

Entanglement of Fermions at Quantum Criticality: Exact Results

Henrik Johannesson
University of Gothenburg, Sweden

in collaboration with

Daniel Larsson
University of Birmingham, UK



Outline

Entanglement: some basics

Outline

Entanglement: some basics

Entanglement and quantum phase transitions (QPTs)

Outline

Entanglement: some basics

Entanglement and quantum phase transitions (QPTs)

Fermionic entanglement at QPTs

Outline

Entanglement: some basics

Entanglement and quantum phase transitions (QPTs)

Fermionic entanglement at QPTs

A case study: the 1D Hubbard model

Outline

Entanglement: some basics

Entanglement and quantum phase transitions (QPTs)

Fermionic entanglement at QPTs

A case study: the 1D Hubbard model

Effects from boundaries and impurities?

Outline

Entanglement: some basics

Entanglement and quantum phase transitions (QPTs)

Fermionic entanglement at QPTs

A case study: the 1D Hubbard model

Effects from boundaries and impurities?

Summary

Outline

Entanglement: some basics

Entanglement and quantum phase transitions (QPTs)

Fermionic entanglement at QPTs

A case study: the 1D Hubbard model

Effects from boundaries and impurities

Summary

Entanglement: some basics

“...best possible knowledge of a whole does not necessarily include the same for its parts. [...] The whole is in a definite state, the parts taken individually are not. [This is] not one, but the essential trait of the new theory, the one which forces a complete departure from all classical concepts.” *Schrödinger, 1935*



Entanglement: some basics

“...best possible knowledge of a whole does not necessarily include the same for its parts. [...] The whole is in a definite state, the parts taken individually are not. [This is] not one, but the essential trait of the new theory, the one which forces a complete departure from all classical concepts.” *Schrödinger, 1935*



Einstein, Podolsky, Rosen 1935



non-local quantum correlations

“...spooky action at a distance” (Einstein)

violation of “local realism” (*Bell’s inequalities*)
verified experimentally (*Aspect et al. 1982*)

Entanglement: some basics

Entanglement is a *physical resource*

Quantum cryptography



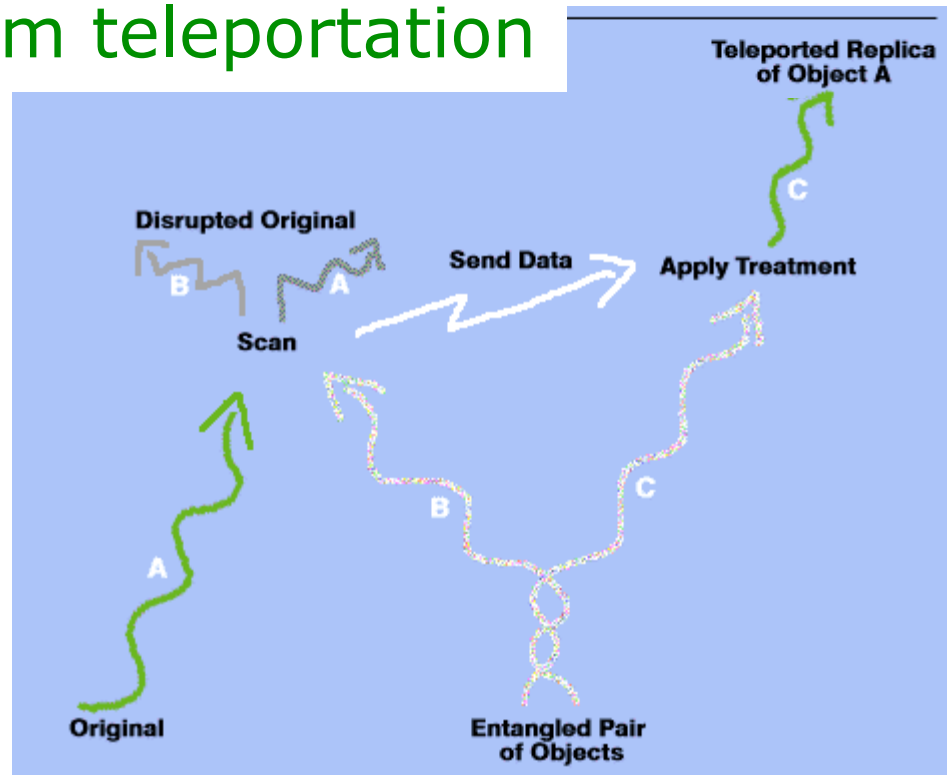
Quantum mechanics at work:
Installing an optical quantum channel
at the Austrian-Croatian border, 2005

