Title: Impurity entanglement entropy and the Kondo model

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Abstract: The entanglement entropy in conformal field theory was predicted to include a boundary term which depends on the choice of conformally invariant boundary condition. We have studied this effect in the Kondo model of a magnetic impurity in a metal, which exhibits a renormalization group flow between conformally invariant fixed points.

Quantum Impurity Entanglement Entropy and the Kondo Model

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Perimeter Institute, May, 2010

Outline

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

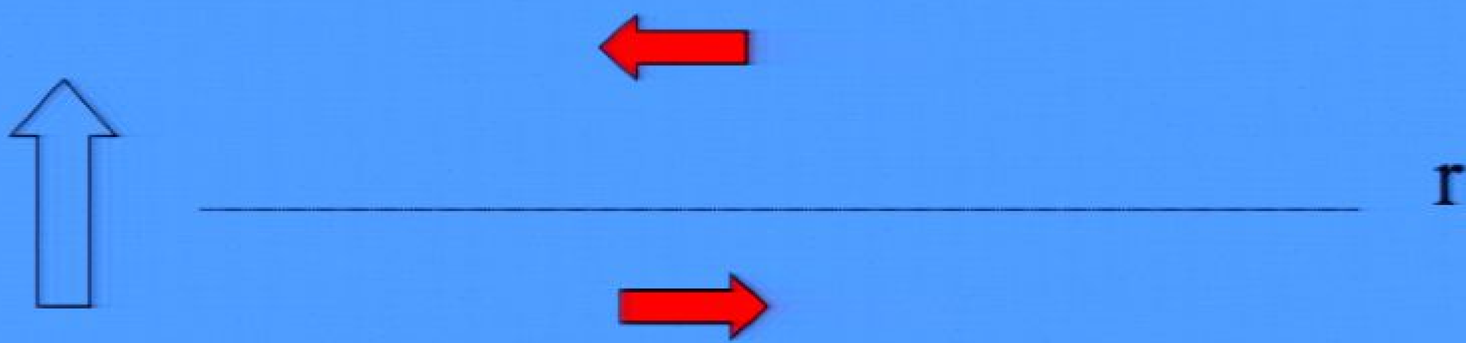
Kondo Effect & Screening Cloud

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

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

- 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:



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

- 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

$$H = H_c + H_s$$

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

$$\vec{J}_R(r) = \vec{J}_L(-r)$$

•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 • $J_K \ll J=1$

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

- 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:

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

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

• 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:

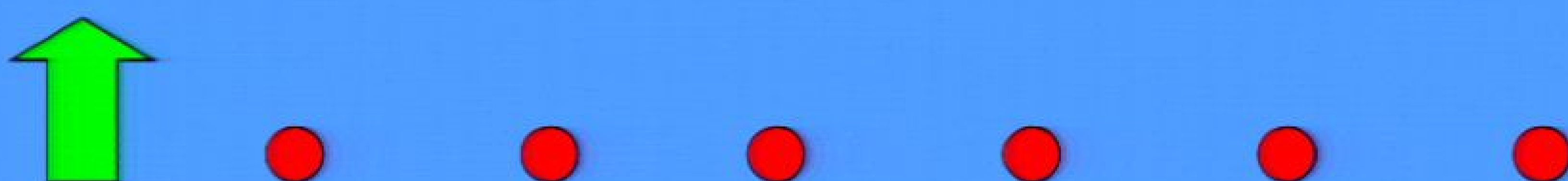
$$|k - k_F| < T_K / v_F \equiv 1/\xi_K$$

• this defines a characteristic *length scale* for the Kondo effect - typically around .1 to 1micron

- $\lambda_{eff} \to \infty$ at low energies ($<<T_K$)

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

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

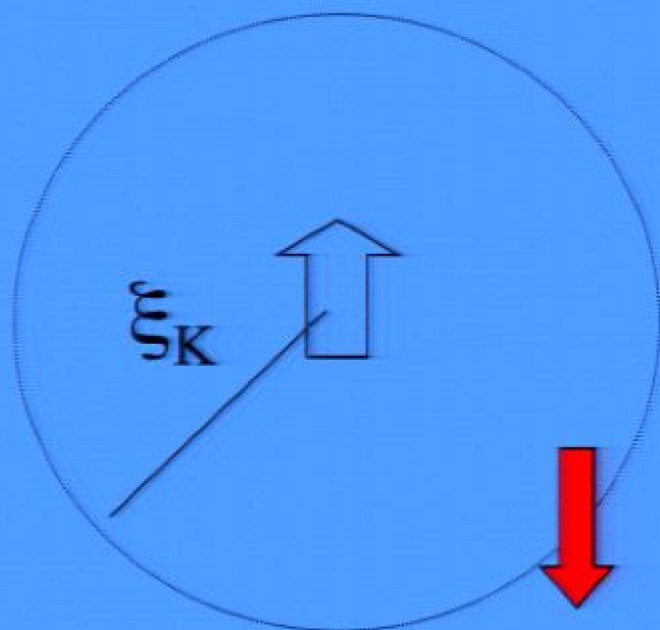


- for J>>t, we simply find ground state of last term:
- 1 electron at j=0 forms spin singlet with impurity: $|\phi_0\rangle=(|\Uparrow\downarrow\rangle-|\Downarrow\uparrow\rangle)/\sqrt{2}$

