Impurity quantum phase transitions: a quantum information perspective

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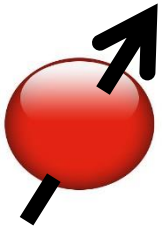
Quantum entanglement

0 or 1



$$\alpha|0\rangle + \beta|1\rangle$$

0 & 1

Two particles (entangled)

$$|\psi\rangle_{AB} = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$$

$$S_{AB} = 0$$

$$\rho_A = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|$$

$$S_A = 1$$

- **Full information about the whole system**
- **No information about the subsystem**

Entanglement is a resource

Quantum computing:

- **far beyond the best current supercomputers**

Quantum communication:

- **Absolute secure communication (banks & military)**

Quantum sensing:

- **Magnetic sensors (military)**
- **Gravity sensors (oil and mining industries)**

Quantum chemistry:

- **efficient solar cells**
- **Personalized medicine**

Delicate entanglement: no free lunch

$$|\psi\rangle_{AB} = \frac{|00\rangle + |11\rangle}{\sqrt{2}} \xrightarrow{\text{Decoherence}} \rho_{AB} = \frac{1}{2}|00\rangle\langle 00| + \frac{1}{2}|11\rangle\langle 11|$$

Challenges:

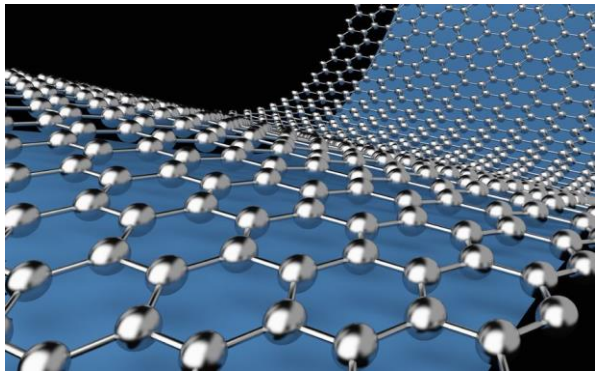
- **Generation**
- **Manipulation**
- **Preservation**

→

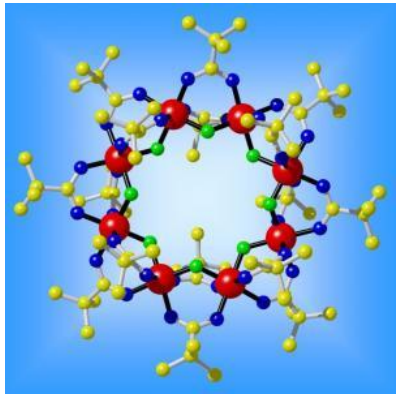
- **Low temperatures**
- **Ultra dilute vacuum**
- **Excellent isolation**

Nature is generous

Strongly correlated many-body systems are highly entangled



Graphene

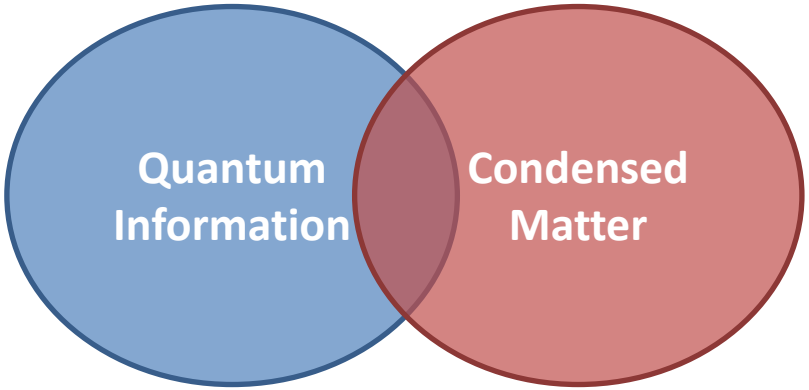


Molecular magnets

Solar cells

Can we use the freely available intrinsic entanglement of many-body systems for useful tasks?

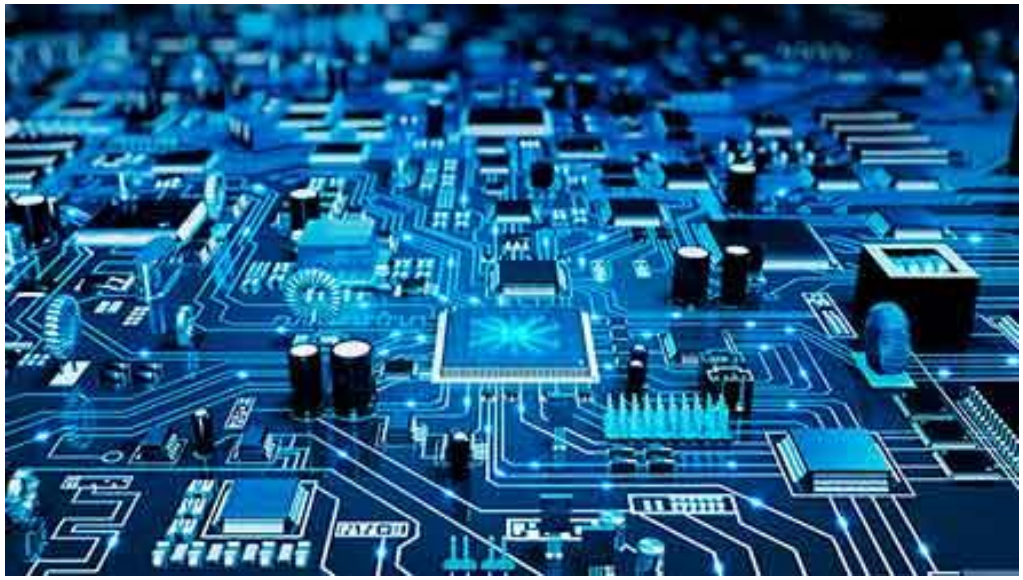
Contents of the talk

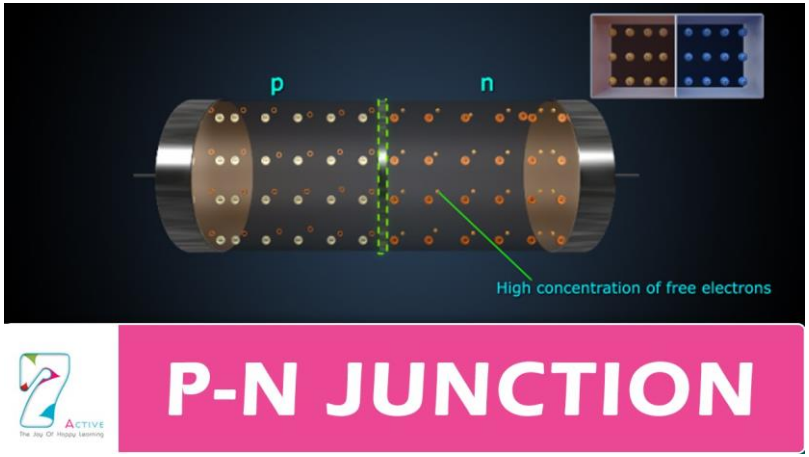


- Impurity quantum phase transitions
- Schmidt gap as an order parameter
- Bipartite entanglement: negativity
- Tri-partite entanglement
- Non-equilibrium dynamics near criticality

Impurity systems

Our technology is based on impurities

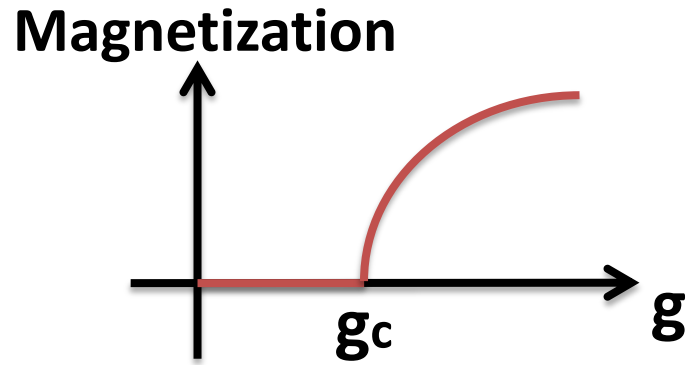




Even a single impurity can change the properties of a material

Quantum Phase Transitions (T=0)

Quantum: $H(g), |GS(g)\rangle$



Landau-Ginzburg paradigm order parameter:

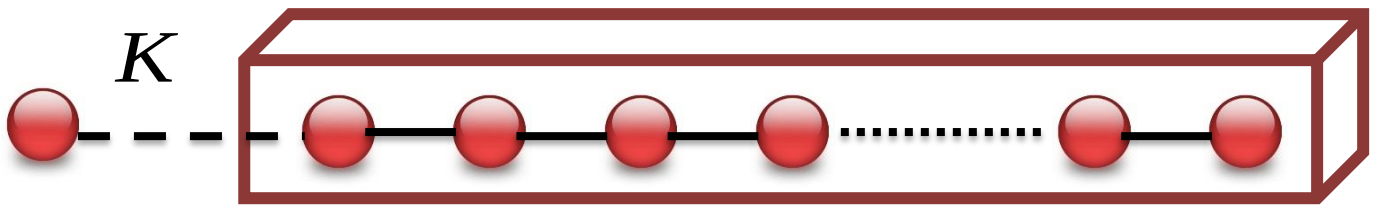
1- is local
2- is associated with a spontaneous symmetry breaking
3- scales near criticality

Bulk vs. Boundary QPT

Bulk phase transition: a global parameter induces the QPT

$$H_{Ising} = \sum_i \sigma_z^i \sigma_z^{i+1} + B \sum_i \sigma_x^i$$

Boundary phase transition: a local parameter induces the QPT

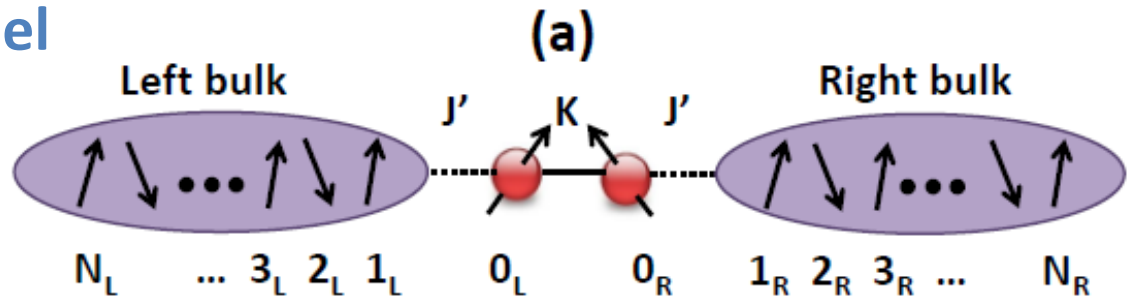


- **There is no order parameter (either local or non-local)**
- **There is no spontaneous symmetry breaking**

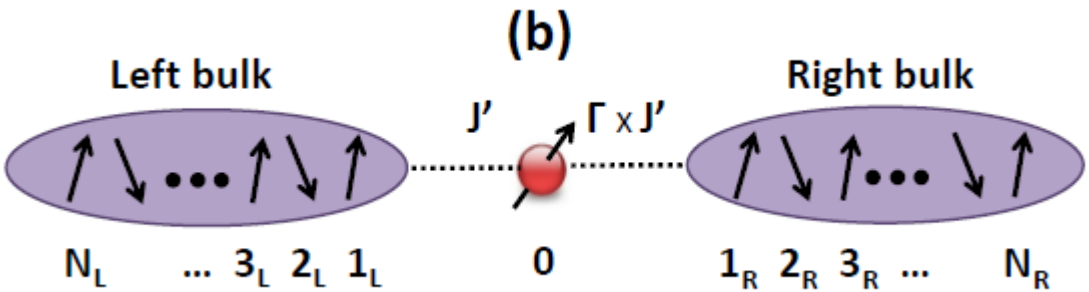
A new machinery needed to address impurity quantum phase transitions!!

Impurity models

- 2-impurity Kondo model

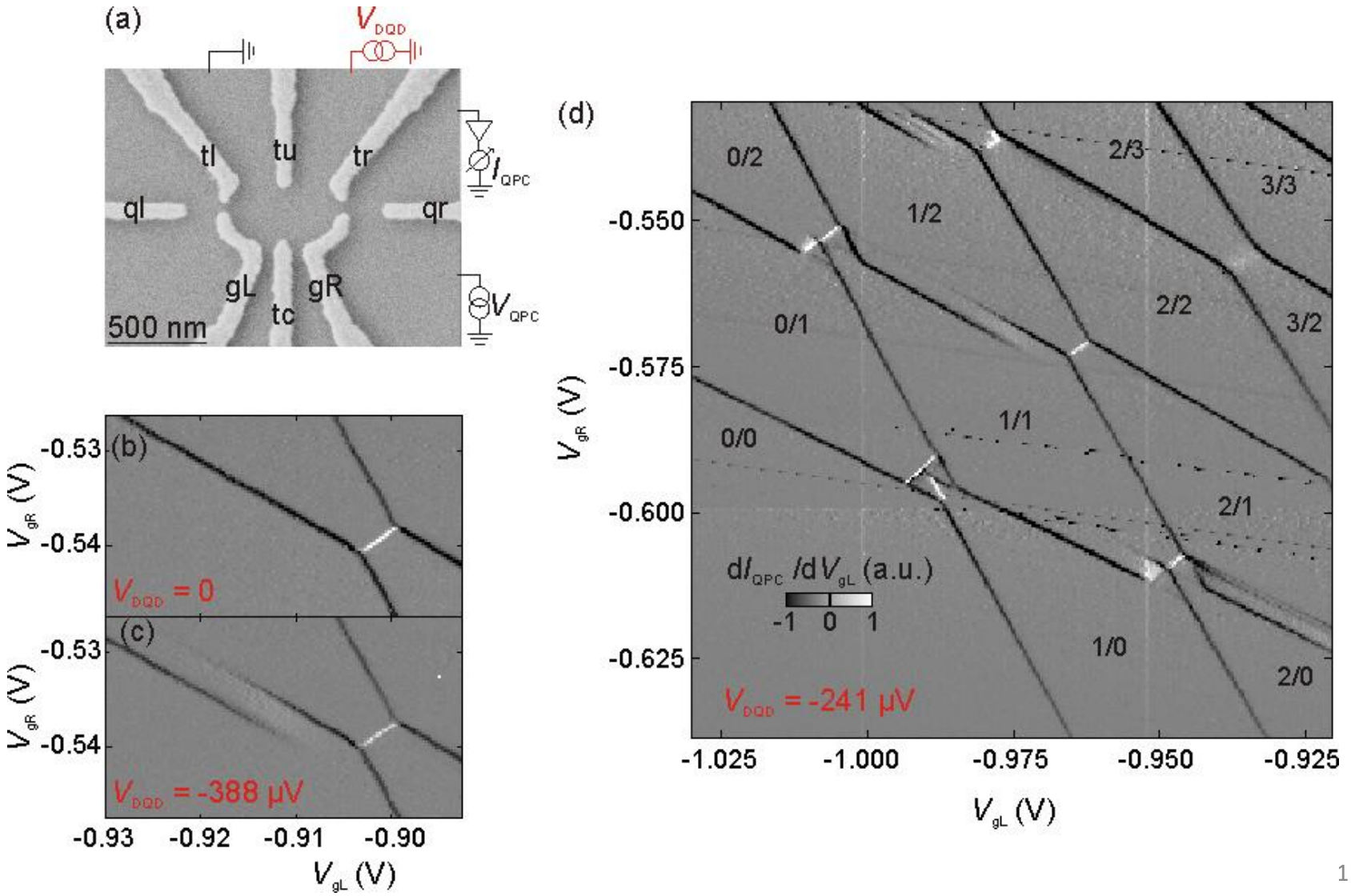


- 2-channel Kondo model



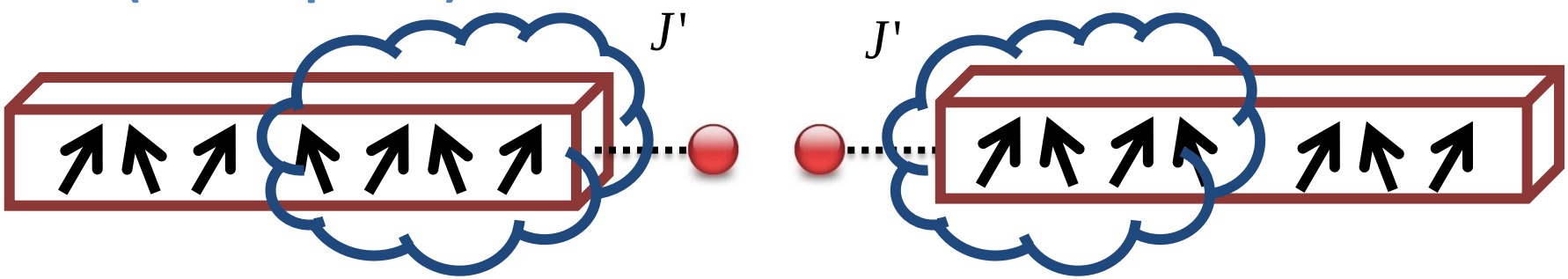
$$H = \sum_k J_k \vec{\sigma}_k . \vec{\sigma}_{k+1}$$