Entanglement: some basics

Entanglement is a *physical resource*

Quantum cryptography

Quantum teleportation



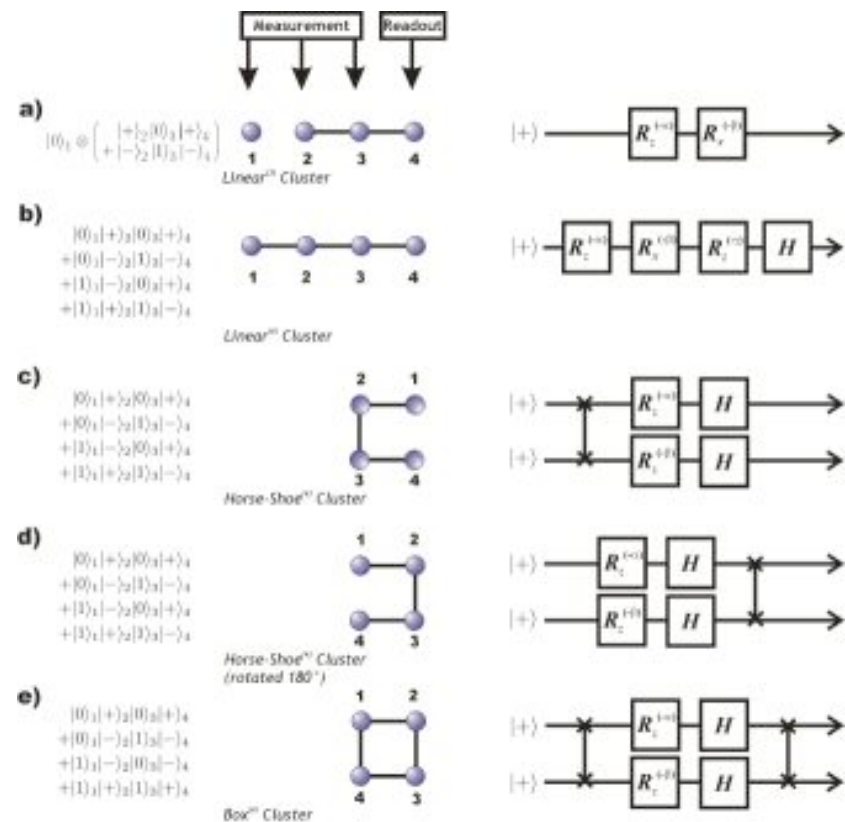
Entanglement: some basics

Entanglement is a *physical resource*

Quantum cryptography

Quantum teleportation

Quantum computing



Entanglement: some basics

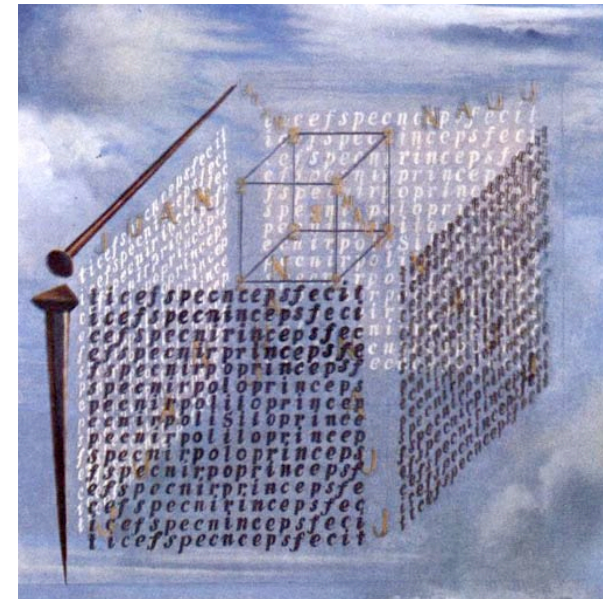
Entanglement is a *physical resource*

Quantum cryptography

Quantum teleportation

Quantum computing

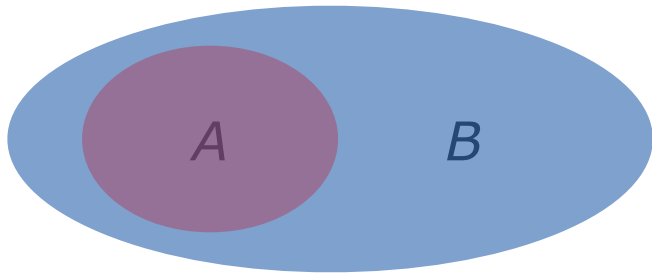
Future technologies?



S. Dali, "Linear Cube"

Entanglement: some basics

If entanglement is a *resource*, how to quantify it?



quantum system in a **pure state** $|\Psi(A, B)\rangle$

How “much” entanglement \mathcal{E} between A and B ?

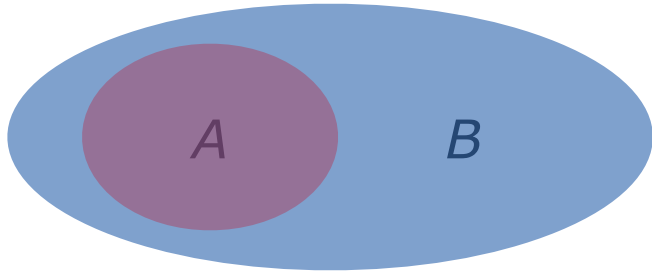
Bennett et al., PRA 53, 2046 (1996):

$$\mathcal{E} = -\text{Tr}(\rho_A \log \rho_A) \quad \text{“von Neumann entropy”}$$

$$\rho_A = \text{Tr}_B \rho = \text{Tr}_B |\Psi(A, B)\rangle \langle \Psi(A, B)|$$

Entanglement: some basics

If entanglement is a *resource*, how to quantify it?



quantum system in a **pure state** $|\Psi(A, B)\rangle$

How “much” entanglement \mathcal{E} between A and B ?

Bennett et al., PRA 53, 2046 (1996):

$$\mathcal{E} = -\text{Tr}(\rho_A \log \rho_A) \quad \text{“von Neumann entropy”}$$



unique measure of (bipartite)
entanglement in a *pure* state

- *non-increasing under local transformations*
- *vanishing for separable states*
- *additive*