- 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

• 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)

$$H = H_c + H_s$$

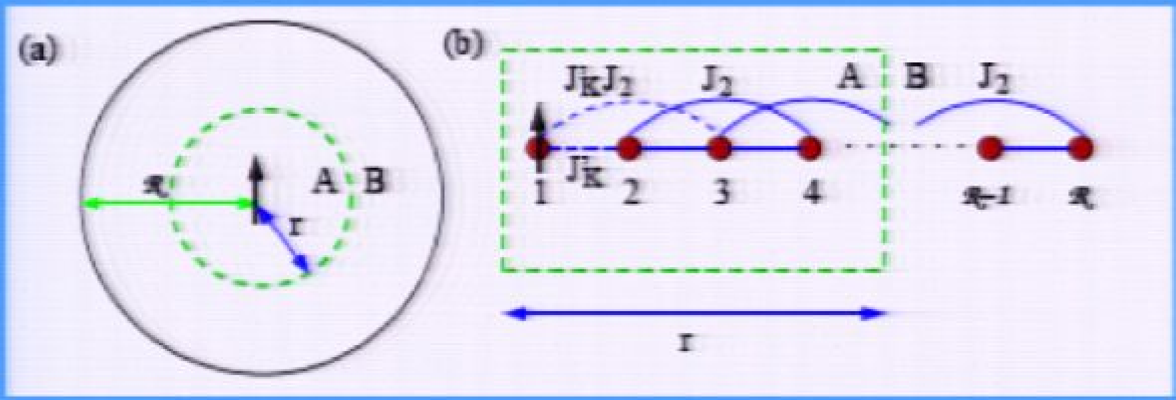
$$H_s = (v/6\pi)\left[\int dr\left[\vec{J}_L\cdot\vec{J}_L + \vec{J}_R\cdot\vec{J}_R\right] - (\xi_K/\pi)\vec{J}_L(0)\cdot\vec{J}_L(0)\right]$$

$$\vec{J}_R(r) = \vec{J}_L(-r)$$

•Leading irrelevant "Fermi liquid" type interaction has dimension 2

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

Quantum Impurity Entanglement Entropy



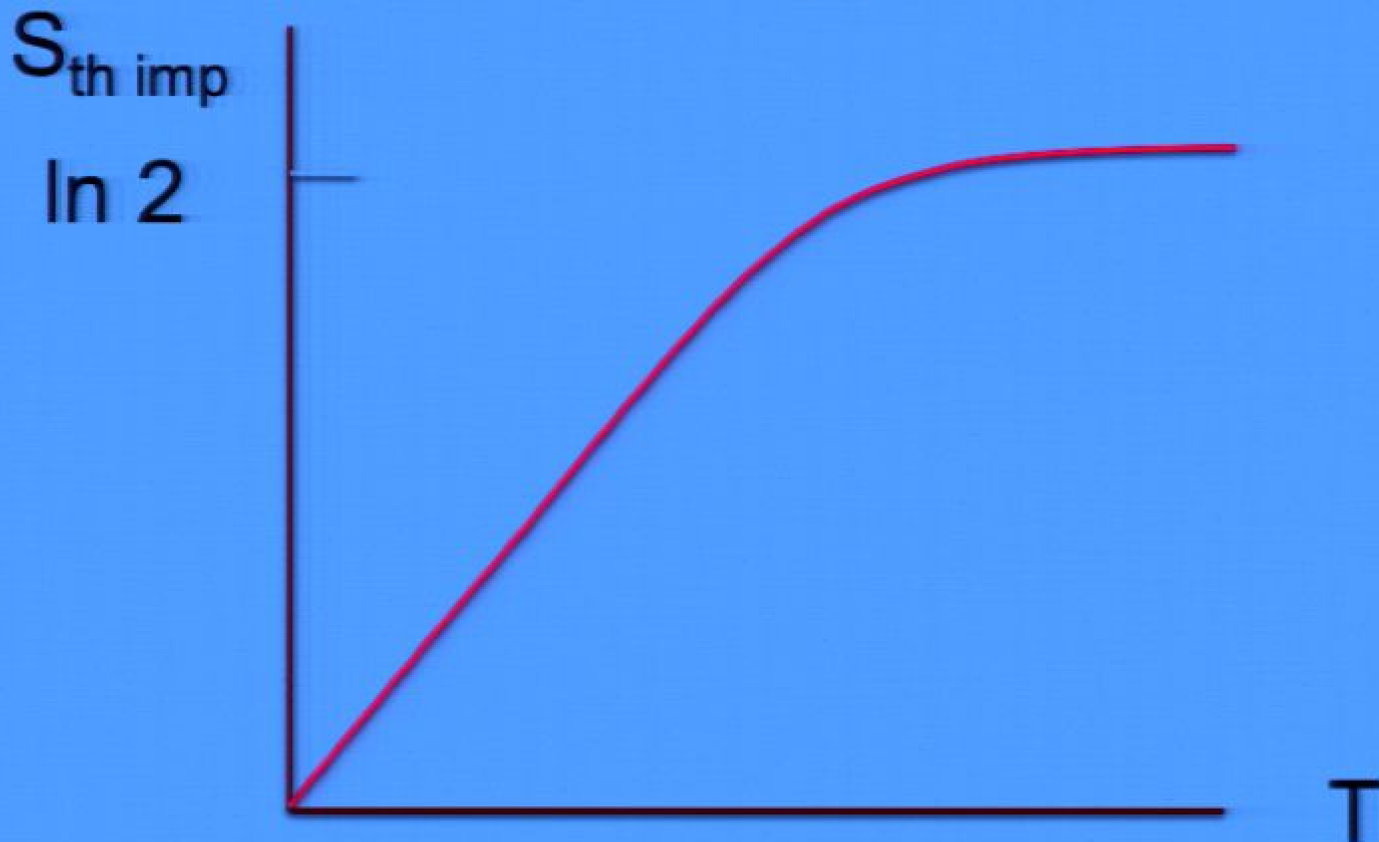
- Region A=impurity spin plus surrounding electrons (or spins) within a distance r
- Reduced density matrix, ρ, obtained from ground state by tracing out rest of system (of size R), S=-tr ρlnρ (natural logarithm)

•Cardy and Calabrese predicted that:
$S_{ent}(r)=(c/6) \ln (r/a)+\ln g$ for conformal field theory in 1D on half-line with a conformally invariant boundary condition characterized by *thermodynamic residual impurity entropy* ln g (IA& AWW Ludwig)

•i.e. if we change boundary condition, non-universal a stays the same, g changes

•For Kondo model: g=2 at weak coupling fixed point and g=1 at strong coupling fixed point

Thermal impurity entropy of Kondo model



- g=2 at T>>TK (weak coupling fixed point)
- g=1 at T=0 (strong coupling fixed point)