Physical realization

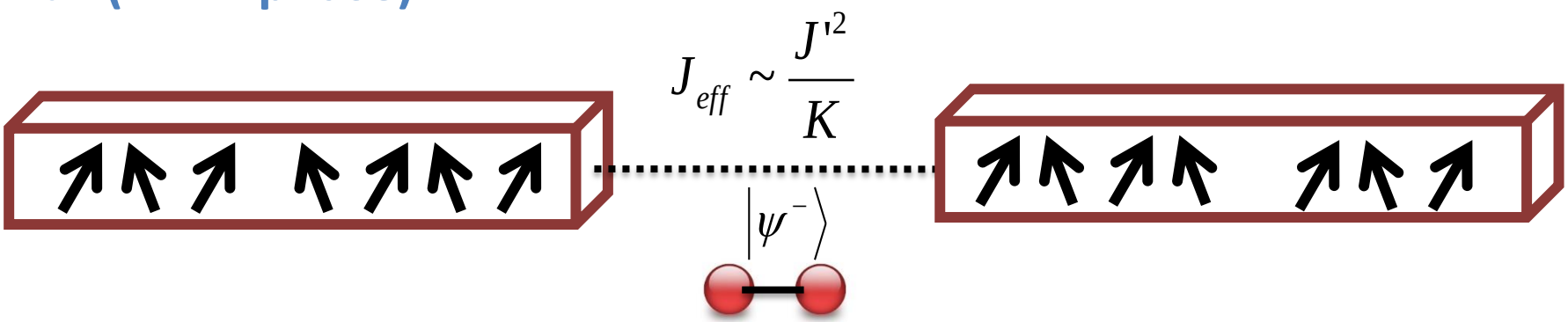


Quantum phases in 2IKM

K<<J' (Kondo phase)



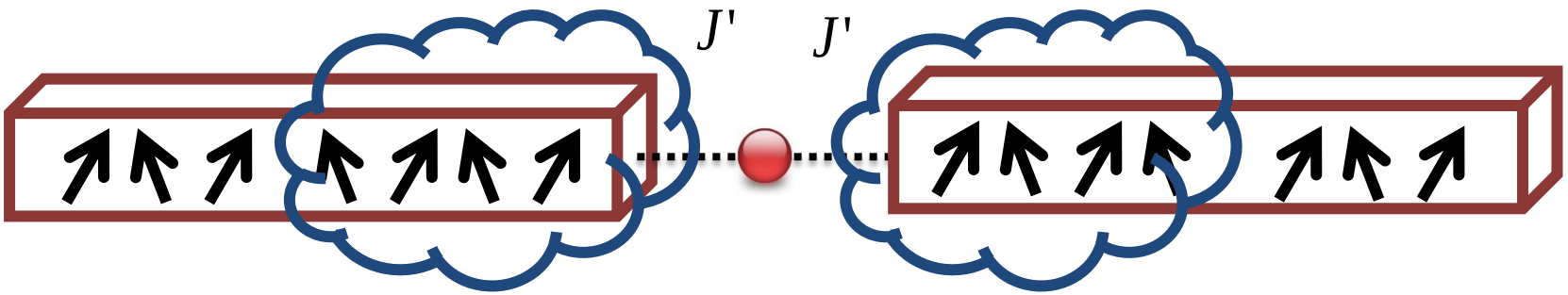
K>>J' (RKKY phase)



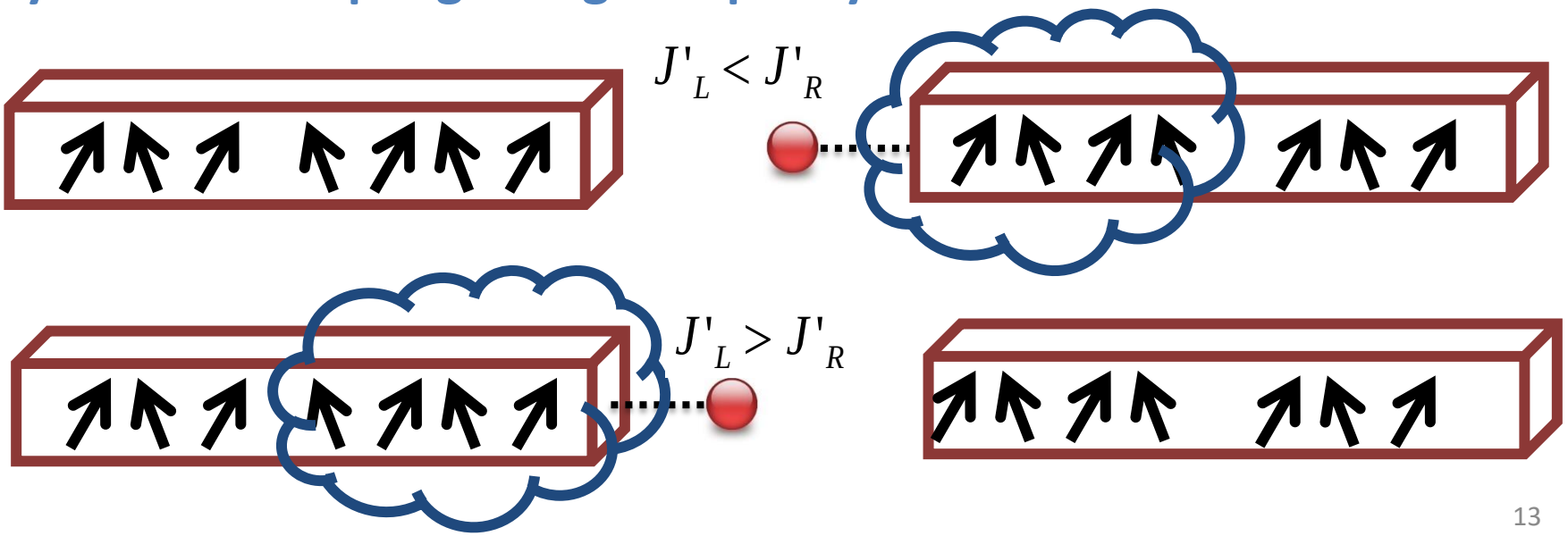
There is no symmetry breaking in the system but quantum states are fully restructured

Quantum phases in 2CKM

Symmetric couplings

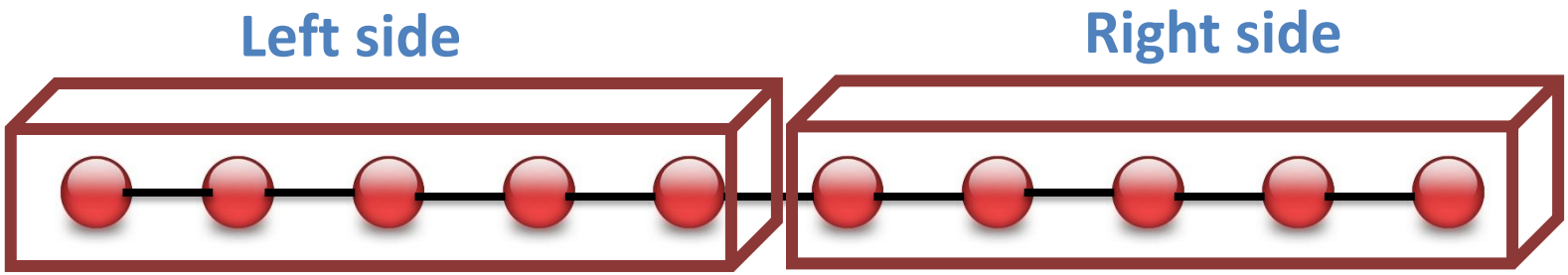


Asymmetric couplings: single impurity Kondo model



Schmidt gap as an order parameter

Entanglement Spectrum



$$|GS\rangle = \sum_k \alpha_{ij} |\tilde{L}_i\rangle \otimes |\tilde{R}_j\rangle$$

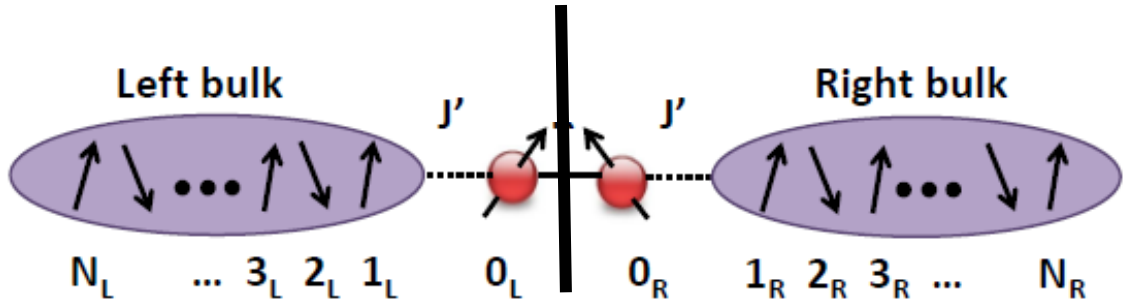
$$|GS\rangle = \sum_k \sqrt{\lambda_k} |L_k\rangle \otimes |R_k\rangle, \quad \lambda_k \geq 0$$ **Schmidt decomposition**

$$\rho_L = \sum_k \lambda_k |L_k\rangle\langle L_k|, \qquad \rho_R = \sum_k \lambda_k |R_k\rangle\langle R_k|$$

Entanglement spectrum: $\lambda_1 \geq \lambda_2 \geq \ldots$

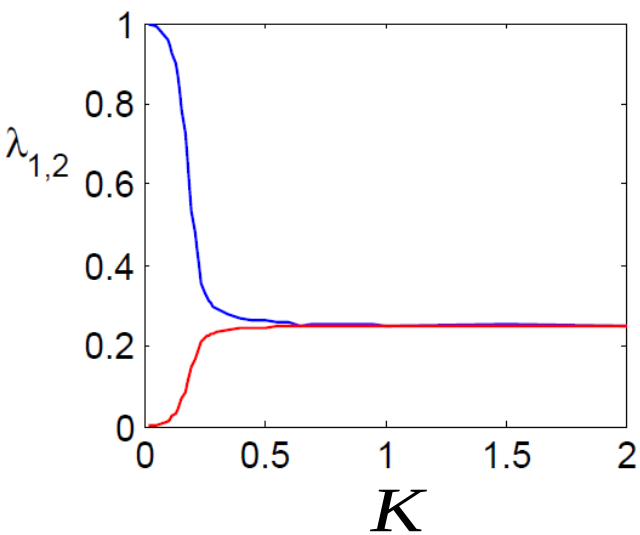
Von Neumann entropy: $s(\rho_L) = s(\rho_R) = -\sum_n \lambda_n \log(\lambda_n)$

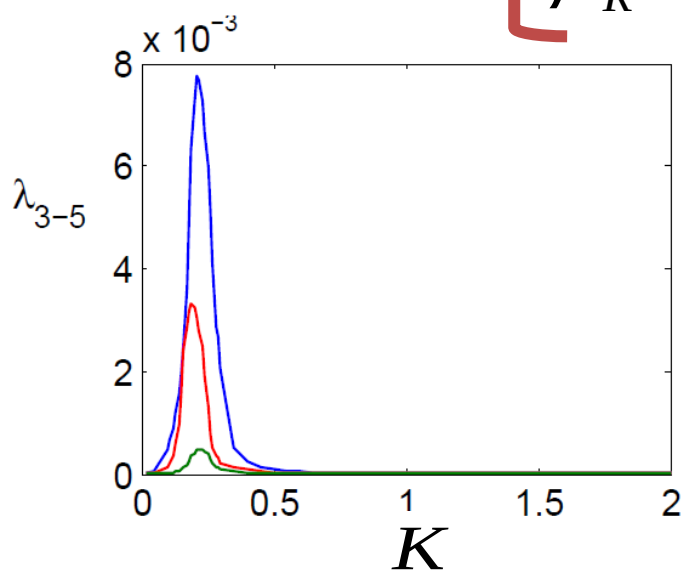
Entanglement Spectrum



$$|GS\rangle = \sum_k \sqrt{\lambda_k}\,|L_k\rangle \otimes |R_k\rangle,\ \lambda_k \geq 0$$

$$\begin{cases} \rho_L = \sum_k \lambda_k |L_k\rangle\langle L_k| \\ \rho_R = \sum_k \lambda_k |R_k\rangle\langle R_k| \end{cases}$$

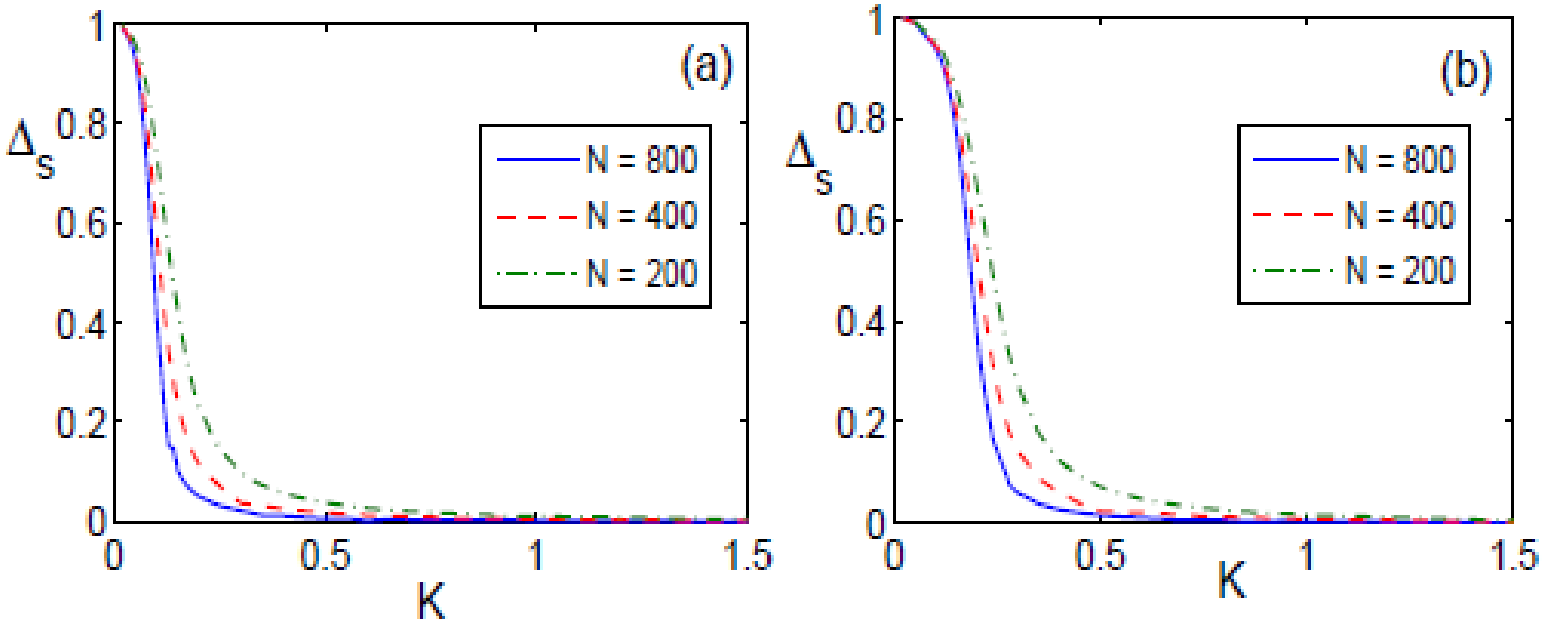




Thermodynamic Behaviour

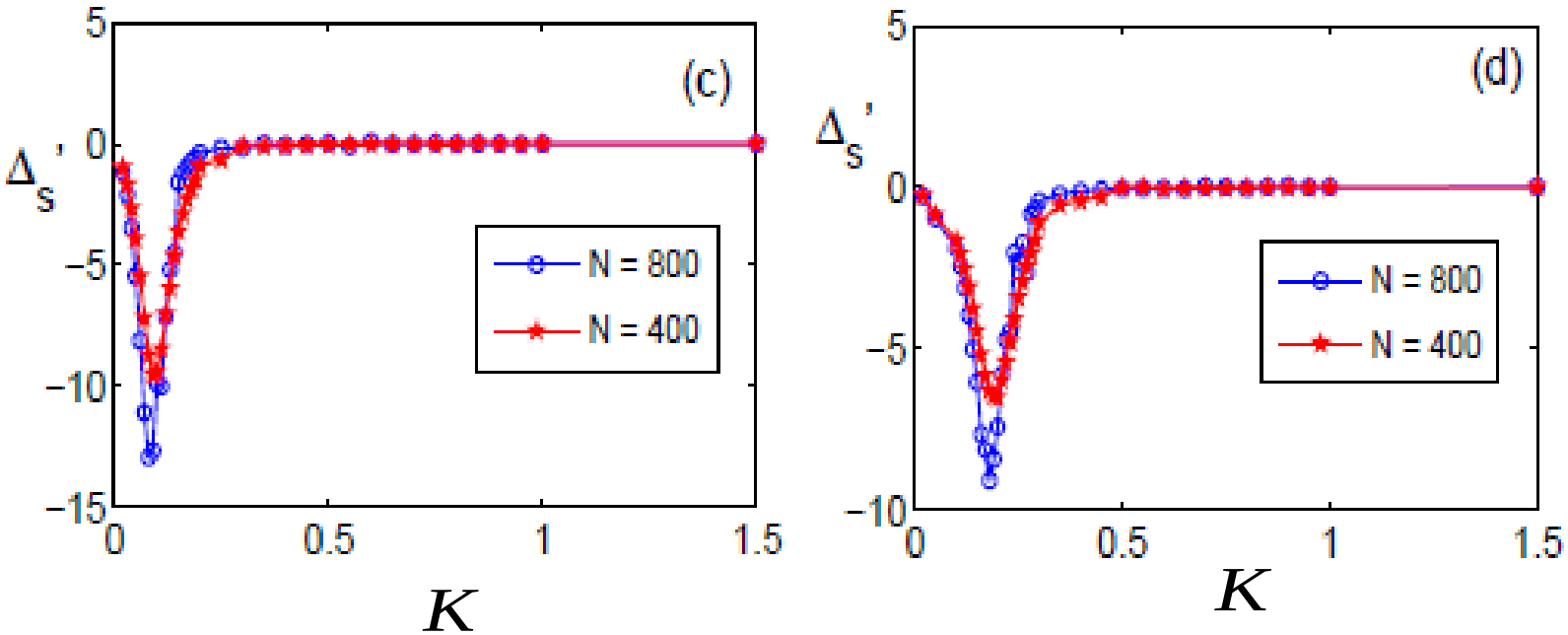
Schmidt gap: $\Delta_S = \lambda_1 - \lambda_2$