Entanglement: some basics

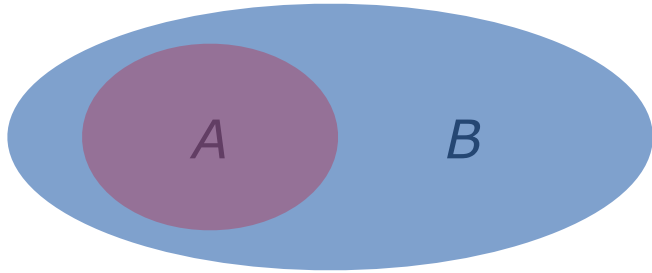
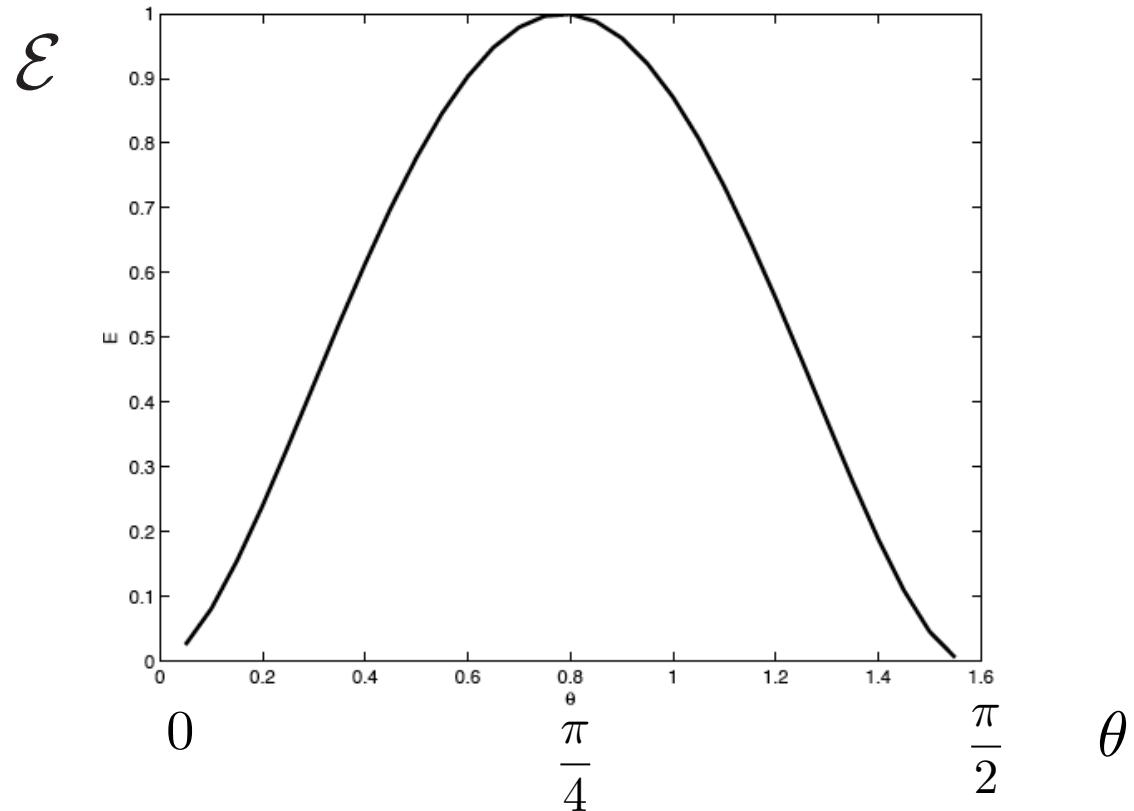
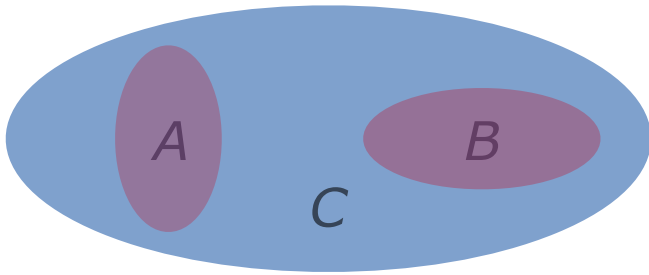


Illustration:

$$|\Psi(A, B)\rangle = \cos \theta |\uparrow\rangle_A |\downarrow\rangle_B + \sin \theta |\downarrow\rangle_A |\uparrow\rangle_B$$



Entanglement: some basics



A+B in a **mixed state** $\rho_{AB} = \sum_i p_i |\psi_i(A, B)\rangle\langle\psi_i(A, B)|$
(after tracing out C)

How “much” entanglement between A and B?

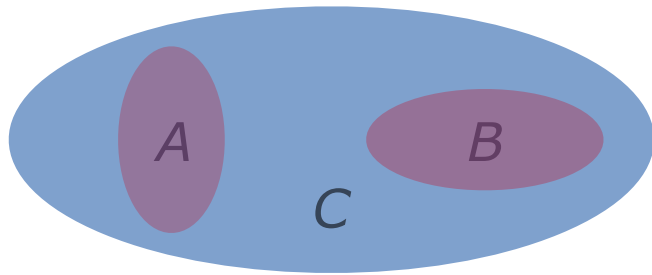
computable measure for **qubit** (“two-level”) systems: CONCURRENCE

$$C = \max\{0, \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}\}$$

$\lambda_1, \lambda_2, \lambda_3, \lambda_4$ ordered eigenvalues to $\rho_{AB} \times (\rho_{AB})^*$