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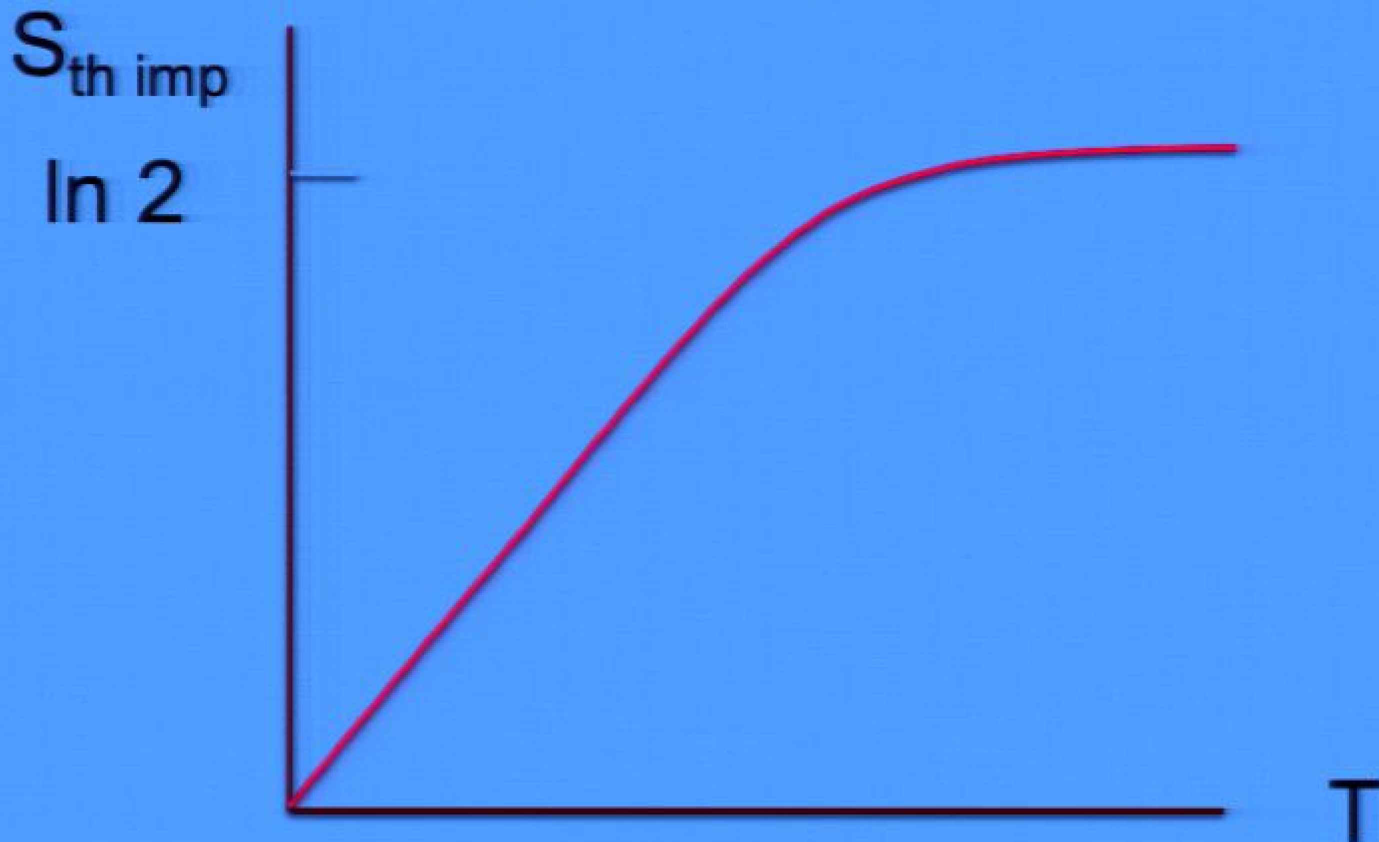

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•N.B. – most of entanglement entropy, S(r,R) is *not* due to impurity

•We are interested in *additional* entanglement entropy caused by introducing impurity

•Analogous to impurity contributions to thermodynamic quantities in Kondo model, measured by Bethe ansatz and experiments

•Technicality: spin chain (and fermion) entanglement has uniform and staggered (or $2k_F$) parts- I focus on uniform part here

•We expect this to be the same for either fermion or spin chain Kondo model

r=0 limit

Entanglement of impurity with bulk, s_{imp}, reduces to (previously studied) ground state impurity magnetization, m_{imp}: (E Sorensen &IA)

$$s_{imp} = -\sum_{\pm}(1/2 \pm m_{imp})\ln(1/2 \pm m_{imp})$$

•for R even, singlet ground state, m_{imp}=0, $\Rightarrow s_{imp}$=ln 2 (maximal entanglement)
•For R odd and a small bare J_K, m_{imp} =1/2,$s_{imp} \cong 0$ for R<<ξ_K, mimln 2 at R>>ξ_K

$$|\phi>=(|\Uparrow>\otimes|\downarrow>-|\Downarrow>\otimes|\uparrow>)/\sqrt{2}$$ (R even)

$$|\phi>=a|\Uparrow>\otimes|0>+b|\Downarrow>\otimes|1,1>$$ (R odd)

- (first factor is impurity spin, second is state of rest of system)
- Impurity magnetization and entanglement entropy can both be easily expressed in terms of parameters a and b

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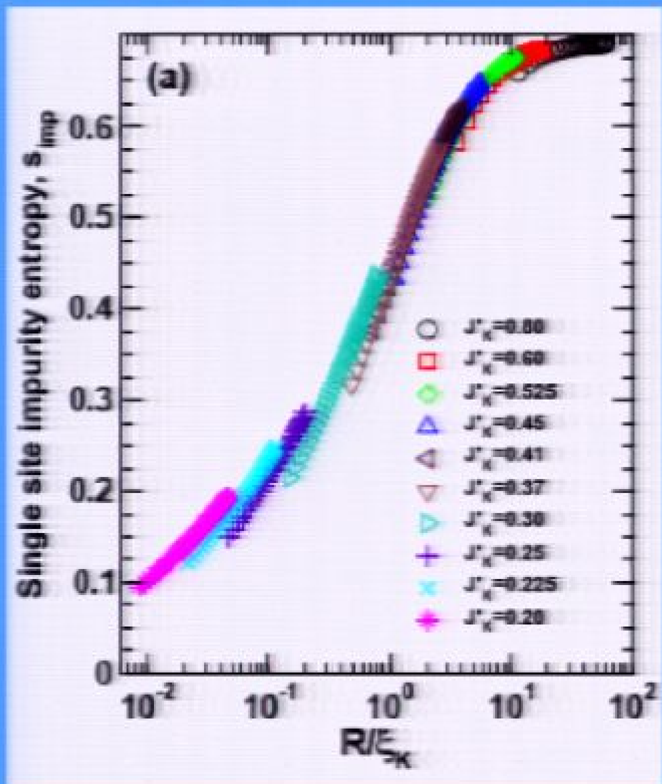