J'=0.4 **J'=0.5**



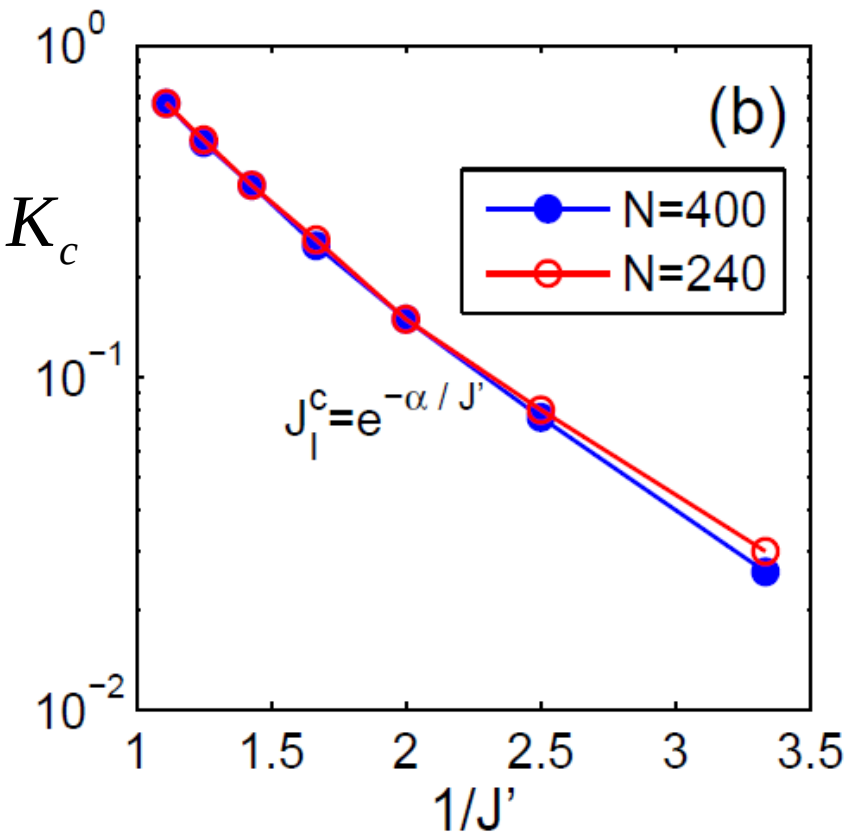
In the thermodynamic limit Schmidt gap vanishes in the RKKY regime

Diverging Derivative



In the thermodynamic limit the first derivative of Schmidt gap diverges

Scaling at the Phase Transition



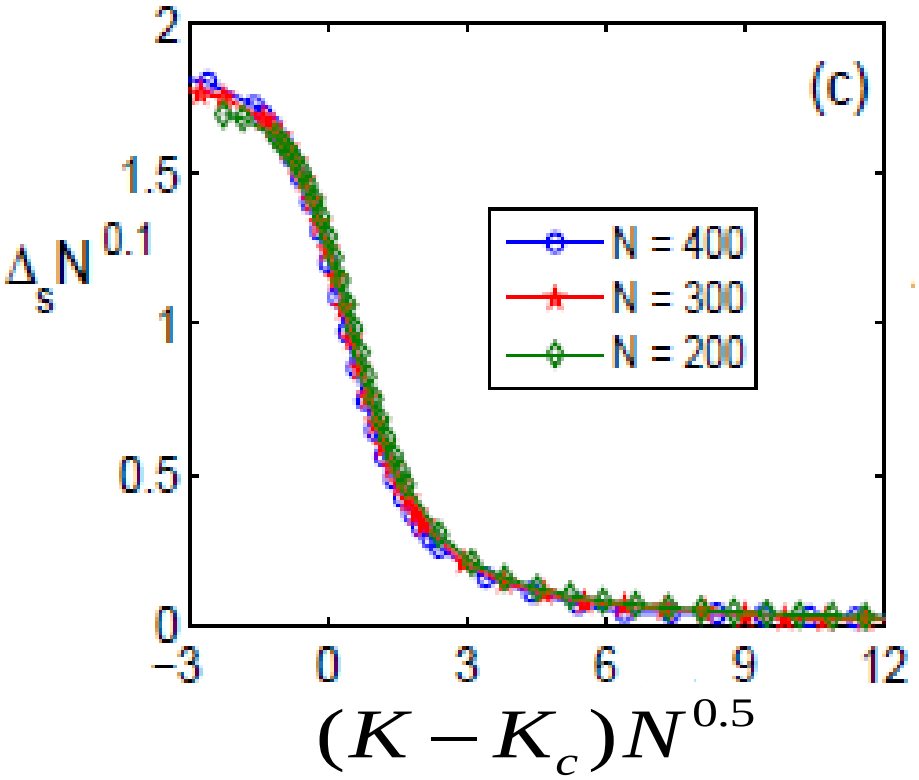
$$K_c \propto T_K \propto \frac{1}{\xi_K} \propto e^{-\alpha / J'}$$

The critical RKKY coupling scales just as Kondo temperature does

Finite Size Scaling

$$\Delta_S = N^{-\beta/\nu} f(|K - K_c| N^{1/\nu}) \Rightarrow$$

$$\Delta_S N^{\beta/\nu} = f(|K - K_c| N^{1/\nu})$$



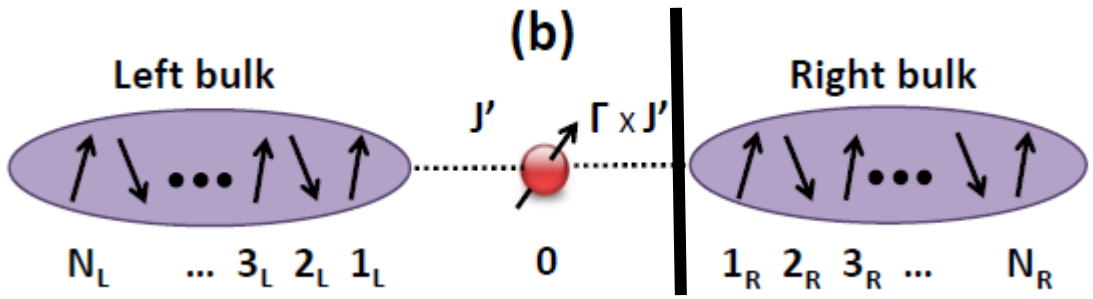
$$\Delta_S = |K - K_c|^{\beta}$$

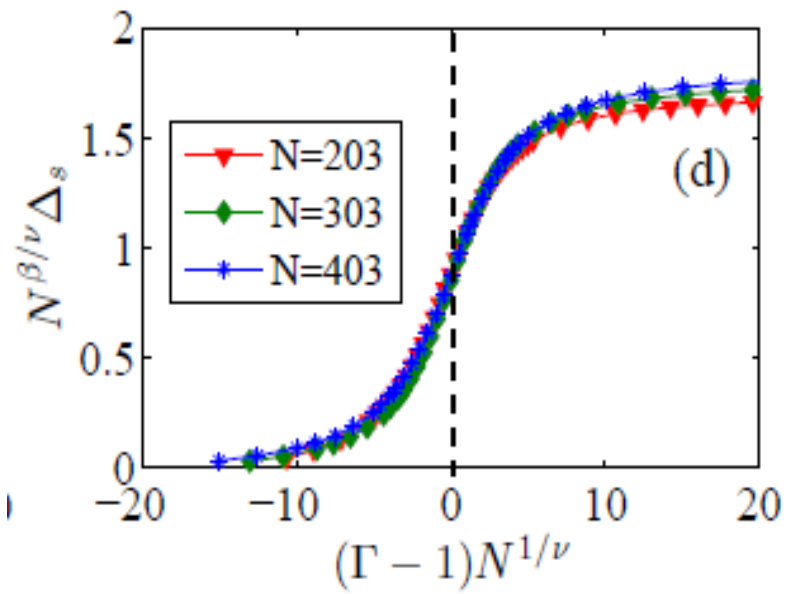
$$\xi = |K - K_c|^{-\nu}$$

$$\beta = 0.2$$

$$\nu = 2$$

Two channel Kondo model





$$\Delta_S = |K - K_c|^{\beta}$$

$$\xi = |K - K_c|^{-\nu}$$

$$\beta = 0.2$$

$$\nu = 2$$

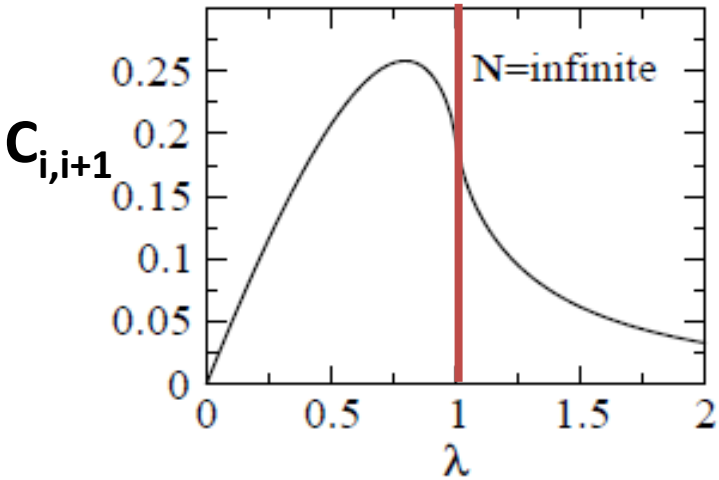
Schmidt gap suggests that 2CKM and 2IKM belong to the same universality class

Entanglement at criticality

$$\xi = | K - K_c |^{-\nu}$$ → Does entanglement peak at criticality?

Entanglement between **what** & **what**?

Transverse Ising



A. Osterloh, L. Amico, G. Falci, R. Fazio, Nature 416, 608 (2002)

Entanglement between one site and the rest does not peak at the critical point either

D. Larsson and H. Johannesson, Phys. Rev. A 73, 042320 (2006)

Total entanglement

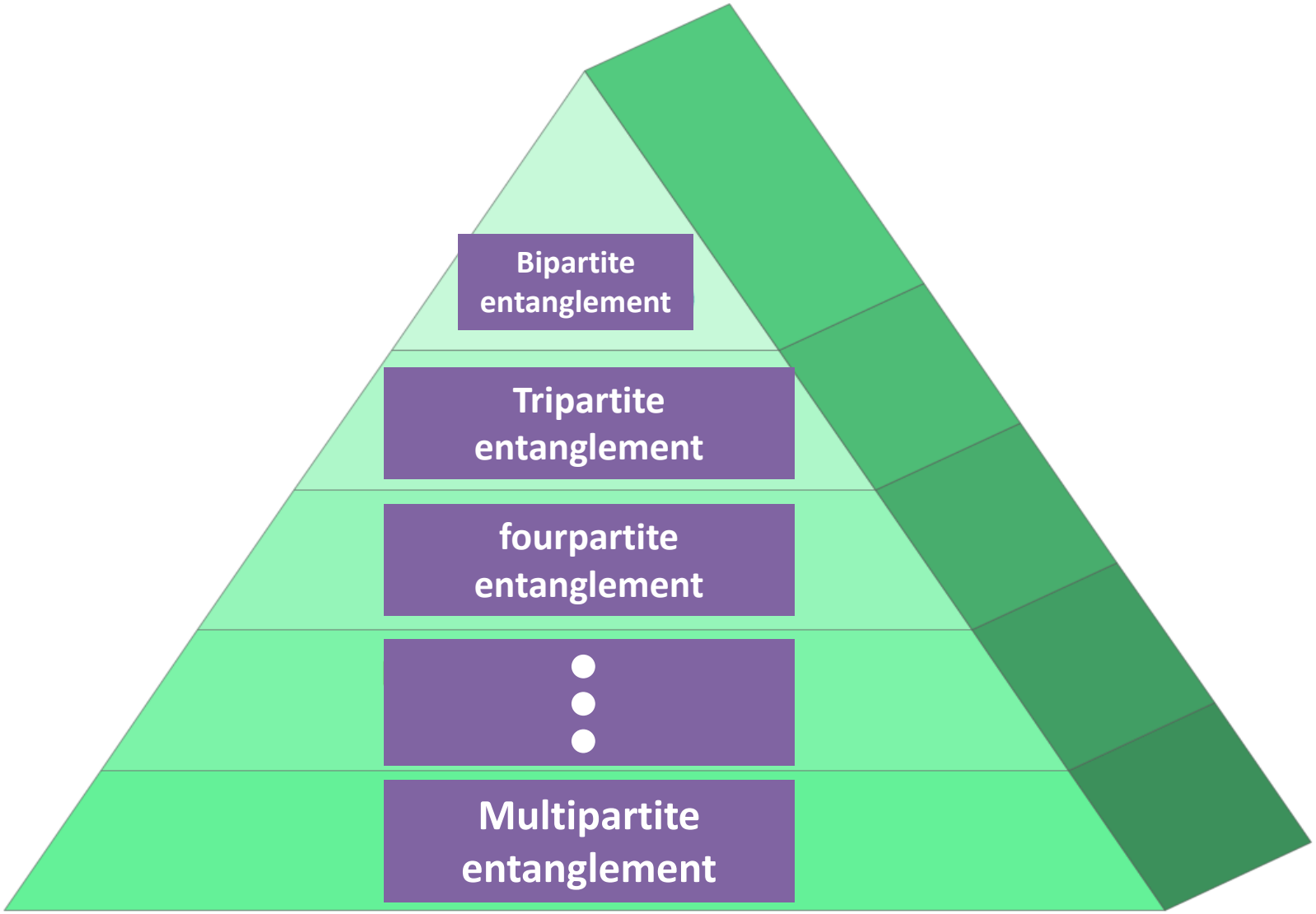
$$\xi = |K - K_c|^{-\nu}$$

Conjecture: It is the total entanglement that is maximum at the critical point.

Quantification of multipartite entanglement is extremely difficult

Entanglement between microscopic constituents may not be practically accessible.