Wootters, PRL 80, 2245 (1998)

Entanglement: some basics



A+B in a **mixed state** $\rho_{AB} = \sum_i p_i |\psi_i(A, B)\rangle\langle\psi_i(A, B)|$
(after tracing out C)

How “much” entanglement between A and B?

encodes the
“Entanglement of formation”

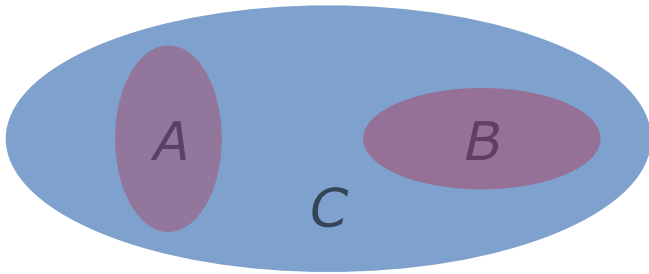
computable measure for **qubit** (“two-level”) systems: CONCURRENCE

$$C = \max\{0, \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}\}$$

$\lambda_1, \lambda_2, \lambda_3, \lambda_4$ ordered eigenvalues to $\rho_{AB} \times (\rho_{AB})^*$

Wootters, PRL 80, 2245 (1998)

Entanglement: some basics



A+B in a **mixed state** $\rho_{AB} = \sum_i p_i |\psi_i(A, B)\rangle\langle\psi_i(A, B)|$

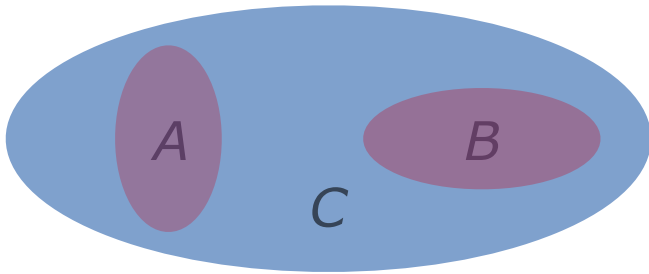
RECIPE
Entanglement of formation



- form all possible ensembles $\Omega = \{p_i, |\psi_i(A, B)\rangle\}$ that realize ρ_{AB}
- for each state in a given Ω , calculate $\mathcal{E}_i = -\text{Tr}(\rho_A \log \rho_A)_i$
- find the minimal average entanglement over all ensembles

$$\mathcal{E}_F(\rho_{AB}) = \min_{\{\Omega\}} \sum_i p_i \mathcal{E}_i$$

Entanglement: some basics



A+B in a **mixed state** $\rho_{AB} = \sum_i p_i |\psi_i(A, B)\rangle\langle\psi_i(A, B)|$

RECIPE
Entanglement of formation



- form all possible ensembles $\Omega = \{p_i, |\psi_i(A, B)\rangle\}$ that realize ρ_{AB}
- for each state in a given Ω , calculate $\mathcal{E}_i = -\text{Tr}(\rho_A \log \rho_A)_i$
- find the minimal average entanglement over all ensembles

$$\mathcal{E}_F(\rho_{AB}) = \min_{\{\Omega\}} \sum_i p_i \mathcal{E}_i$$

Wootters, PRL 80, 2245 (1998) $\mathcal{E}_F = h\left(\frac{1}{2}(1 + \sqrt{1 - C(\rho)^2})\right)$ for qubit systems

Why study entanglement of many-body quantum systems?