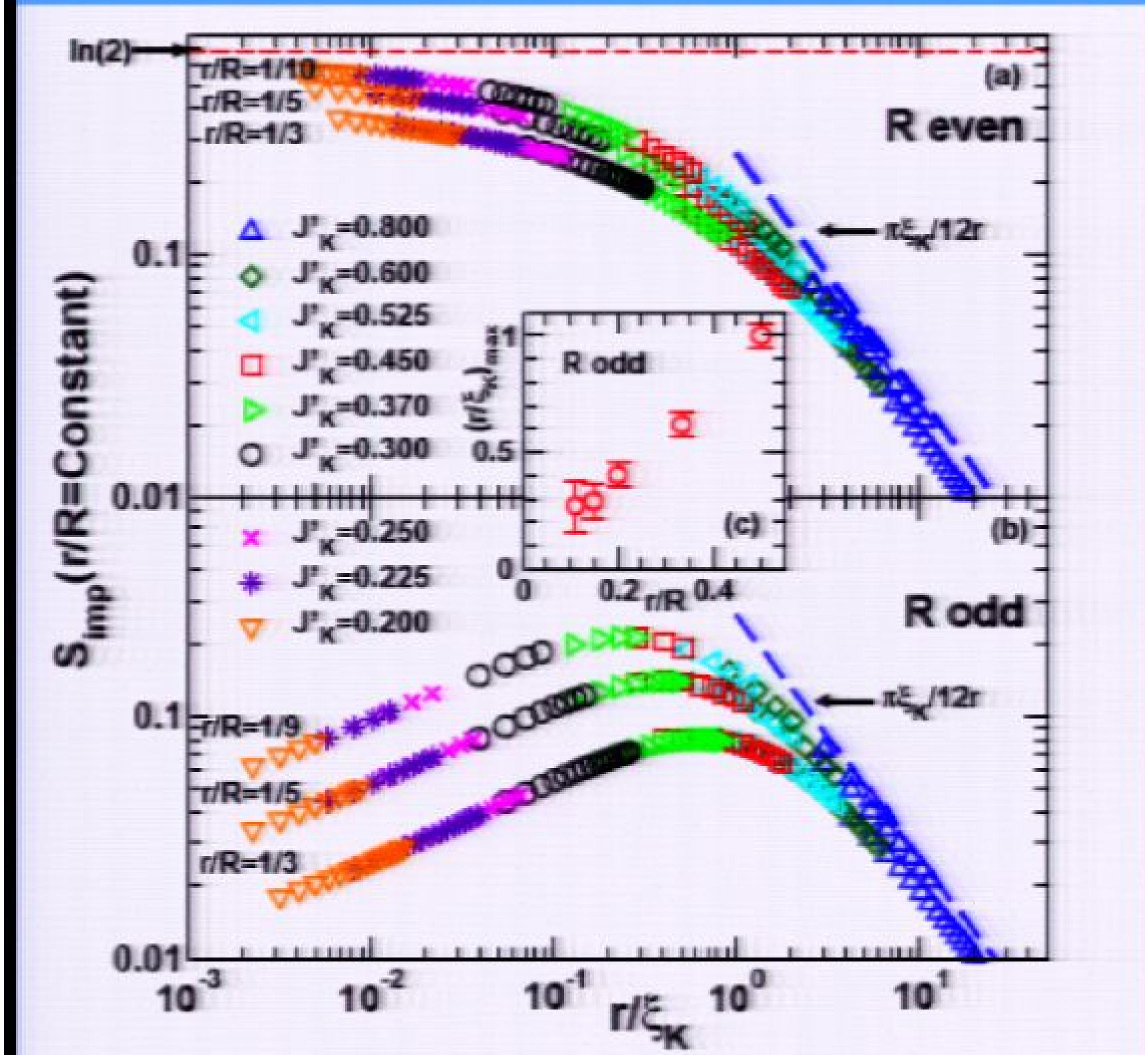
←DMRG results

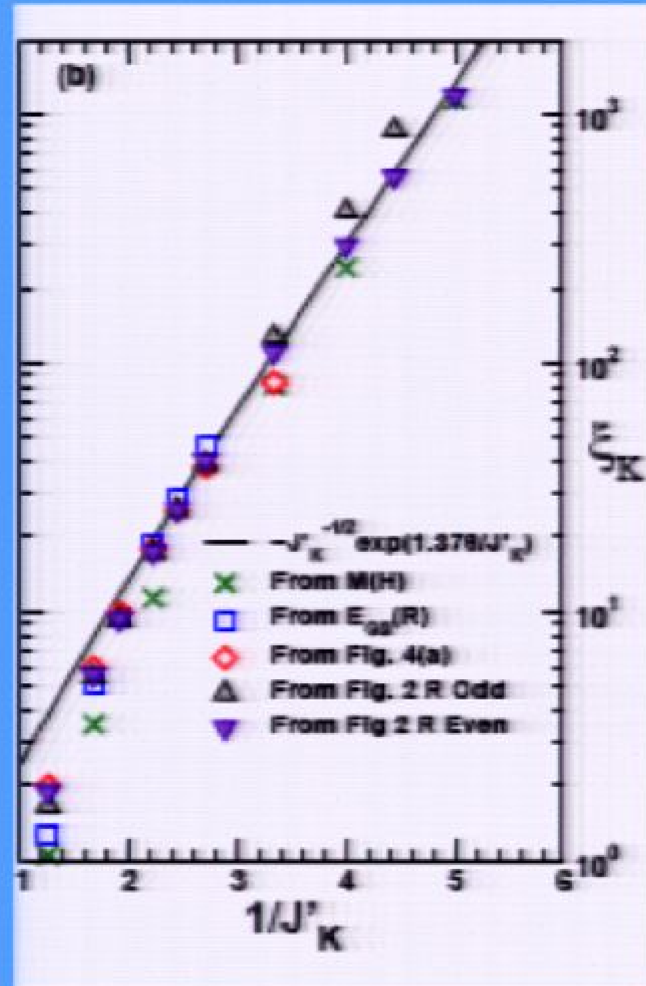
s_{imp} is *not* a pure scaling function of R/ξ_K since impurity spin operator has an anomalous dimension

