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## Entanglement Probe of Two-Impurity Kondo Physics in a Spin Chain

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in collaboration with

Abolfazl Bayat (Universität Ulm & UCL) Sougato Bose (UCL) Pasquale Sodano (University of Perugia & IIP)



# Outline

Background...

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Basics on two-impurity Kondo model

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Realization in the lab: double-quantum dot systems

Basics on two-impurity Kondo model

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#### Applications: two-qubit gates for quantum computing?

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## A new view through quantum entanglement...

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Spin chain modeling

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Negativity and von Neumann entropy from DMRG

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Results: Entanglement structure, Kondo cloud, and more...

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# A new view through quantum entanglement... Spin chain modeling

Negativity and von Neumann entropy from DMRG

Results: Entanglement structure, Kondo cloud, and more...

from J. Ziman, "The Principles of the Theory of Solids"







 $H_{\rm RKKY}$ \_



$$H_{ ext{el-imp}} = JS \cdot \sigma$$
  
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#### $H = H_{\rm kin} + J \boldsymbol{S}_1 \cdot \boldsymbol{\sigma} + J \boldsymbol{S}_2 \cdot \boldsymbol{\sigma} + K(R) \boldsymbol{S}_1 \cdot \boldsymbol{S}_2$

VOLUME 47, NUMBER 10

PHYSICAL REVIEW LETTERS

7 September 1981

#### **Two-Impurity Kondo Problem**

C. Jayaprakash

Nordisk Institut for Teoretisk Atomfsyik, DK-2100 Copenhagen Ø, Denmark, and Department of Physics, Cornell University, Ithaca, New York 14853

and

H. R. Krishna-murthy Nordisk Institut for Teoretisk Atomfsyik, DK-2100 Copenhagen Ø, Denmark, and Department of Physics, Indian Institute of Science, Bangalore, India

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J. W. Wilkins Nordisk Institut for Teoretisk Atomfsyik, DK-2100 Copenhagen Ø, Denmark, and Department of Physics, Cornell University, Ithaca, New York 14853 (Received 28 May 1981)

The two-impurity Kondo problem is studied by use of perturbative scaling techniques. The physics is determined by the interplay between the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction between the two impurity spins and the Kondo effect. In particular, for a strong ferromagnetic RKKY interaction the susceptibility exhibits three structures as the temperature is lowered, corresponding to the ferromagnetic locking together of the two impurity spins followed by a two-stage freezing out of their local moments by the conduction electrons due to the Kondo effect. competition between RKKYinteraction and Kondo screening

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> RKKY-coupled spin-singlet, no Kondo screening

 $K(R) \to -\infty$ 

### $H = H_{\rm kin} + JS_1 \cdot \boldsymbol{\sigma} + JS_2 \cdot \boldsymbol{\sigma} + K(R)S_1 \cdot S_2$

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competition between RKKYinteraction and Kondo screening!

RKKY-coupled spin-triplet, Kondo screened by conduction electrons RKKY-coupled spin-singlet, no Kondo screening

 $K(R) \to -\infty$ 

$$\delta=\pi/2$$
 P. Nozières and A. Blandin, J. Phys. (Paris) 41, 193 (1980)

 $\delta = 0$ 

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 $K(R) \to -\infty$ 

particle-hole symmetry  $\longrightarrow \delta = 0$  or  $\delta = \pi/2$ 

A. Millis et al. Field Theories in Condensed Matter Physics ed. Z. Tesanovic, 1990

 $\delta = \pi/2$ 

RKKY-coupled spin-triplet, Kondo screened by conduction electrons  $\delta = 0$ 

RKKY-coupled spin-singlet, no Kondo screening

 $K(R) \to -\infty$ 



 $K(R) \to \infty$ 

 $K(R) \to -\infty$ 

T



## At the quantum critical point...



$$\frac{C_{\rm imp}}{T} = \gamma \mathop{\longrightarrow}_{T \to 0} \frac{T_K}{(K - K_c)^2}$$

$$S_{\rm imp} \equiv \lim_{T \to 0} \lim_{L \to \infty} [S(L,T) - S_0(L,T)] = \ln \sqrt{2}$$

۰:

I.Affleck et al., PRB 52, 9528 (1995)