Coarse-grained entanglement

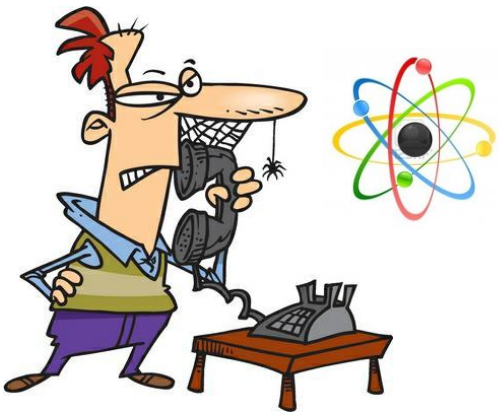


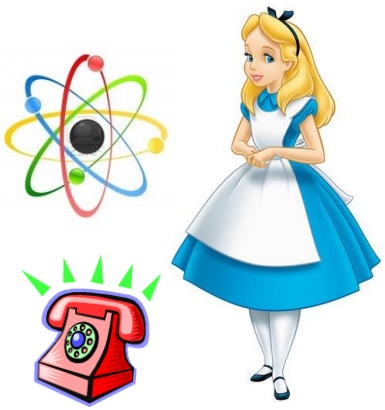
Negativity:
a true bipartite entanglement measure

Separable States

Separable states: $$\rho_{AB} = \sum_i p_i \rho_i^A \otimes \rho_i^B$$

$$p_i \geq 0, \quad \sum_i p_i = 1$$





Entangled states: $$\rho_{AB} \neq \sum_i p_i \rho_i^A \otimes \rho_i^B$$

Negativity

For any density matrix: $\rho \Rightarrow \rho^T$ **is also a density matrix**

Separable:

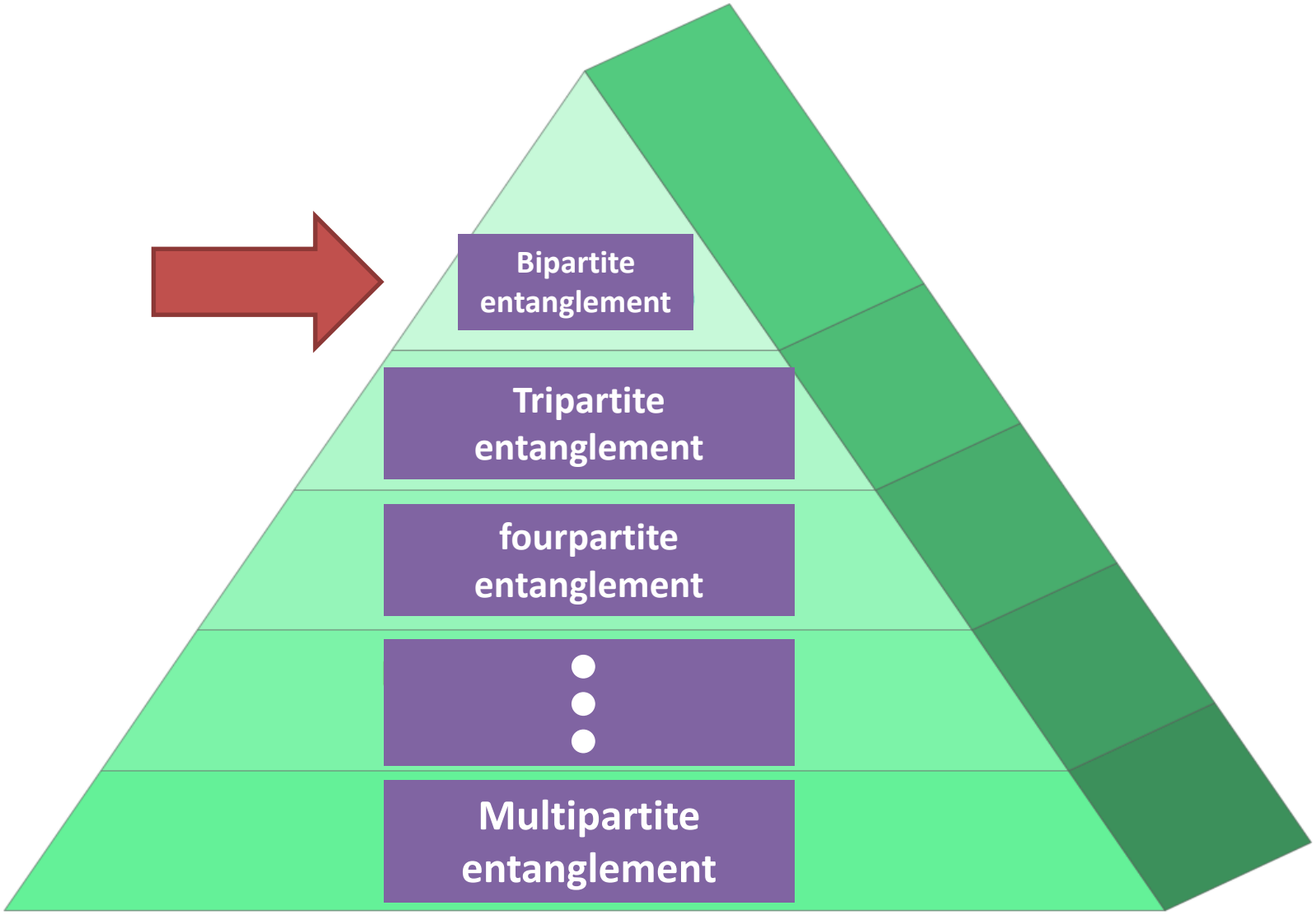
$$\rho = \sum_i p_i \, \rho_i^A \otimes \rho_i^B \Rightarrow \rho^{T_A} = \sum_i p_i \, \boxed{(\rho_i^A)^t} \otimes \boxed{\rho_i^B} \Rightarrow \rho^{T_A} \geq 0 \checkmark$$

Valid density matrices

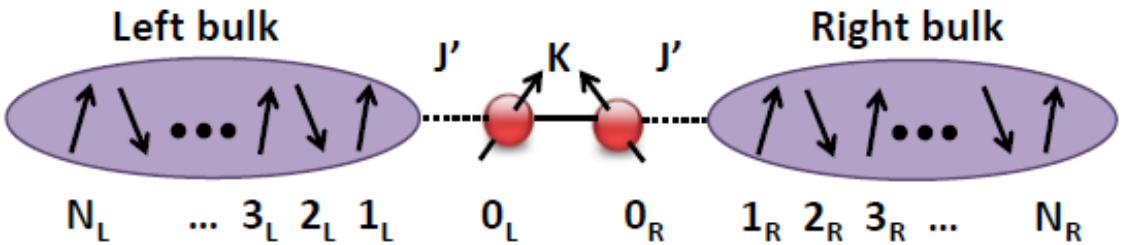
Entangled: $\rho^{T_A} |\lambda\rangle = \lambda |\lambda\rangle \quad (\lambda < 0)$

Negativity: $N(\rho) = 2\sum_{\lambda<0} |\lambda|, \qquad \rho^{T_A} |\lambda\rangle = \lambda |\lambda\rangle$

Bipartite entanglement

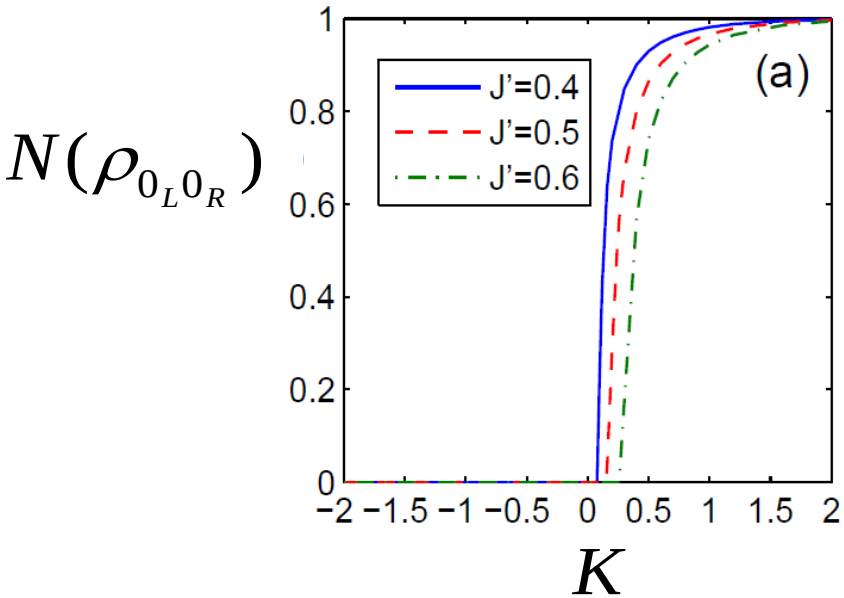


Impurities

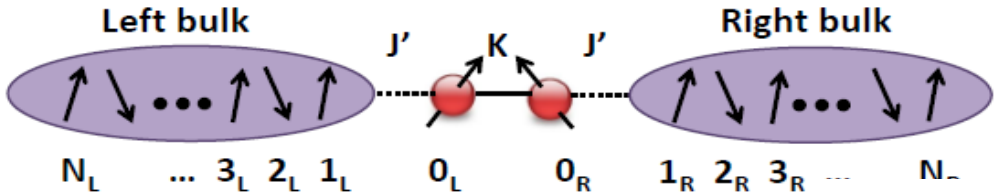


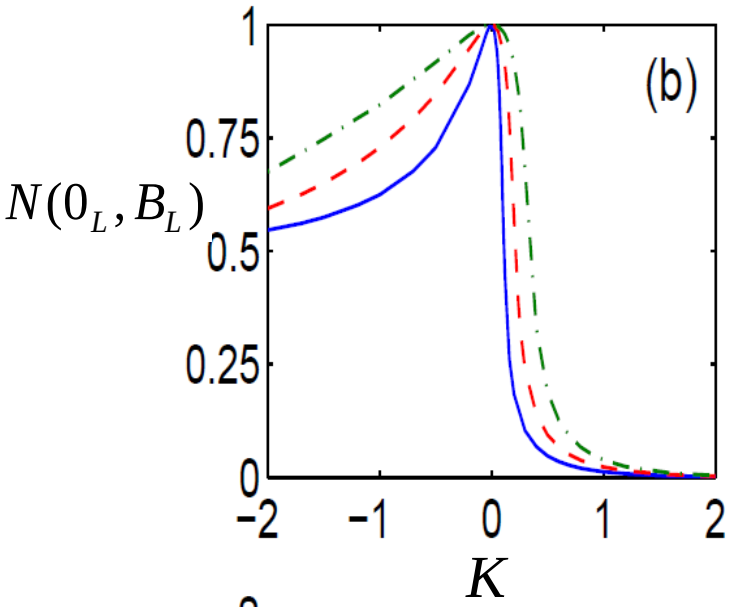
$$|GS\rangle \Rightarrow \rho_{0_L 0_R} = p|\psi^-\rangle\langle\psi^-| + \frac{1-p}{3}\sum_{k=0,\pm}|T^k\rangle\langle T^k|$$