• $m_{imp} \cong (1+\lambda_K{}^0/2+\ldots)f(R/\xi_K)$

• $S_{imp}(r,R)$ is different

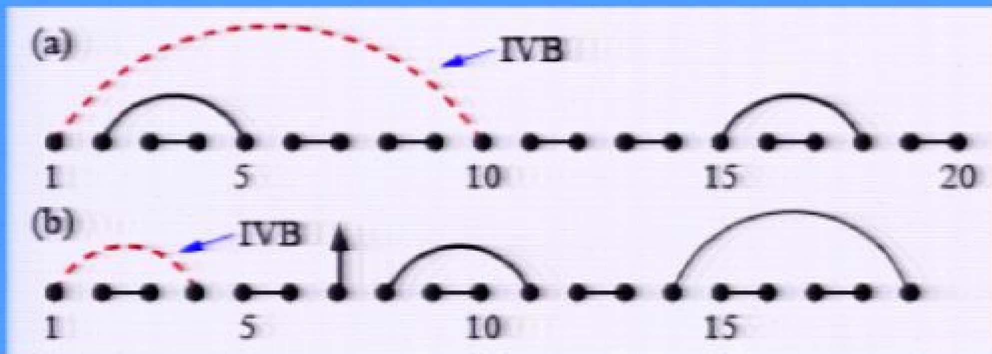
• appears to be a pure scaling function (zero anomalous dimension) for r>>1





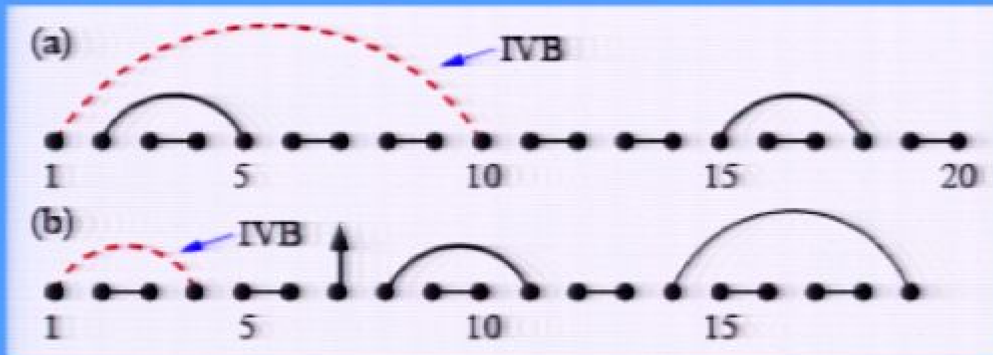
- $S_{imp}(r/R, r/\xi_K)$ scales, with expected ξ_K
- S_{imp} is different for R even/odd
- Large r/ξ_K limit the same, given by CFT

Intuitive Picture



•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)



(R even)

(Rodd)

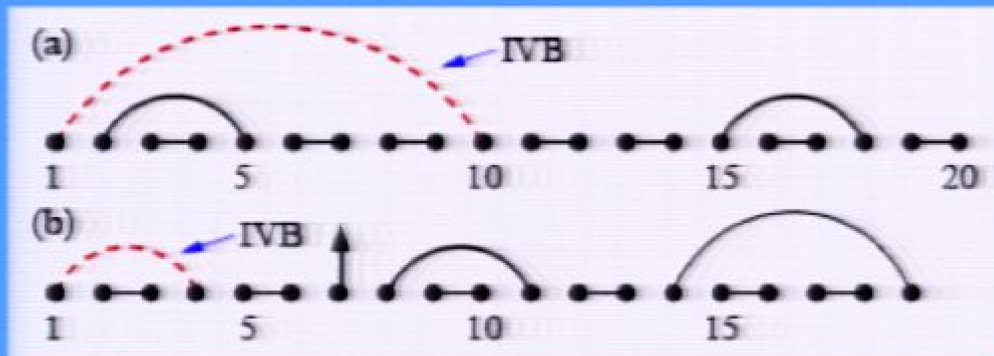
- Typical length of IVB is ξ_K so, for R even, S_{imp} decreases monotonically with r on scale ξ_K
- For R odd, there may be no IVB since there is an unpaired spin somewhere in chain
- Unpaired spin is impurity for λ=0: S_{imp}=0
- With decreasing ξ_K, (i.e. increasing λ) probability of having an IVB 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}, for fixed r/R, at $R\sim\xi_K$ (agrees well with DMRG data)

•For $R>>r$, ξ_K, $S_{imp} \to S_{imp}(r/\xi_K)$, the same universal function for R even or odd

•$S_{imp}(r/\xi_K)$ decreases from ln 2 at $r<<\xi_K$ to 0 at $r>>\xi_K$ as predicted by Cardy and Calabrese



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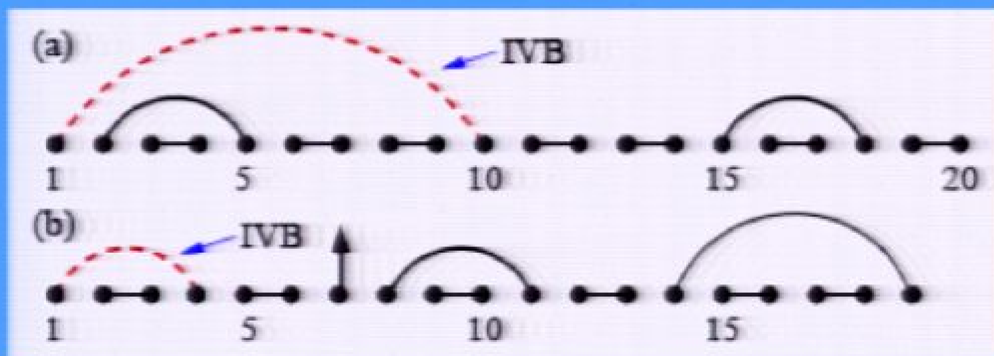