"fractional ground state degeneracy"  $g^A = \sqrt{2}$ 

$$G \approx G_0(1 - \lambda_1 T^{1/2})$$

G. Zaránd et al., PRL 97, 166802 (2006)

## Realization in double quantum-dot systems









**RKKY coupling**  $K(R) \propto (J^2/R^2) \cos(k_F R)$ 



**RKKY** coupling  $K(R) \propto (J^2/R^2) \cos(k_F R)$ 

Kondo temperature  $T_K \propto D \exp(-1/\pi \rho J)$ 











#### $H_{\text{int}} = J_1 S_1 \cdot \boldsymbol{\sigma}_1 + J_2 S_2 \cdot \boldsymbol{\sigma}_2 + K(R) S_1 \cdot S_2$

No transfer of electrons between 1 and 2: quantum critical point  $K_c \approx 2.2T_K$  is stable against electron-hole symmetry breaking and breaking of parity

G. Zaránd et al., PRL 97, 166802 (2006)

### Realization in double quantum-dot systems

N. J. Craig et al., Science 304, 565 (2004)





## Realization in double quantum-dot systems

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#### Nota Bene:

The central dot supports both RKKY and Kondo screening. This experiment does *not* probe quantum criticality. Instead, **important for proving gate-controlled RKKY!** 



### *Possible application* "Long-distance" control of two-qubit gates...



$$H_{s}(t) = J(t)\vec{S}_{1}\cdot\vec{S}_{2}$$
$$U_{s}(t) = T \exp\{-i\int_{0}^{t}H_{s}(t')dt'\}$$
$$U_{s}(\tau_{s} = \pi\hbar/J_{0}) = U_{sw}$$
$$U_{sw} \mid ij \rangle = \mid ji \rangle, \quad i, j = \uparrow, \downarrow$$

Loss–DiVincenzo proposal for spin-based quantum computing

PRA 57, 120 (1998)

#### *Possible application* "Long-distance" control of two-qubit gates...



Loss–DiVincenzo proposal for spin-based quantum computing

PRA 57, 120 (1998)



 $U_{\rm CNOT}$  + "single-qubit gates" (single-spin rotations)

"universal" quantum computing
"Long-distance" control of two-qubit gates...?







N. J. Craig *et al.*, Science **304**, 565 (2004) M.G.Vavilov and L.I. Glazman, PRL **94**, 086805 (2005)



N. J. Craig *et al.*, Science **304**, 565 (2004) M.G.Vavilov and L.I. Glazman, PRL **94**, 086805 (2005) What about *spin decoherence* caused by the conduction electrons via RKKY?



Y. Rikitake and H. Imamura, PRB 72, 033308 (2005)



Quantum information processing requires **entanglement** of qubits. What about the competition from Kondo screening?

N. J. Craig et al., Science **304**, 565 (2004) M.G. Vavilov and L.I. Glazman, PRL **94**, 086805 (2005)

Quantum information processing requires **entanglement** of qubits. What about the competition from Kondo screening?

A dual scenario: nonlocal control of two-qubit entanglement from Kondo screening + quantum **quench...** P. Sodano, A. Bayat, and S. Bose, PRB **81**, 100412 (2010)

N. J. Craig *et al.*, Science **304**, 565 (2004) M.G.Vavilov and L.I. Glazman, PRL **94**, 086805 (2005) Quantum entanglement probe of the two-impurity Kondo groundstates for different RKKY couplings

### Quantum entanglement probe of the two-impurity Kondo groundstates for different RKKY couplings

S.Y. Cho and R. H. McKenzie, PRA **73**, 012109 (2006) A. Ramsak *et al.*, PRB **74**, 241305 (2006)

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A. Bayat, S. Bose, P. Sodano, H.J., PRL 109, 066403 (2012)

How is entanglement distributed between impurities and electrons? Is there an RKKY threshold for impurity-bulk decoupling? How does entanglement behave at the quantum critical point? What can we learn about the *Kondo screening cloud*? and more....

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#### A. Bayat, S. Bose, P. Sodano, H.J., PRL 109, 066403 (2012)

How is entanglement distributed between impurities and electrons?

How to make the impurities decouple from the bulk?

How does entanglement behave at the quantum critical point?

What can we learn about the Kondo screening cloud?