- Identify useful Hamiltonians to produce and control entangled states
 - New schemes for quantum computing...
“topological quantum computing”, “one-way quantum computing”,...
 - Get information about properties of complex ground state wave functions (without calculating them explicitly!)
- Identify and characterize ***quantum phase transitions (QPTs)***
A. Osterloh et al., Nature 416, 608 (2002)
T. Osborne and M. Nielsen, PRA 66, 032110 (2002)

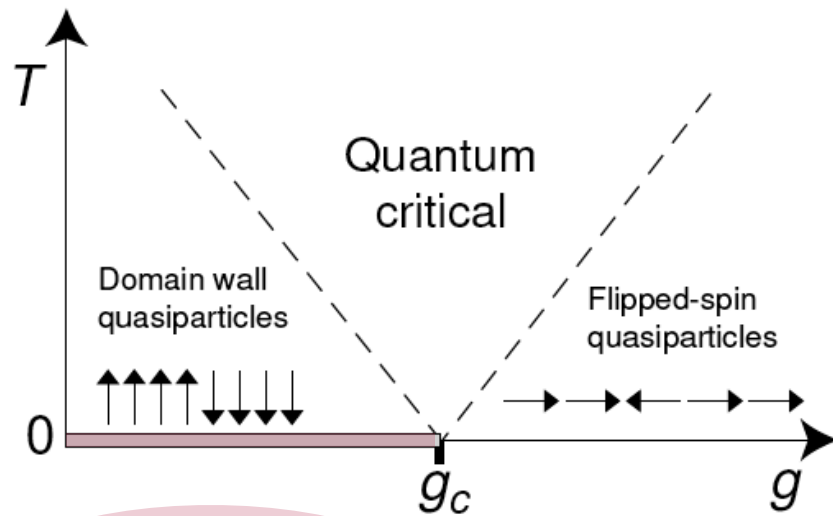
What is a quantum phase transition?

Example: quantum Ising chain

$$H_I = -J \sum_{j=1}^{N-1} \hat{\sigma}_j^z \hat{\sigma}_{j+1}^z - gJ \sum_{j=1}^N \hat{\sigma}_j^x,$$

What is a quantum phase transition?

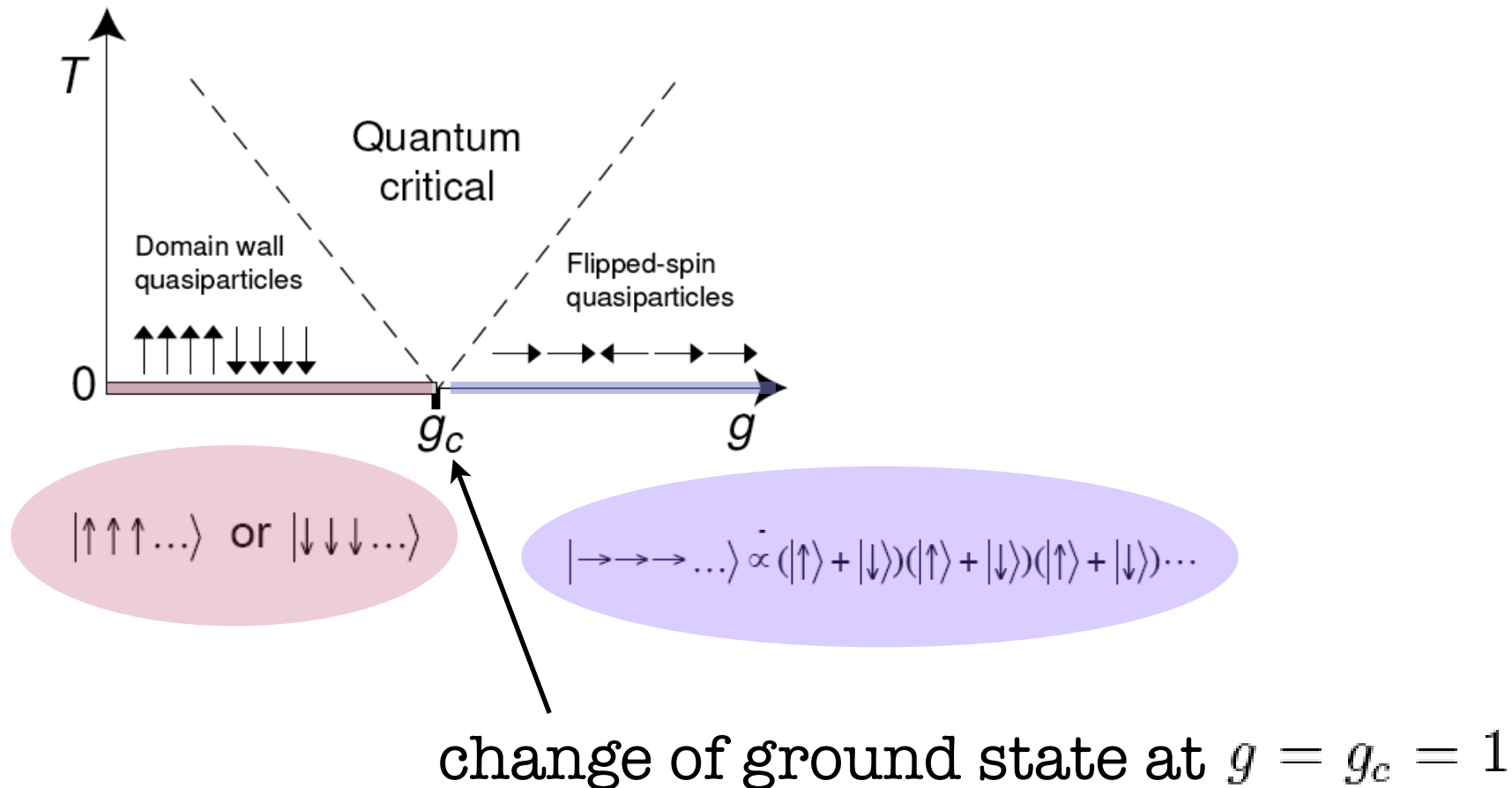
$$H_I = -J \sum_{j=1}^{N-1} \hat{\sigma}_j^z \hat{\sigma}_{j+1}^z - gJ \sum_{j=1}^N \hat{\sigma}_j^x,$$