Negativity: $N(\rho_{0_L 0_R}) = \max\{0, 2p-1\}$



Impurity-Block Entanglement

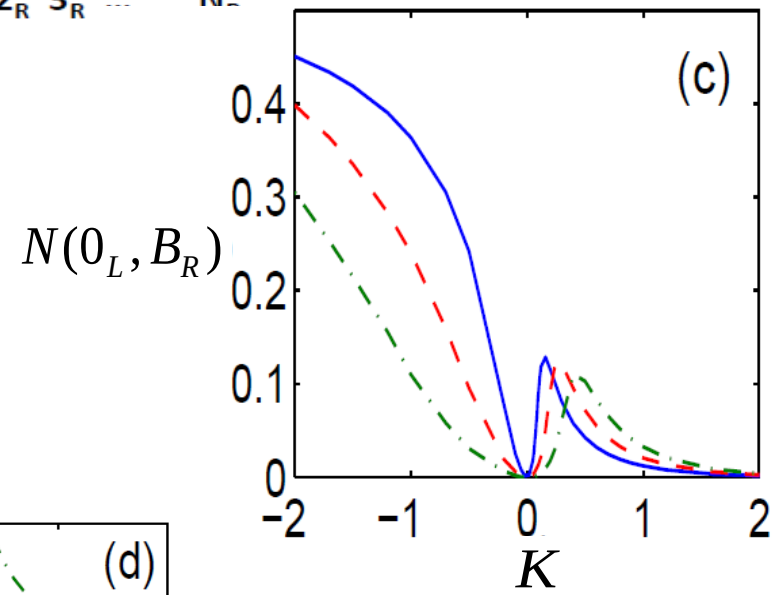


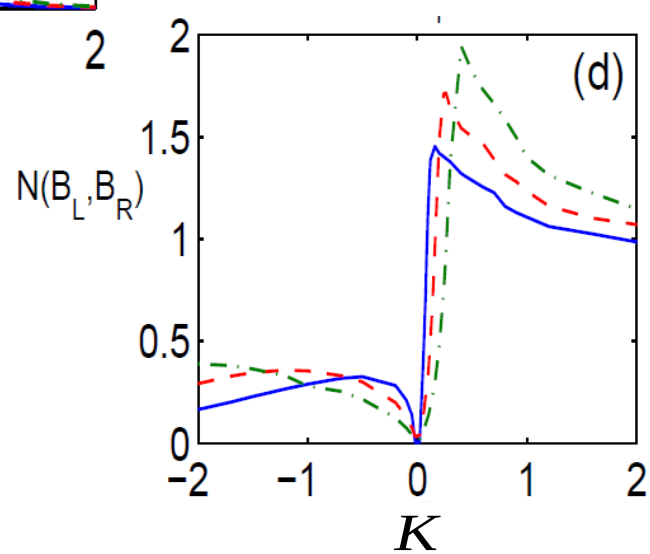


J'=0.4

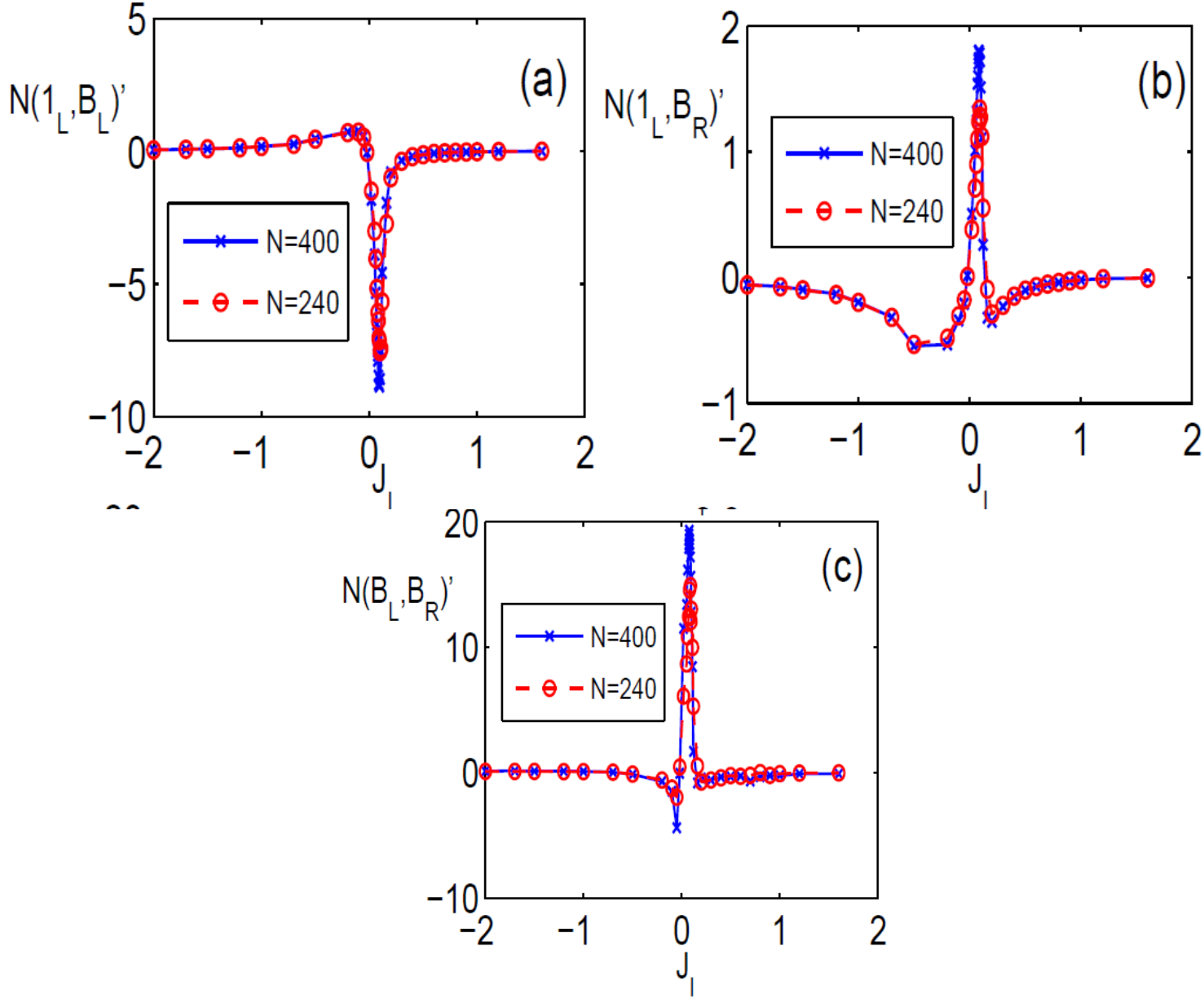
J'=0.5

J'=0.6

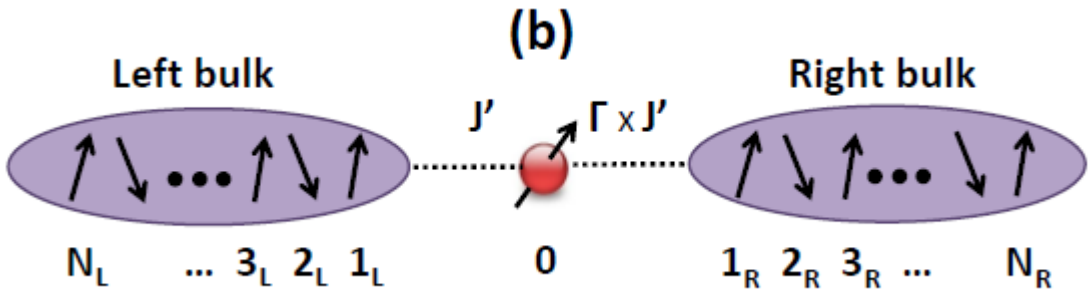




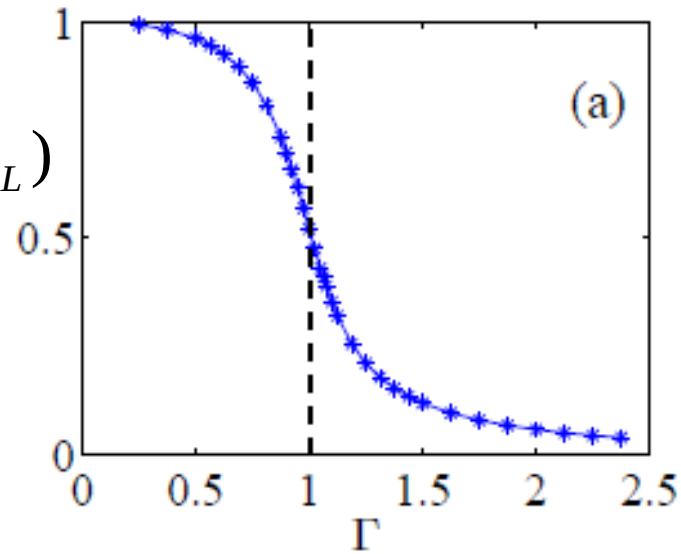
2nd Order Phase Transition



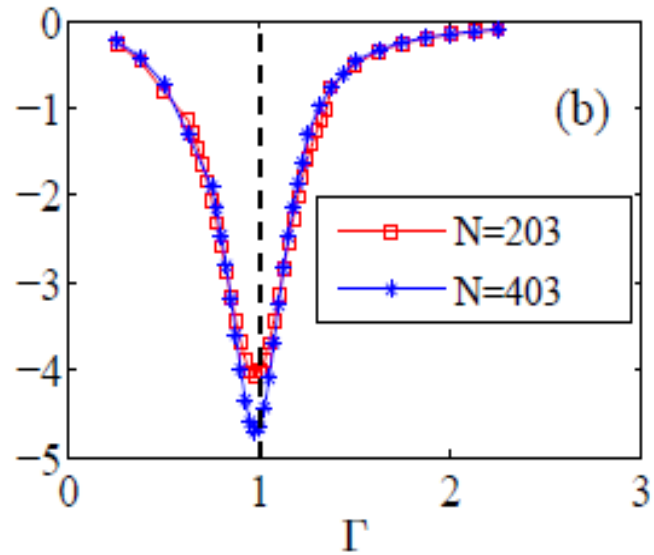
Negativity in 2CKM



$N(0, B_L)$



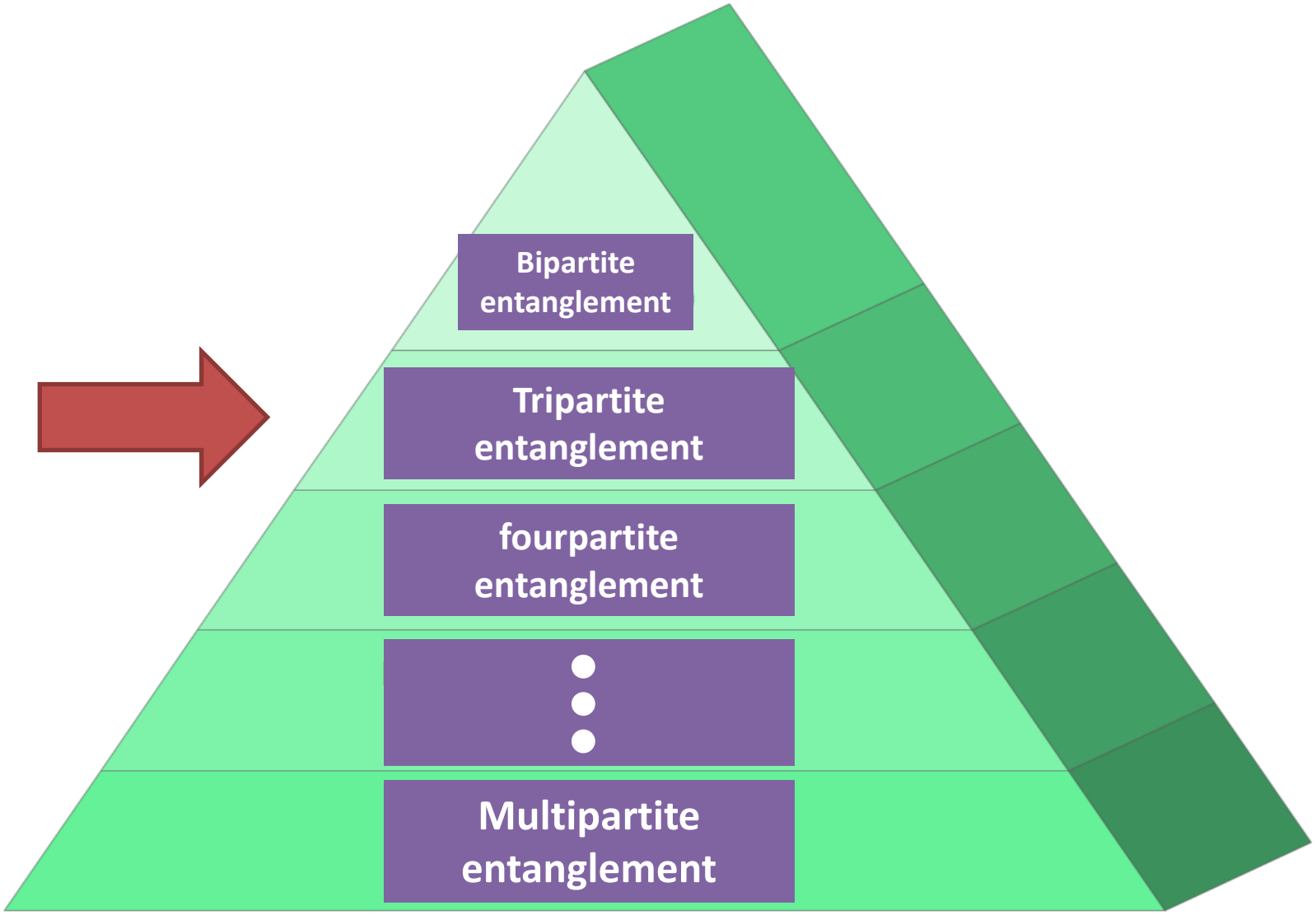
$N'(0, B_L)$



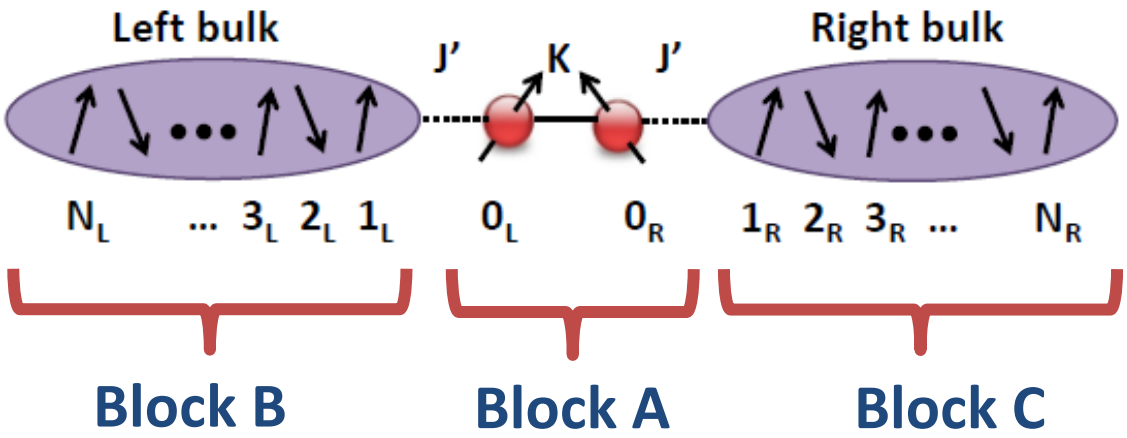
Summary 1

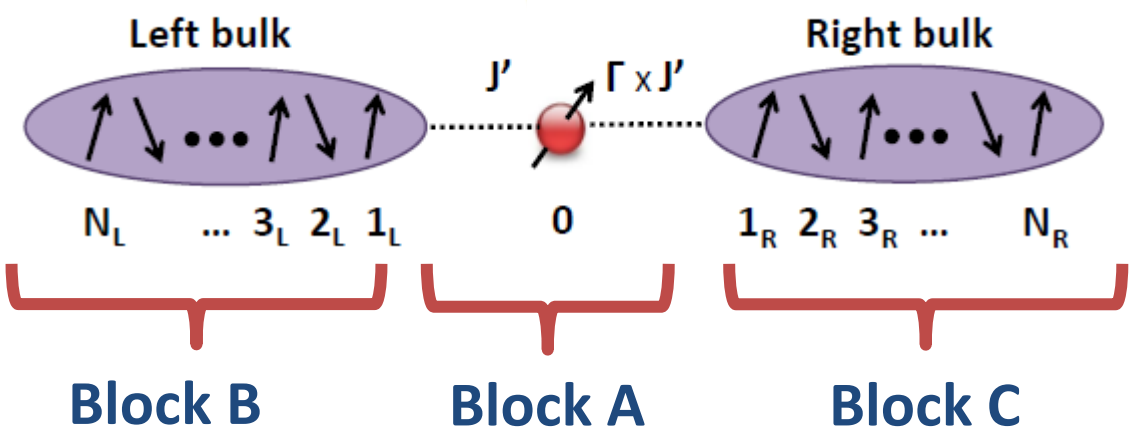
- **Bipartite entanglement (impurity-bulk & bulk-bulk) can detect iQPT.**
- **Bulk-bulk entanglement peaks at criticality**

Tripartite entanglement



Tripartite entanglement





Three qubits

- **Class 1: GHZ-states**

$$|GHZ\rangle_{ABC} = \frac{|000\rangle_{ABC} + |111\rangle_{ABC}}{\sqrt{2}} \Rightarrow \rho_{AB} = \underbrace{\frac{1}{2}|00\rangle\langle 00| + \frac{1}{2}|11\rangle\langle 11|}_{\text{Separable}}$$

- **Class 2: w-states**

$$|W\rangle_{ABC} = \frac{|001\rangle_{ABC} + |010\rangle_{ABC} + |100\rangle_{ABC}}{\sqrt{3}} \Rightarrow \rho_{AB} = \underbrace{\frac{1}{3}|00\rangle\langle 00| + \frac{2}{3}|\psi+\rangle\langle\psi+|}_{\text{Entangled}}$$

Where: $|\psi+\rangle = \frac{|01\rangle + |10\rangle}{\sqrt{2}}$

Such classification does not exist for higher dimensions

Quantification of tripartite entanglement

- **Measure 1:** $$E_1 = [N_{A,BC} N_{B,AC} N_{C,AB}]^{1/3}$$

S. Campbell and M. Paternostro, Phys. Rev. A 82, 042324 (2010)

- **Measure 2:**

$$\pi_A = N_{A,BC}^2 - N_{A,B}^2 - N_{A,C}^2$$

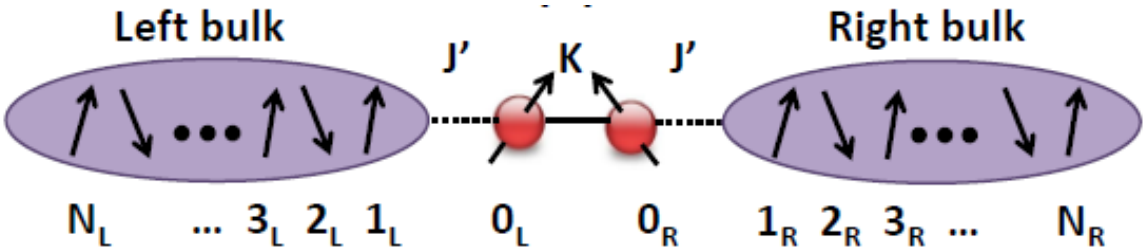
Conjecture: $\pi_A \geq 0$

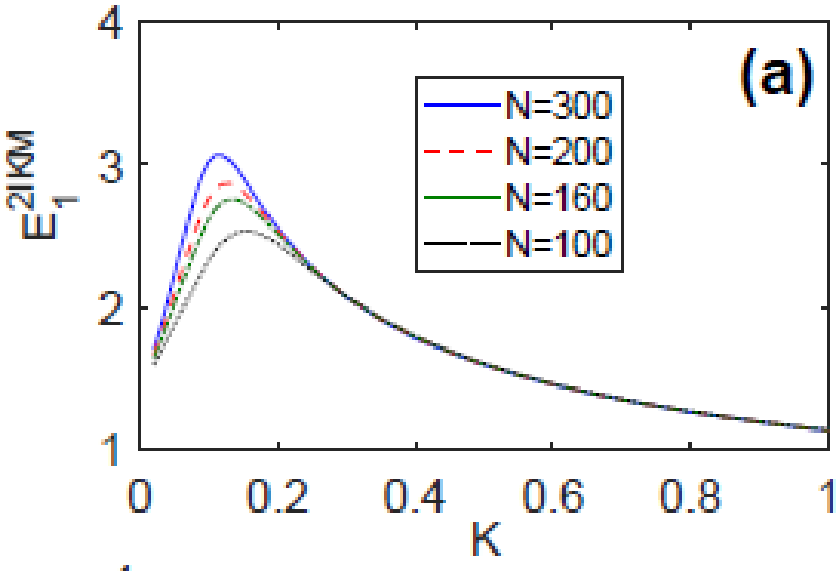
Proved for three qubits: Y.-C. Ou and H. Fan, PRA A 75, 062308 (2007).

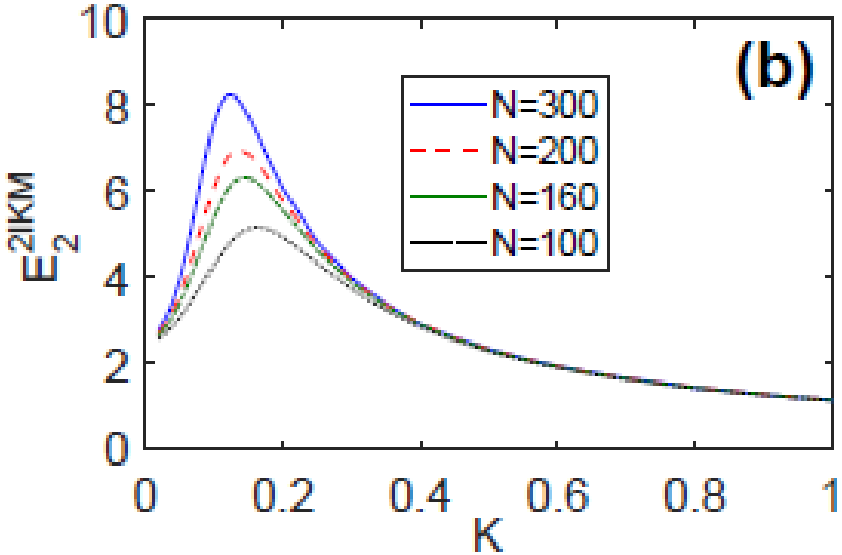
Numerically verified for 4-level systems: H. He and G. Vidal, PRA 91, 012339 (2015).