Method: DMRG computation of *negativity* and *von Neumann entropy* via a spin chain emulation of the two-impurity Kondo model

## Spin chain modeling useful for DMRG and intuition!

start with the single-impurity Kondo model

 $H = \int \mathrm{d}^{3} \boldsymbol{r} [\psi^{\dagger} (-\nabla^{2}/2m)\psi + J_{K}\delta^{3}(0)\psi^{\dagger}\boldsymbol{\sigma}\psi \cdot \boldsymbol{S}_{\mathrm{imp}}]$ 

# Spin chain modeling useful for DMRG and intuition...

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## Spin chain modeling useful for DMRG and intuition...

start with the single-impurity Kondo model



## Spin chain modeling useful for DMRG and intuition...

start with the single-impurity Kondo model



This is the low-energy effective theory of a spin chain with a weak boundary link!



$$H = J_1 \sum_{i=2}^{N-1} S_i \cdot S_{i+1} + J' J_1 S_1 \cdot S_2 \quad J' < 1$$

Jordan-Wigner + bosonization

 $m{S}_i = m{J}_L(ai) + m{J}_R(ai) + (-1)^i ext{constant} \cdot m{n}(ai)$ = lattice spacing + continuum limit

$$H_{\rm spin} = \frac{v_F}{6\pi} \int_0^\infty dx (\boldsymbol{J}_L \cdot \boldsymbol{J}_L + \boldsymbol{J}_R \cdot \boldsymbol{J}_R) + v_F \lambda \boldsymbol{J}_L(0) \cdot \boldsymbol{S}_{\rm imp}$$

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+ marginally irrelevant + irrelevant terms



+ marginally irrelevant + irrelevant terms

S. Eggert, PRB 54, 9616(R) (1996)

$$H = \sum_{j=1}^{2} J_j \left( J' \boldsymbol{S}_1 \cdot \boldsymbol{S}_{j+1} + \sum_{i=2}^{N-j} \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+j} \right)$$

same low-energy physics as the (spin sector) of the single-impurity Kondo model

S. Rommer and S. Eggert, PRB **62**, 4370 (2000) N. Laflorencie *et al.*, J. Stat. Mech. P02007 (2008)

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### Implication for two-impurity Kondo model?



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### Implication for two-impurity Kondo model?



two RKKY-coupled 'Kondo spin chains' (a.k.a. 'two-impurity Kondo chain')

#### 'Two-impurity Kondo spin chain'



Well adapted for DMRG... and entanglement probes!





John von Neumann in the 1940s

von Neumann entropy

 $S_A = -\mathrm{Tr}\rho_A \log_2 \rho_A$ 

 $\rho_A = \mathrm{Tr}_B |\Psi\rangle \langle \Psi|$ 





Computable entanglement measure for this case: *Negativity* 

В

Α

G.Vidal and R.F. Werner, PRA **65**, 032314 (2002)

$$\mathcal{N}(\rho_{AB}) = \sum_{i} |a_{i}| - 1$$
$$a_{i} \text{ eigenvalues of } \rho_{AB}^{T^{A}}$$
$$\rho_{AB} = \operatorname{Tr}_{(AB)^{c}} |\Psi\rangle\langle\Psi|$$

Computable entanglement measure for this case: *Negativity* 

B



Α

$$\begin{split} \mathcal{N}(\rho_{AB}) &= \sum_{i} |a_{i}| - 1\\ a_{i} \text{ negative eigenvalues of } \rho_{AB}^{T^{A}}\\ \rho_{AB} &= \operatorname{Tr}_{(AB)^{c}} |\Psi\rangle \langle \Psi| \end{split}$$

First-time (?) application in condensed matter: Entanglement probe of (single-impurity) Kondo chain



A. Bayat, P. Sodano, and S. Bose, PRB 81, 064429 (2010)

Using negativity (and von Neumann entropy!) to explore the entanglement properties of the **two-impurity Kondo chain** with DMRG...

What do we learn?

negativity for two qubits in a Werner state = concurrence

Entanglement between the two impurities





**Entanglement between the two impurities** R0 0 0.8 J'=0.4 0 N(1<sub>L</sub>,1<sub>R</sub>) J'=0.5 0 0.6 J'=0.6 0 0 0.4 0.2 0 0-2-1.5-1-0.5 Q.5 1.5 2 0 1 J  $J_I^c$  "quantum critical point...!" S.Y. Cho and R. H. McKenzie, PRA 73, 012109 (2006)

•

negativity for two qubits in a Werner state = concurrence



- Signature of the quantum phase transition at  $J_1^c$ 



- Signature of the quantum phase transition at  $J_1^{\,c}$ 



• Signature of the quantum phase transition at  $J_1^c$ 



Entanglement structure





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. . .