$|\uparrow\uparrow\uparrow\dots\rangle$ or $|\downarrow\downarrow\downarrow\dots\rangle$

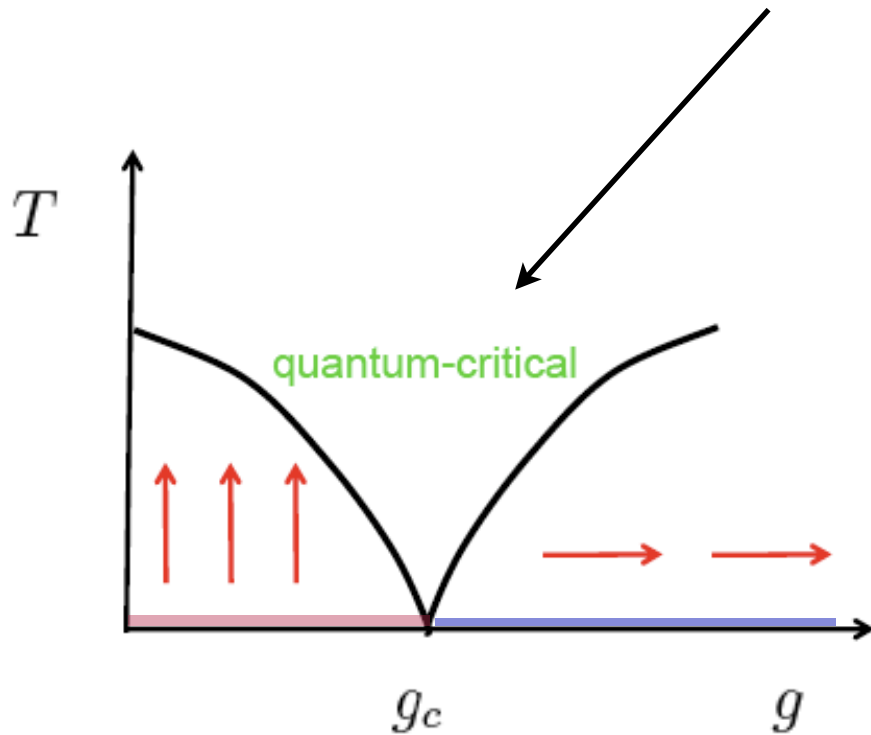
What is a quantum phase transition?

