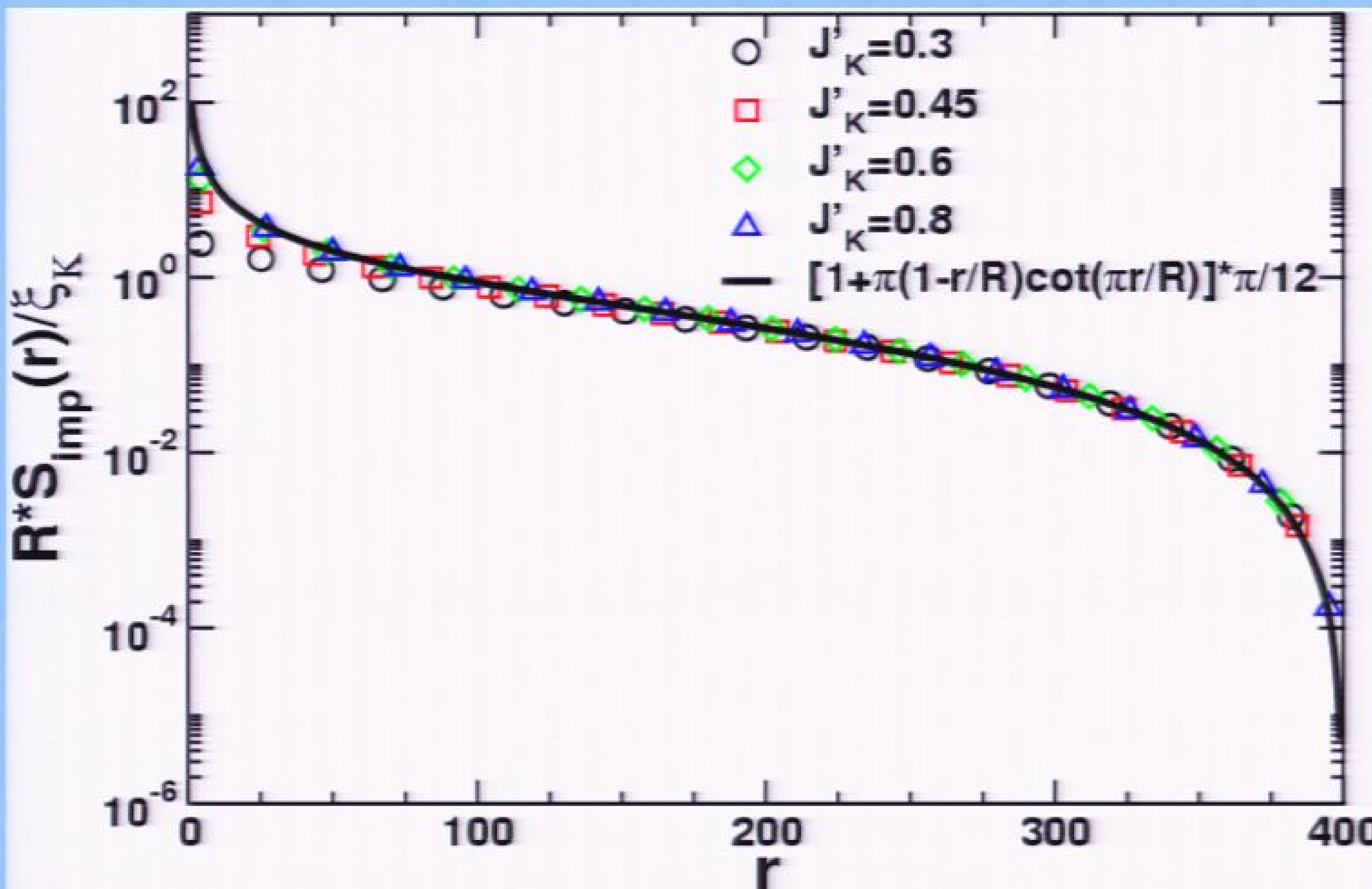
- *Heuristically* S_{imp} is ln 2 times probability of the IVB being present and stretching into region B (>r)