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Background: single-impurity Kondo model...

One-loop RG equations: 
$$\frac{d\lambda}{d\ln D} = -\nu\lambda^2 + \dots$$

effective scale-dependent coupling  $\lambda$  becomes of  $\mathcal{O}(1)$  at

$$T_K = D_0 \exp(-\text{const.}/\lambda_0)$$

Background: single-impurity Kondo model...

1-loop RG equations: 
$$\frac{d\lambda}{d\ln D} = -\nu\lambda^2 + ...$$

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$$T_K = D_0 \exp(-\text{const.}/\lambda_0)$$

 $\mathbf{\xi}_{K} = \frac{v_{F}}{T_{K}}$  dynamically generated energy scale KONPO TEMPERATURE

> dynamically generated length scale: KONDO SCREENING LENGTH

Heuristics: single-impurity Kondo model...



Heuristics: single-impurity Kondo model...



Heuristics: single-impurity Kondo model...



Theoretical construct.... ...so far no experimental signal...

Does the Kondo cloud really exist?

... and what about the two-impurity Kondo model?



... and what about the two-impurity Kondo model?



Entanglement probe:

- Trace out, compute the negativity between the impurities and the rest of the system
- Define  $\xi_E \equiv$  length beyond which the negativity is smaller than some cutoff (here, = 0.01)





![](_page_83_Figure_1.jpeg)

![](_page_84_Figure_1.jpeg)

![](_page_85_Figure_1.jpeg)

Kondo resonance narrowing

![](_page_86_Figure_1.jpeg)

Experiments indicate that the width of the Kondo resonance narrows with larger impurity spin (at exact screening)

M.D. Daybell and W.A. Steyert, RMP 40, 380 (1968)

Perturbative scaling theory suggests

 $T_K = D_0 \exp(-2S \times \text{const.}/\lambda_0)$ 

A. H. Nevidomskyy and P. Coleman, PRL 103, 147205 (2009)

Kondo resonance narrowing

![](_page_87_Figure_1.jpeg)

$$\xi_K \sim \exp(\alpha(J_I)/J')$$

$J_I$	-3.00	-2.50	-2.00	-1.50	-1.00	-0.50	0.00
$\alpha(J_I)$	) 3.2175	3.1407	2.9403	2.6838	2.3106	2.0718	1.7686

$$\rightarrow \alpha(-\infty) \approx 2.5\alpha(0)$$

Nevidomskyy-Coleman predicts

 $\alpha(-\infty) = 2\alpha(0)$ 

• Effective decoupling of impurities

![](_page_88_Figure_1.jpeg)

$$\begin{aligned} H_{I}^{eff} &= \frac{J'^{2}J_{1}}{2J_{I}}\boldsymbol{S}_{2}^{L}\cdot\boldsymbol{S}_{2}^{R} + \frac{J'^{2}J_{2}}{2J_{I}J_{1}}\boldsymbol{S}_{3}^{L}\cdot\boldsymbol{S}_{3}^{R} \\ &+ \frac{J'^{2}J_{2}}{2J_{I}}(\boldsymbol{S}_{2}^{L}\cdot\boldsymbol{S}_{3}^{L} + \boldsymbol{S}_{2}^{R}\cdot\boldsymbol{S}_{3}^{R} - \boldsymbol{S}_{2}^{R}\cdot\boldsymbol{S}_{3}^{L} - \boldsymbol{S}_{2}^{L}\cdot\boldsymbol{S}_{3}^{R}) \end{aligned}$$

Effective decoupling of impurities

![](_page_89_Figure_1.jpeg)

effective impurity-bulk decoupling already for intermediate values of RKKY

## Summary

Two-impurity Kondo model, DMRG entanglement probe A. Bayat, S. Bose, P. Sodano, H.J., PRL **109**, 066403 (2012)

- nonperturbative diagnostic of Kondo-RKKY quantum phase transition
- Kondo cloud reconstruction for any (subcritical) RKKY and Kondo couplings
- test of Kondo resonance narrowing
- quantitative measure of impurity-bulk decoupling
- entanglement spectrum work in progress
- negativity scaling work in progress