$$E_2 = \frac{\pi_A + \pi_B + \pi_C}{3}$$

2IKM

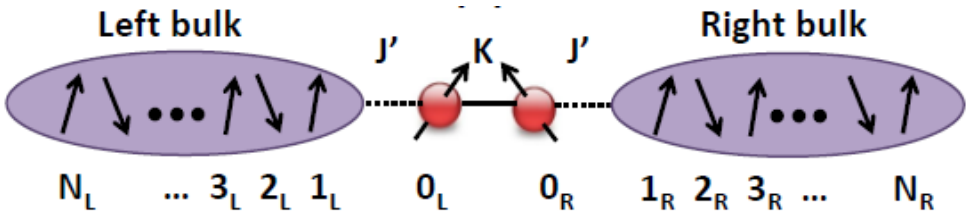


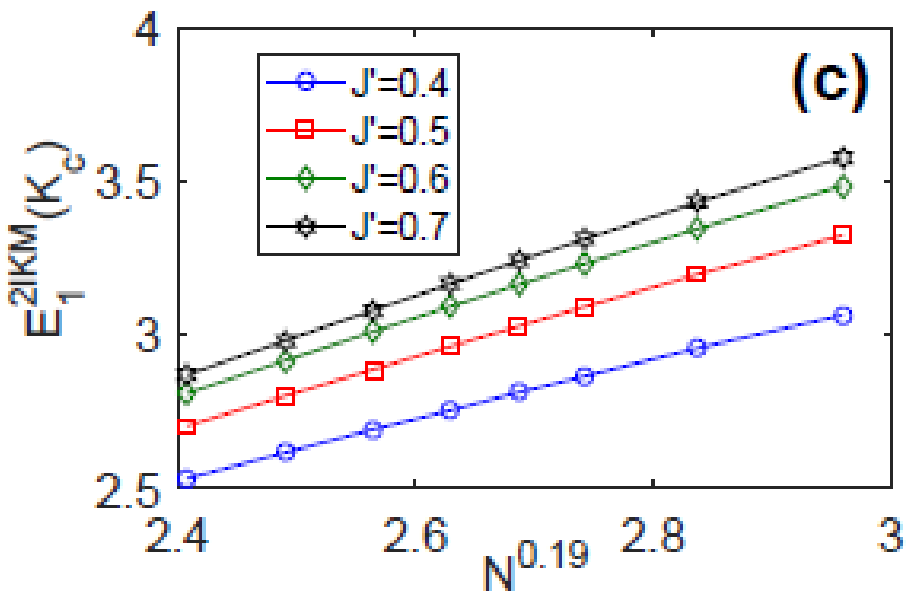


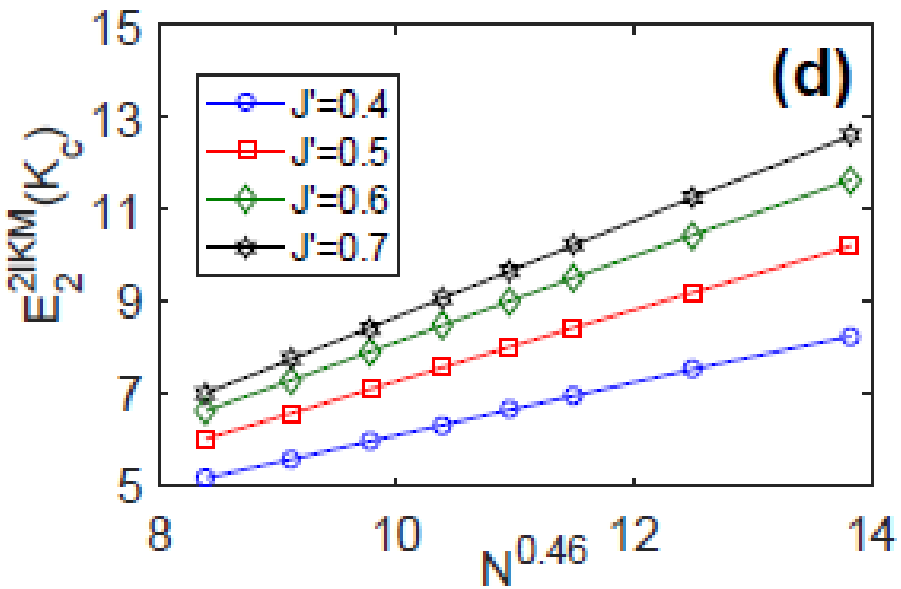


Tripartite entanglement diverges at criticality for 2IKM

Divergence at criticality







$$E_j(K_c) = N^{\lambda_j}$$

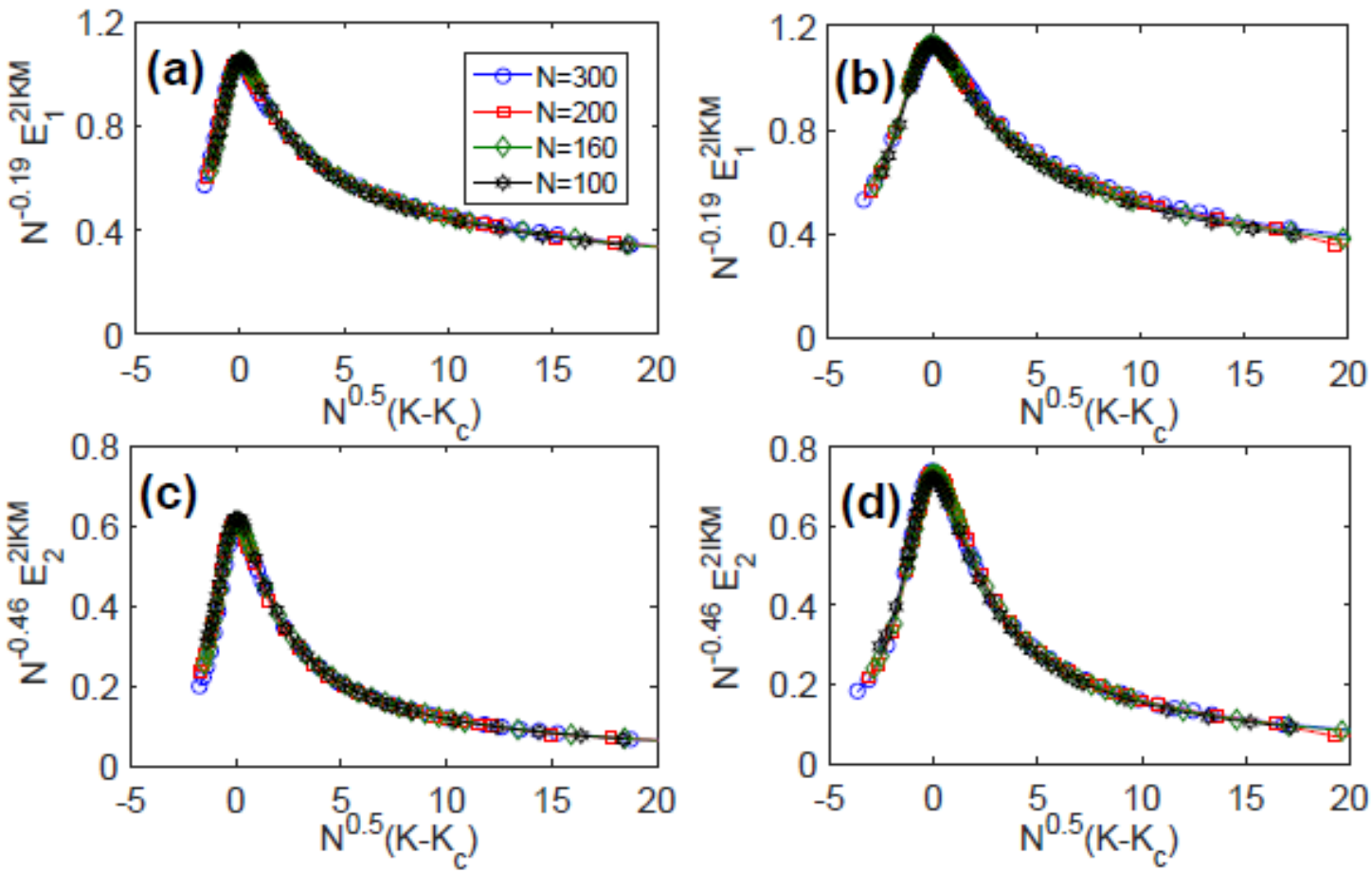
Finite size scaling (2IKM)

$$E_j = N^{\beta_j/\nu} f(N^{1/\nu}|K - K_c|)$$

$$\nu = 2$$

$$\beta_1^{2IKM} = 0.38$$

$$\beta_2^{2IKM} = 0.92$$



Critical exponents (2IKM)

$$\nu = 2$$

$$\beta_1^{2IKM} = 0.38, \quad \lambda_1^{2IKM} = 0.19$$

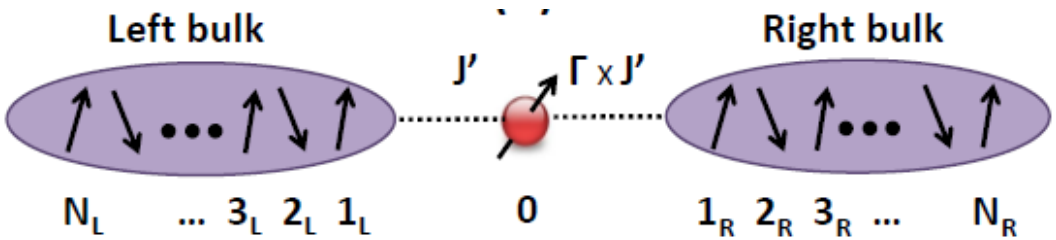
$$\beta_2^{2IKM} = 0.92, \quad \lambda_2^{2IKM} = 0.46$$

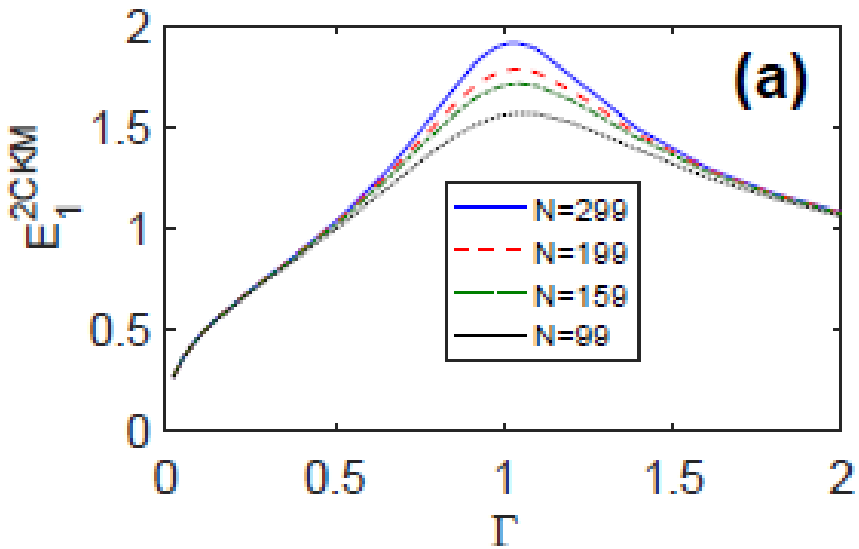
$$E_j = N^{\beta_j/\nu} f(N^{1/\nu}|K - K_c|) \xRightarrow{K=K_C} E_j = N^{\beta_j/\nu} f(0) \Rightarrow \lambda_j = \beta_j / \nu$$

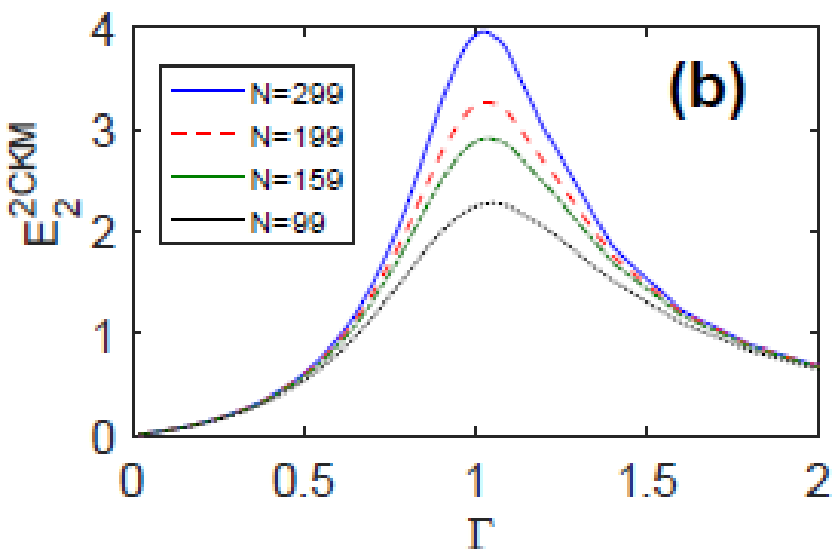
$$\beta_1^{2CKM} = 0.38, \quad \lambda_1^{2CKM} = 0.19, \quad \nu = 2$$

$$\beta_2^{2CKM} = 1, \quad \lambda_2^{2CKM} = 0.5, \quad \nu = 2$$

2CKM

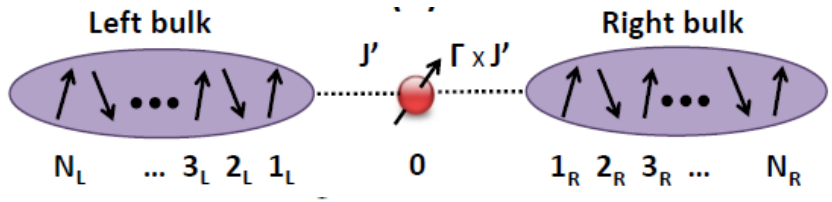


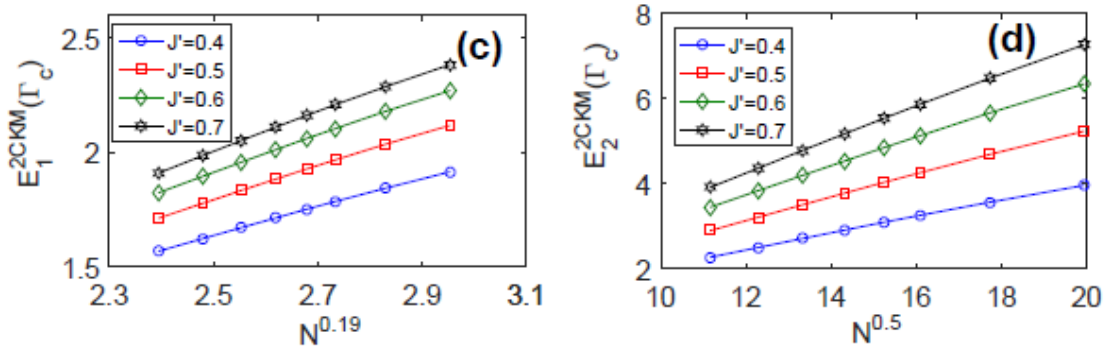




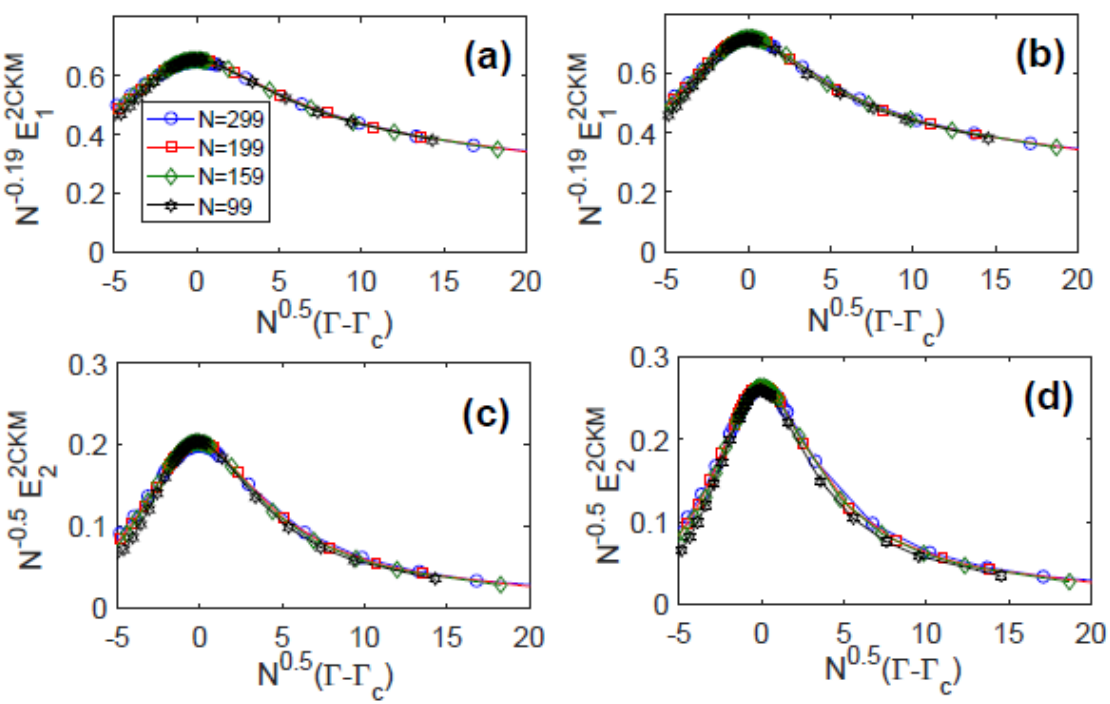
Tripartite entanglement diverges at criticality for 2CKM

2CKM





$$E_j(\Gamma_c) = N^{\lambda_j}$$



$$E_j = N^{\beta_j/\nu} f(N^{1/\nu}|\Gamma - \Gamma_c|)$$

$$\nu = 2$$

$$\beta_1^{2CKM} = 0.38, \quad \lambda_1^{2CKM} = 0.19$$

$$\beta_2^{2CKM} = 1, \quad \lambda_2^{2CKM} = 0.5$$

$$\lambda_j = \frac{\beta_j}{\nu}$$

Universality class

For E_1

2IKM	2CKM
$\upsilon = 2$	$\upsilon = 2$
λ_1=0.19	$\lambda_1 = 0.19$
$\beta_1 = 0.38$	$\beta_1 = 0.38$