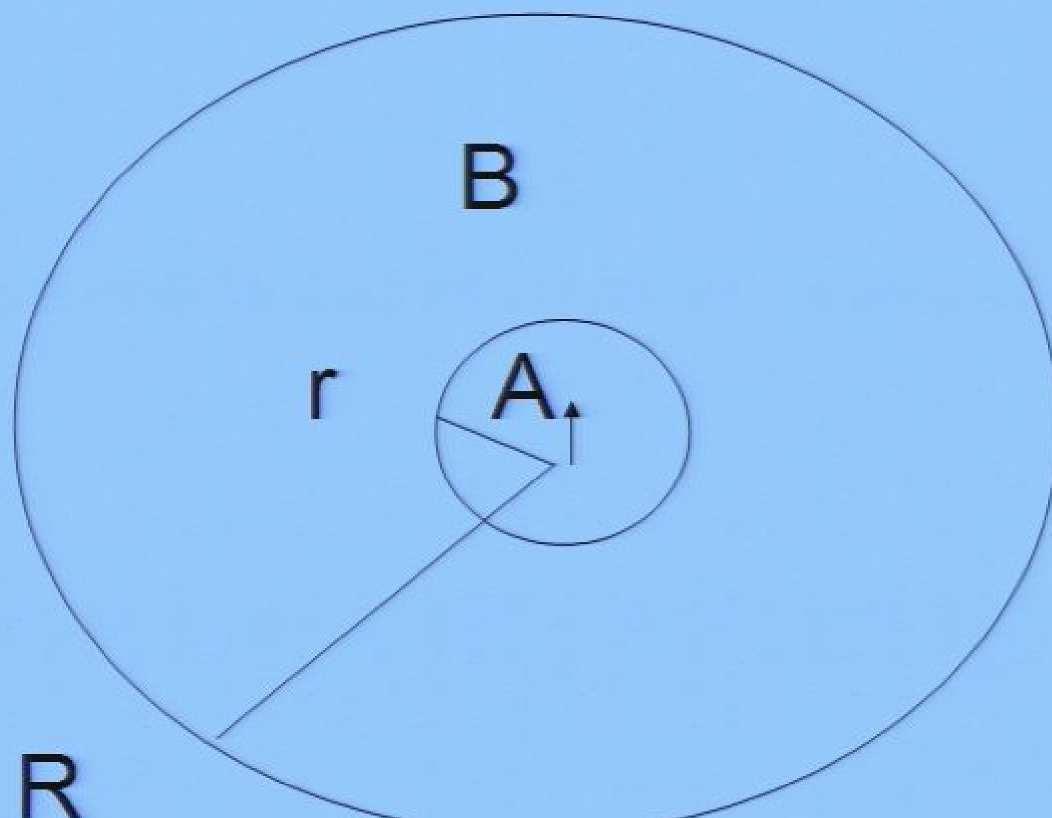
- Naively, expect IVB to be equally likely to have any length implying
$S_{imp}\ (\xi_K=0, r/R)=(1-r/R)\ln 2$
- This is approximately true



DMRG data compared to Fermi Liquid Theory For S_{imp}



We expect this calculation to apply equally well to Kondo model for free fermion in 2 or 3 dimensions



For spherically symmetric model with δ-function Kondo interaction, for example, S_0 is a sum of terms from all angular momentum channels (l,m)

$$S_0 = \sum_{l,m} S_{l,m}$$

each term can be calculated in a 1D model with a centrifugal potential:

$$V_l(r) = \frac{l(l+1)}{2mr^2}$$

- Only the l=0 (s-wave) channel couples to the impurity spin so only $S_{l=0}$ is modified by Kondo interaction
- Again:

$S(r,R)=S_0(r,R) + S_{imp}(r,R)$

- Now $S_0(r) \propto r^2 \ln r$ in 3 dimensions
- $S_{imp}(r/R, r/\xi_K)$ is same universal scaling function as before