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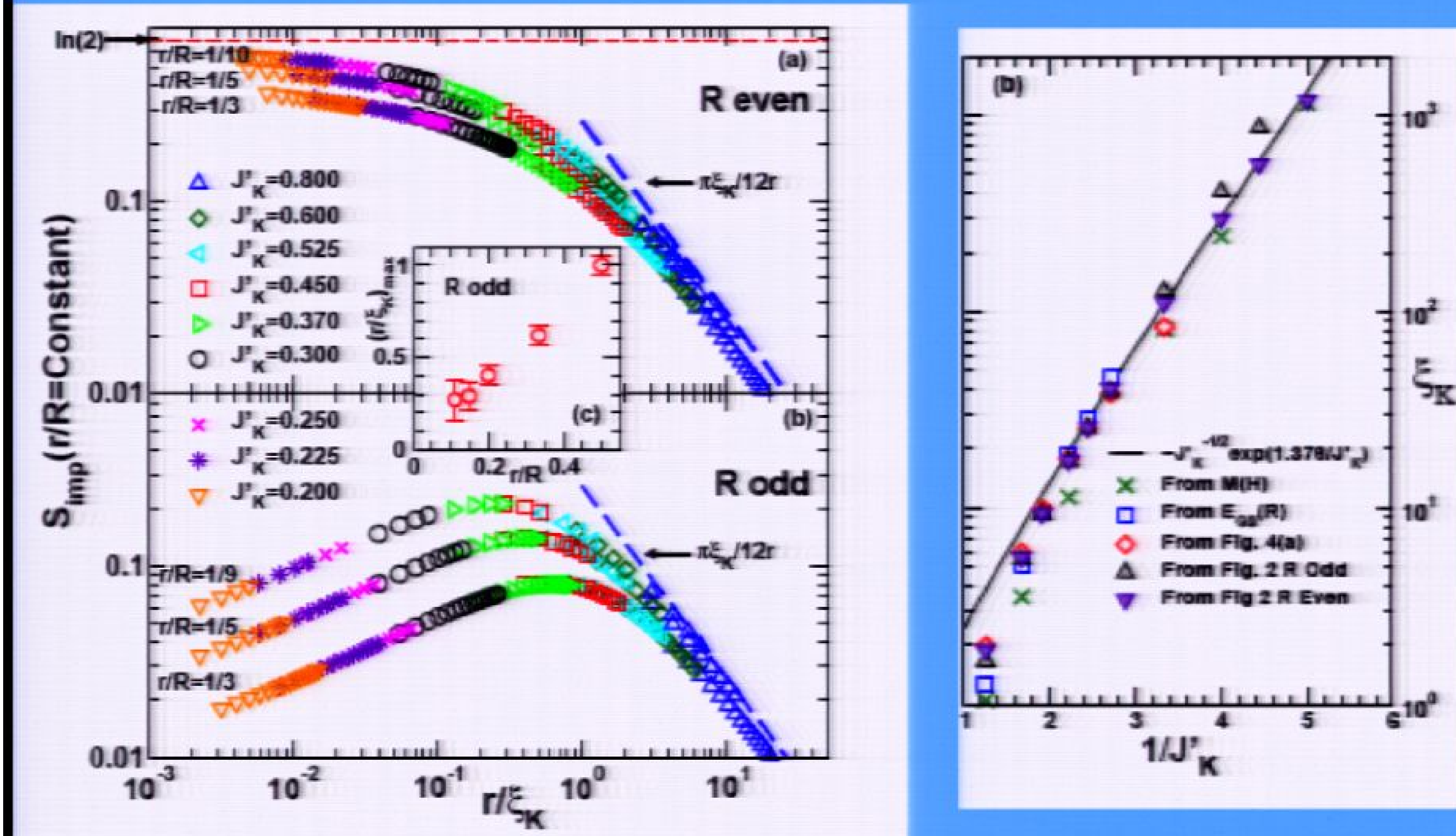

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•We can find a simple analytic expression for S_{imp} when ξ_K<<r by doing lowest order perturbation theory in Fermi liquid interaction

$$H_s = (v/6\pi)\int dr \left[\vec{J}_L\cdot\vec{J}_L + \vec{J}_R\cdot\vec{J}_R\right] + (v\xi_K/6\pi^2)\vec{J}_L(0)\cdot\vec{J}_L(0)$$