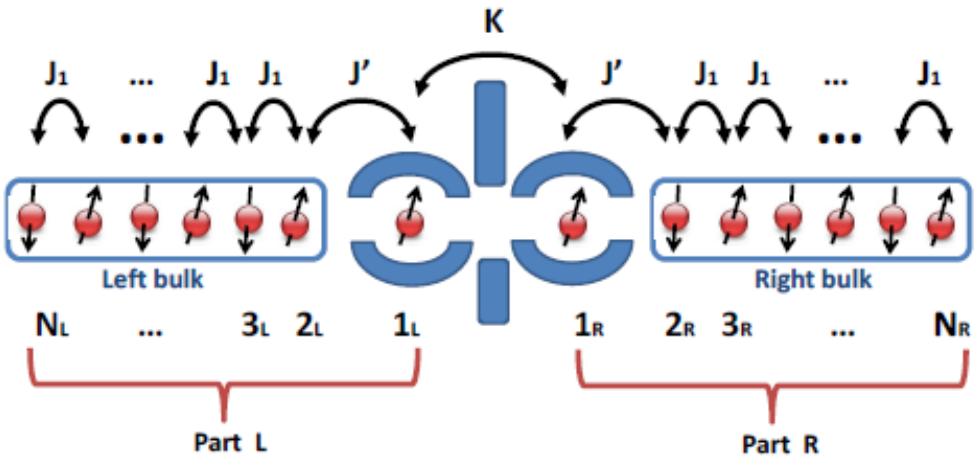
For E_2

2IKM	2CKM
$\upsilon = 2$	$\upsilon = 2$
λ_2=0.46	λ_2=0.5
$\beta_2 = 0.92$	$\beta_2 = 1$

The two measures give almost equal critical exponents for 2IKM and 2CKM

Quantum quench

Quantum quench



System is initialized in the RKKY phase (Impurities form a singlet)

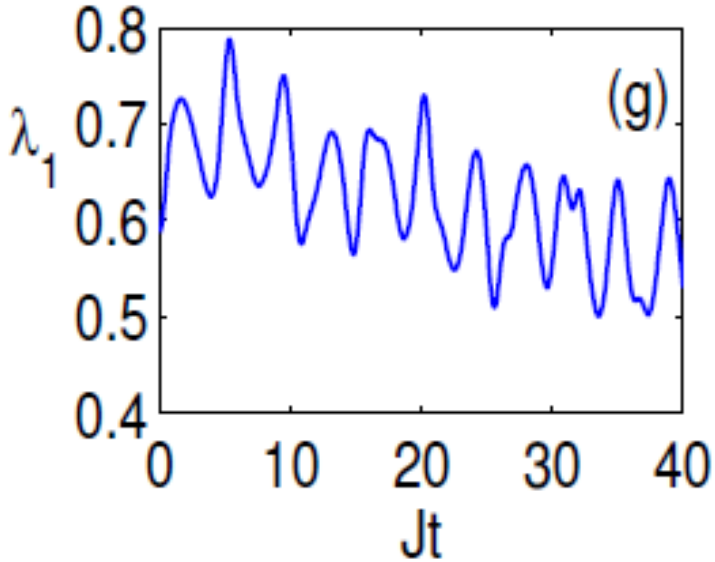
$$K = K_1 > K_c : \qquad |\Psi(0)\rangle = |GS(K_1)\rangle$$

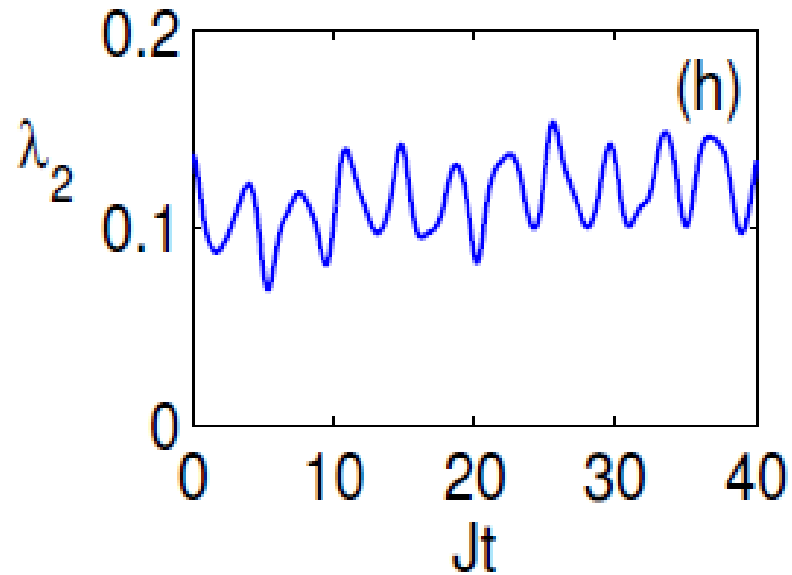
$$K = K_1 \rightarrow K = K_2 < K_c : \qquad |\Psi(t)\rangle = e^{-iH_2 t}|\Psi(0)\rangle$$

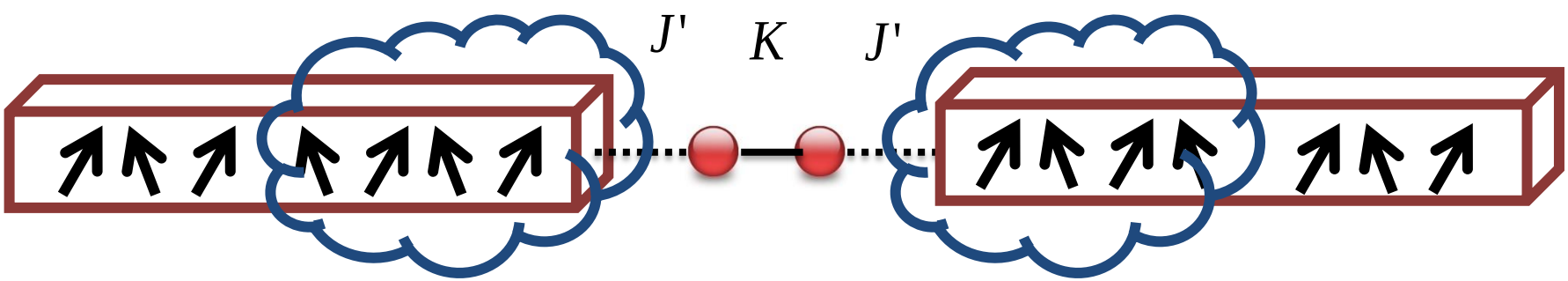
$$|\Psi(t)\rangle = \sum_k \sqrt{\lambda_k(t)}\,|L_K(t)\rangle \otimes |R_K(t)\rangle$$

Non-optimality

$$\xi(K_2, J') < N$$



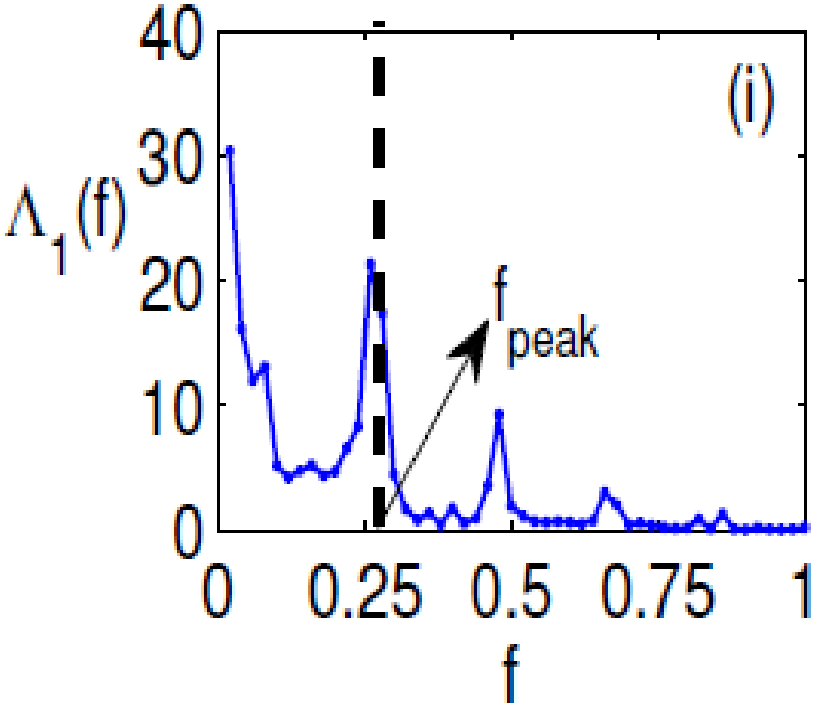


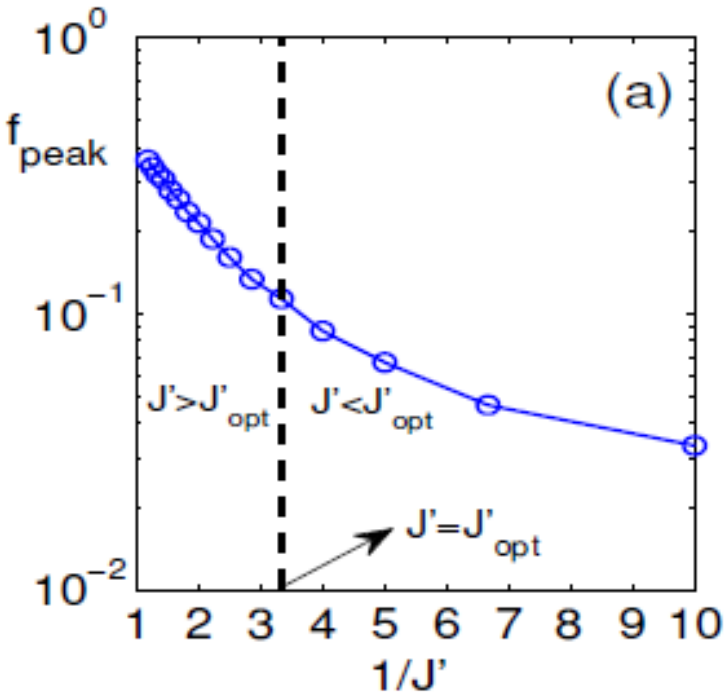


The extra spins play like environment making the dynamics dispersive

Entanglement spectrum

$$\Lambda_n(f) \equiv \mathcal{F}[\lambda_n(t)] = \frac{1}{\sqrt{2\pi}} \int \lambda_n(t) e^{i2\pi f t} dt, \; n = 1, 2$$

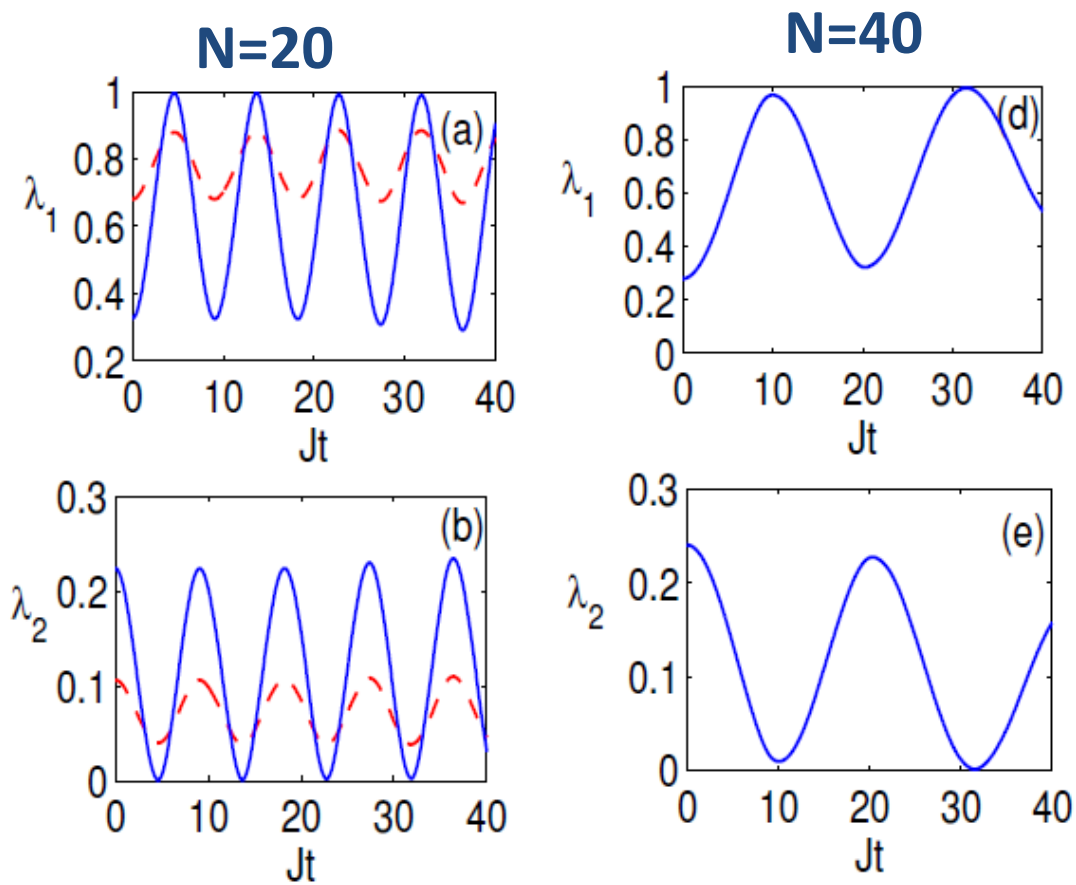


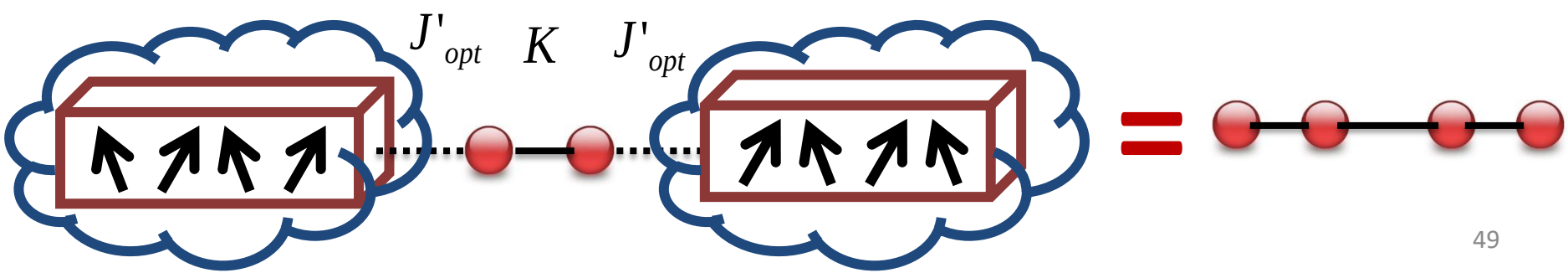


$$f_{peak} \sim \frac{1}{\xi(K_2, J')} \sim e^{-\alpha / J'} \sim T_K$$

Optimal Chain

$$\xi(J'_{opt}, K) \approx N$$

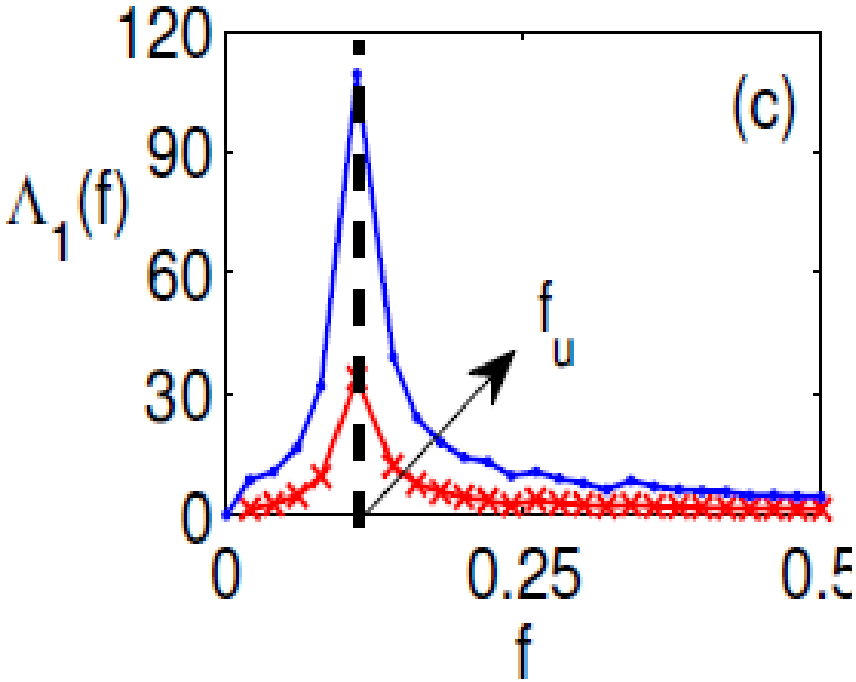




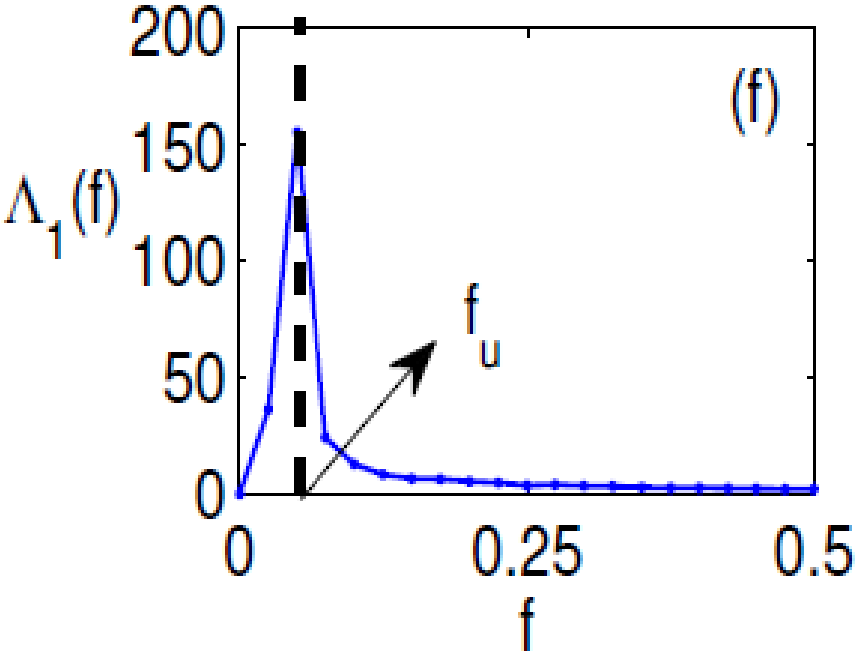
Fourier transform

$$\Lambda_n(f) \equiv \mathcal{F}[\lambda_n(t)] = \frac{1}{\sqrt{2\pi}} \int \lambda_n(t) e^{i2\pi f t} dt, \; n = 1, 2$$