For spherically symmetric model with δ-function Kondo interaction, for example, S_0 is a sum of terms from all angular momentum channels (l,m)

$$S_0 = \sum_{l,m} S_{l,m}$$

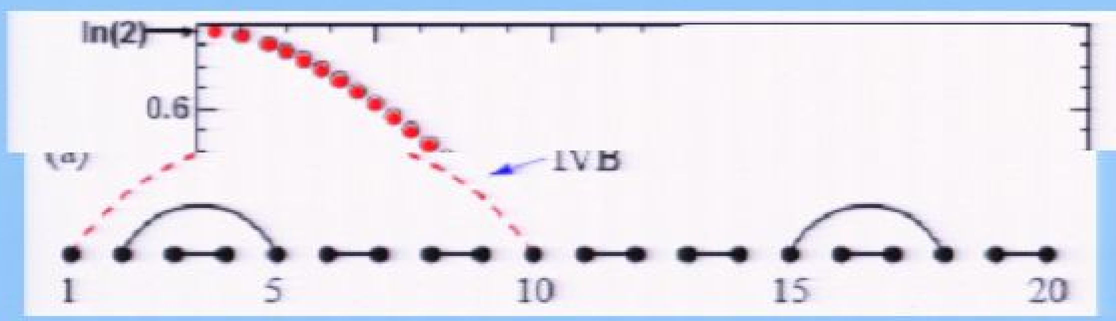
each term can be calculated in a 1D model with a centrifugal potential:

$$V_l(r) = \frac{l(l+1)}{2mr^2}$$

- Naively, expect IVB to be equally likely to have any length implying

$S_{imp}\ (\xi_K=0, r/R)=(1-r/R)\ln 2$

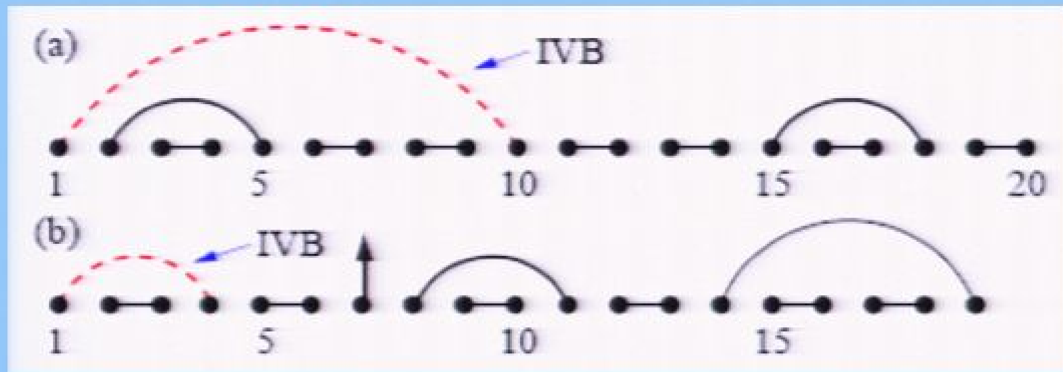
- This is approximately true



Conclusions

- Impurity entanglement entropy is a useful probe for quantum impurity problems
- S_{imp} a universal scaling function of r/ξ_K , r/R
- $\Delta S=\Delta(\ln g)=-\ln 2$ from $r<<\xi_K$ to $r>>\xi_K$
- S_{imp} is given by simple analytical expression for $\xi_K<<r$

•R/ξ_K controls strength of effective Kondo interaction (strong for $\xi_K<R$)
•Prob (IVB) versus average length of IVB trade off to produce a maximum in S_{imp} at $R\sim\xi_K$ (agrees well with DMRG data)



- Typical length of IVB is ξ_K so, for R even, S_{imp} decreases monotonically on scale ξ_K
- For R odd, there may be no IVB since there is an unpaired spin somewhere in chain
- Unpaired spin is impurity for λ=0: S_{imp}=0
- With decreasing ξ_K, (i.e. increasing λ) probability of having an IVB increases but its length (when it exists) decreases