•Will give $S_{imp} \propto \xi_K/r$

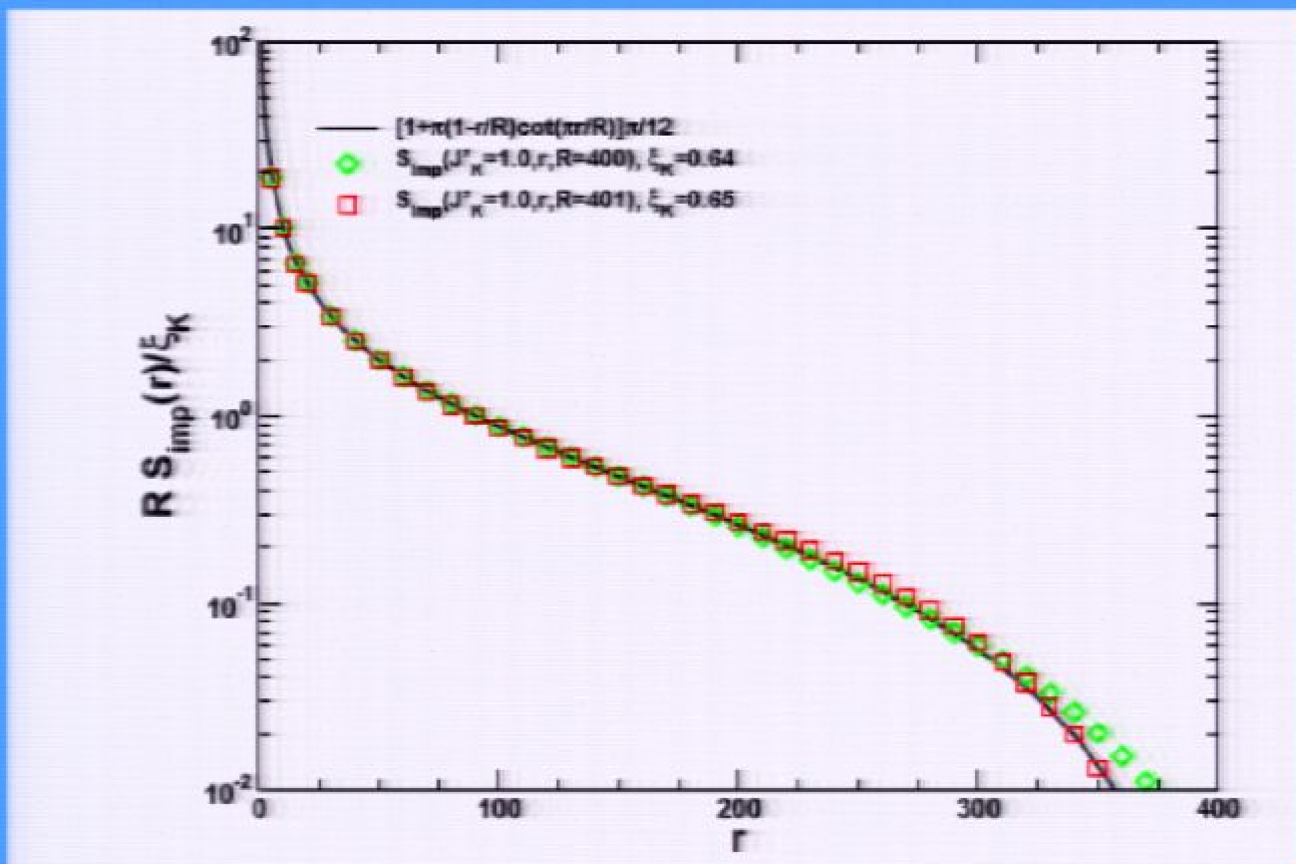
•Following Cardy and Calabrese, S is obtained from partition function Z_n on n-sheeted Riemann surface with sheets joined along cut from 0 to r, using replica trick (n→1)

- 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 ξ_K<<r

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

This agrees very 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 $r>>\xi_K$
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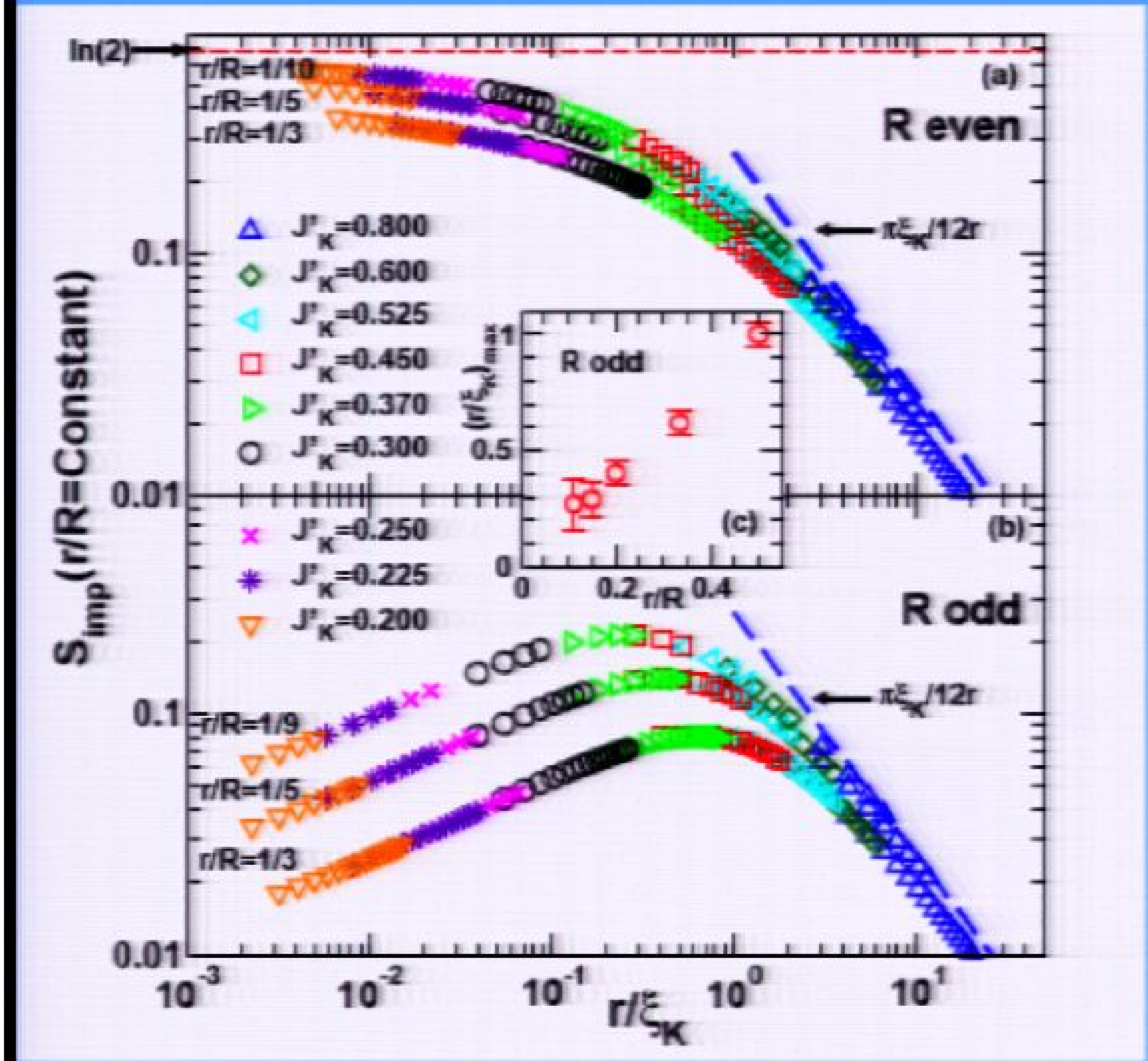