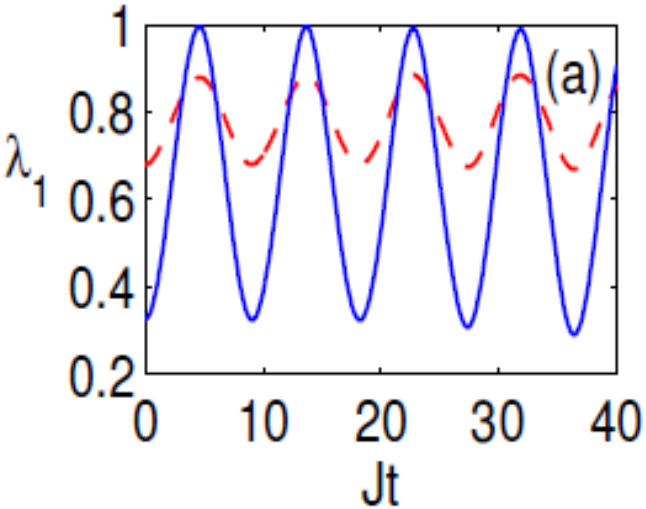
N=20



N=40



Independence of K1 & K2



The frequency fu is independent of K1 (we should only start from RKKY phase)

By changing K2 one can retune the impurity coupling J' to that:

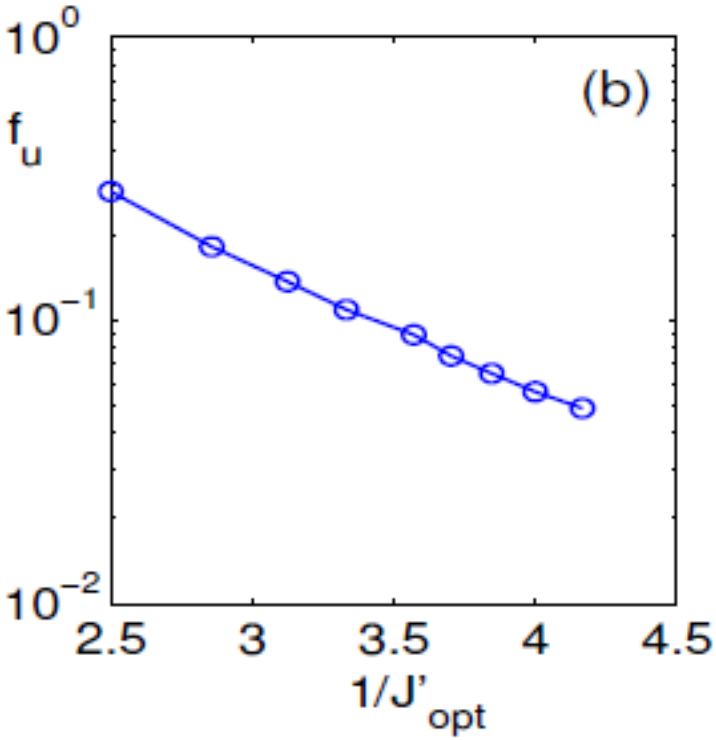
$$\xi(K_2, J'_{opt}) = N$$

For instance in a chain of N=20 (Kc=0.2):

- **K2=0.19, J'opt=0.300 → fu=0.11**
- **K2=0.10, J'opt=0.315 → fu=0.11**

Scaling

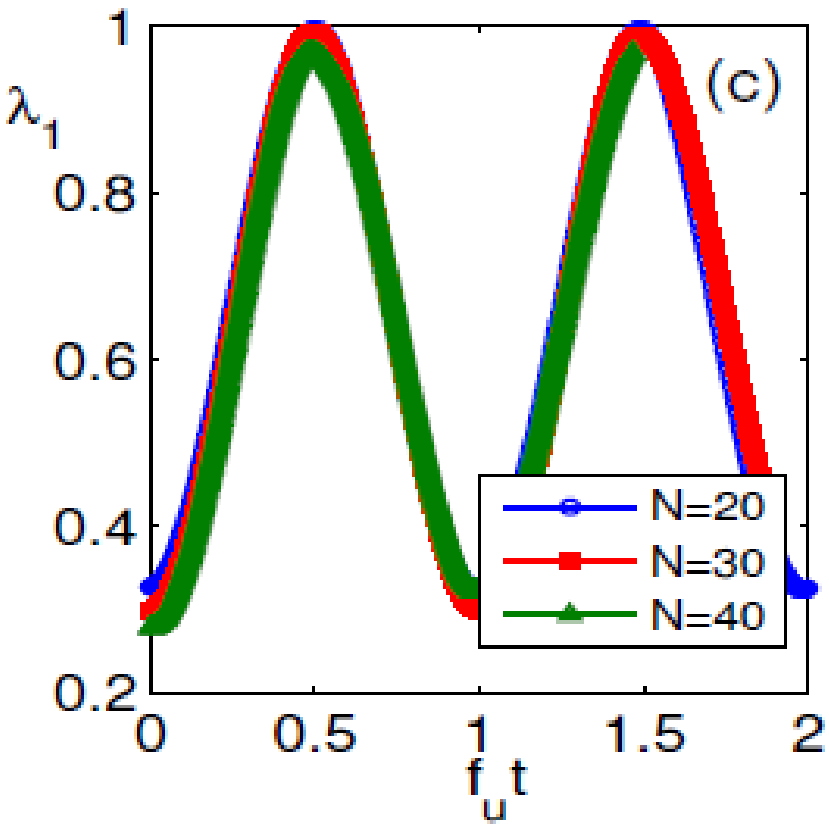
Universal frequency is indeed proportional to the Kondo temperature



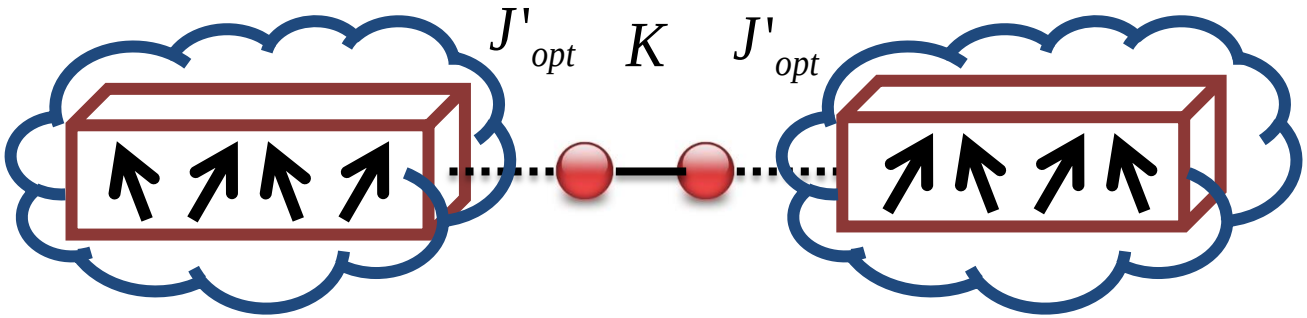
$$f_u \sim e^{-\alpha / J'_{opt}} \sim T_K \sim \frac{1}{\xi(K, J'_{opt})} = \frac{1}{N}$$

N	8	12	16	20	24	28	32	36	40
$f_u N$	2.250	2.184	2.192	2.180	2.136	2.100	2.080	2.01	2.000

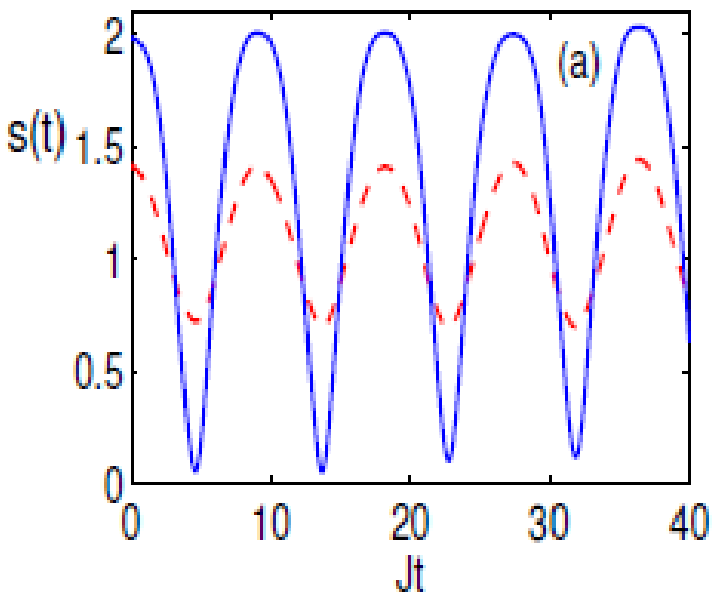
The scale invariant dynamics

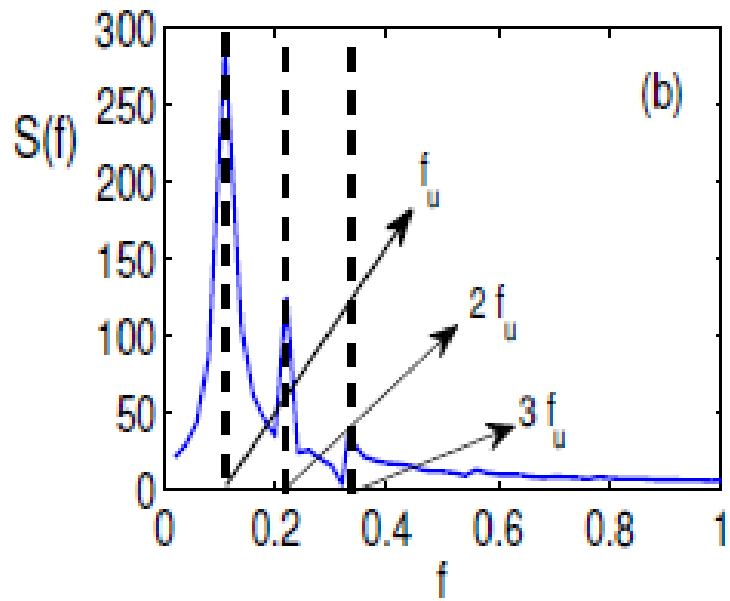


Von Neumann entropy

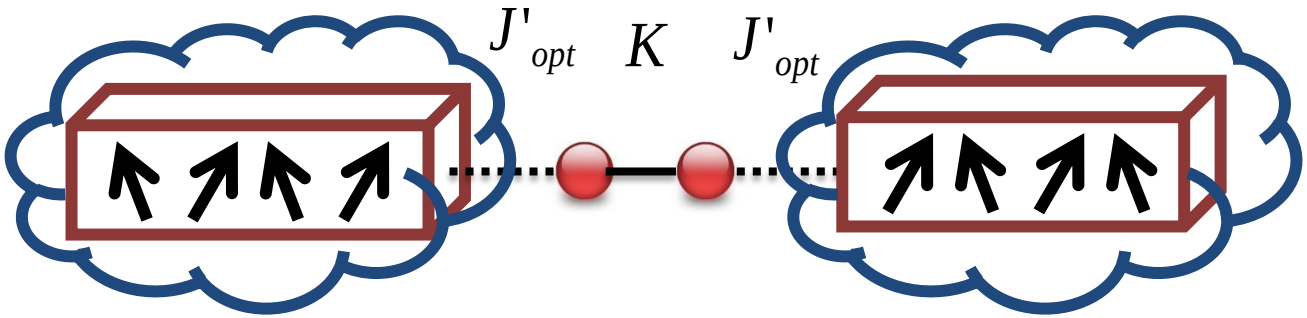


$$s(\rho_L) = s(\rho_R) = -\sum_n \lambda_n \log(\lambda_n)$$

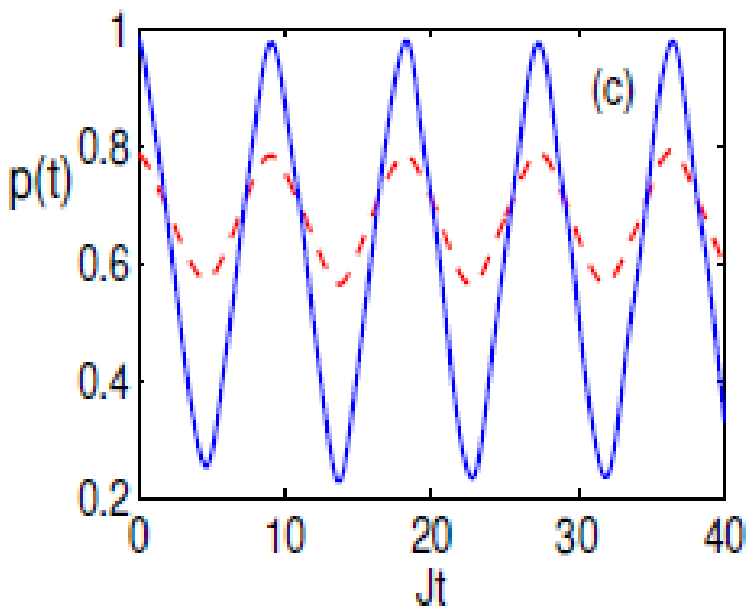


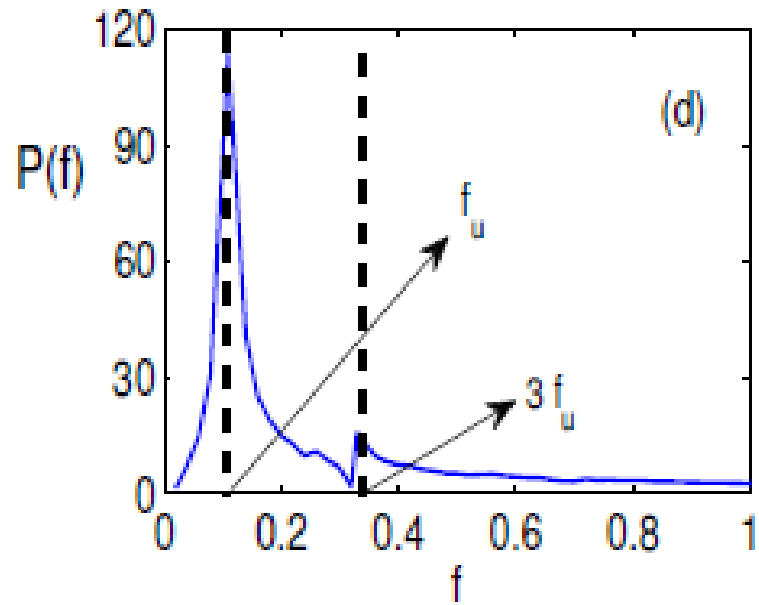


Singlet fraction



$$\rho_{1_L,1_R}(t) = p(t)|\psi^-\rangle\langle\psi^-| + \frac{1-p(t)}{3}\sum_{n=0,\pm}|T^n\rangle\langle T^n|$$





Summary

- Impurity systems show exotic quantum phase transitions which do not fit in the Landau-Ginzburg paradigm.
- The emergence of a diverging length scale near criticality implies that entanglement has to be multi-partite.
- In order to capture the multipartite entanglement one has to take more complex quantities such as Schmidt gap and Negativity.
- Schmidt gap plays like an order parameter for iQPTs.
- Negativity, as both bipartite and tripartite entanglement, provides a coarse-grained view of multipartite entanglement via scaling.

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  E. S. Sørensen, K. Le Hur
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  A. Bayat, S. Bose, P. Sodano, H. Johannesson
  Phys. Rev. Lett. 109, 066403 (2012)