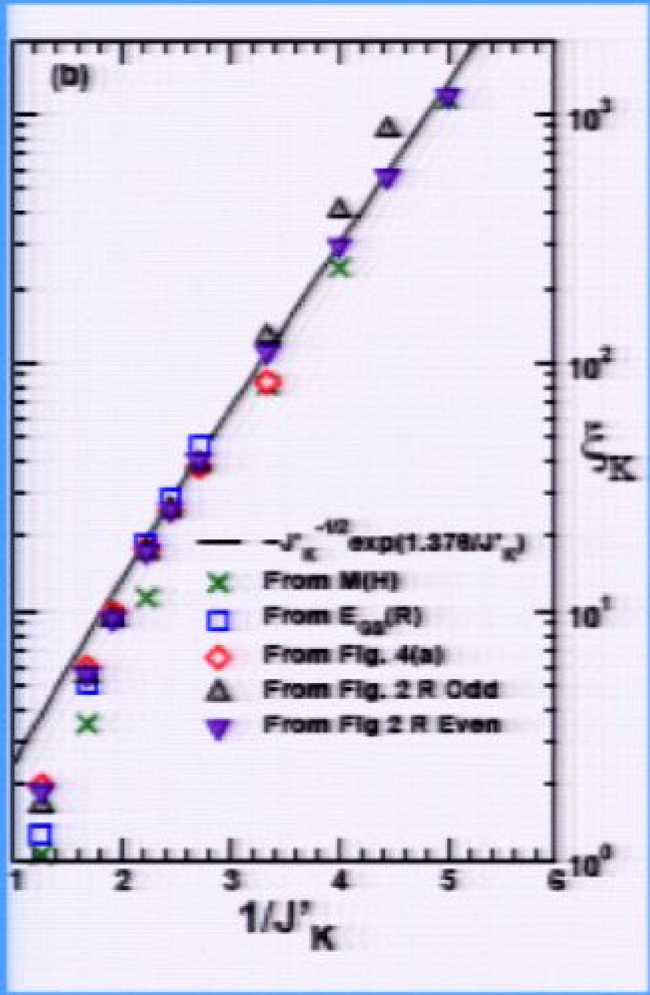

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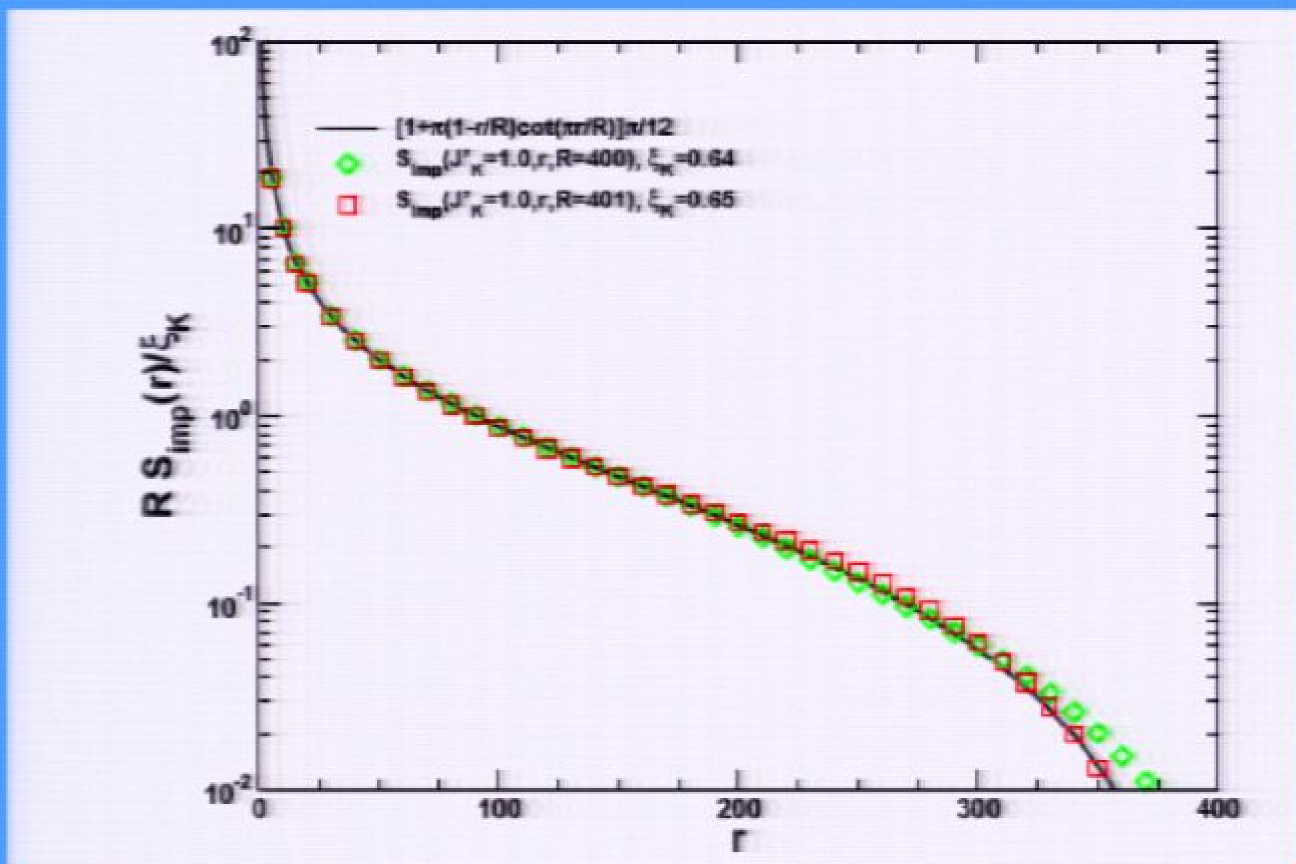

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