$$H_I = -J \sum_{j=1}^{N-1} \hat{\sigma}_j^z \hat{\sigma}_{j+1}^z - gJ \sum_{j=1}^N \hat{\sigma}_j^x,$$



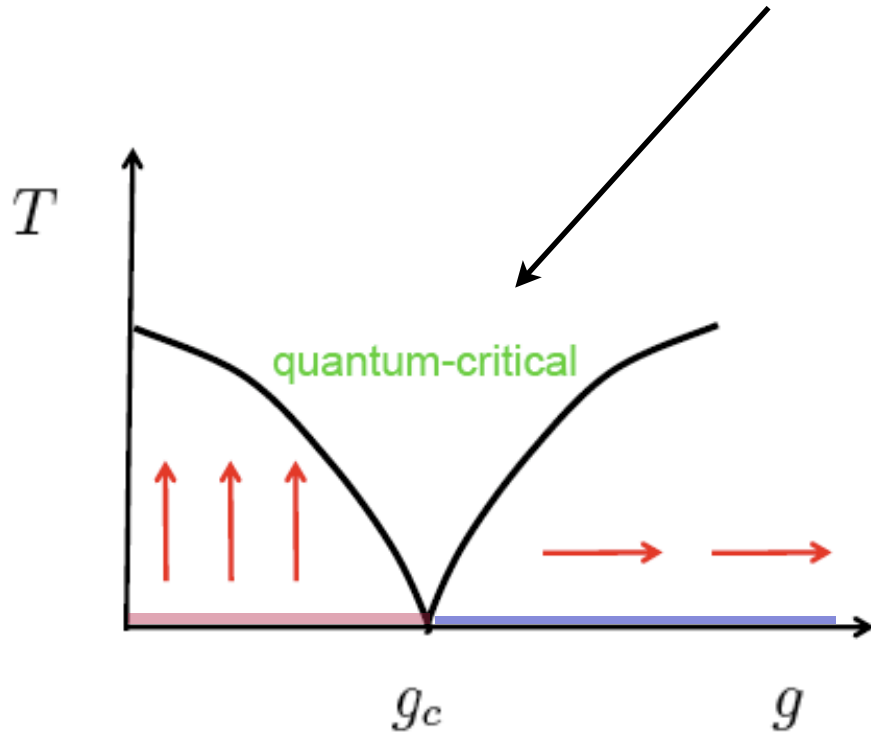
What is a quantum phase transition?

breakdown of “text book” condensed matter physics:
anomalous **non-Fermi liquid behavior** (“heavy electrons”, high T_c ?,...)

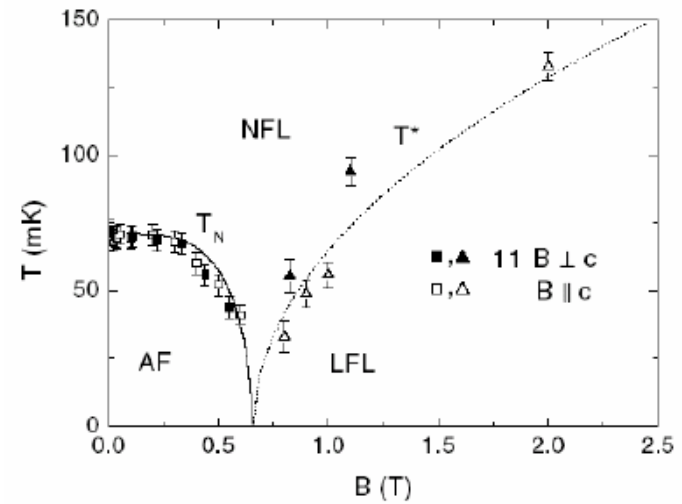


What is a quantum phase transition?

breakdown of “text book” condensed matter physics:
anomalous **non-Fermi liquid behavior** (“heavy electrons”, high T_c ?,...)

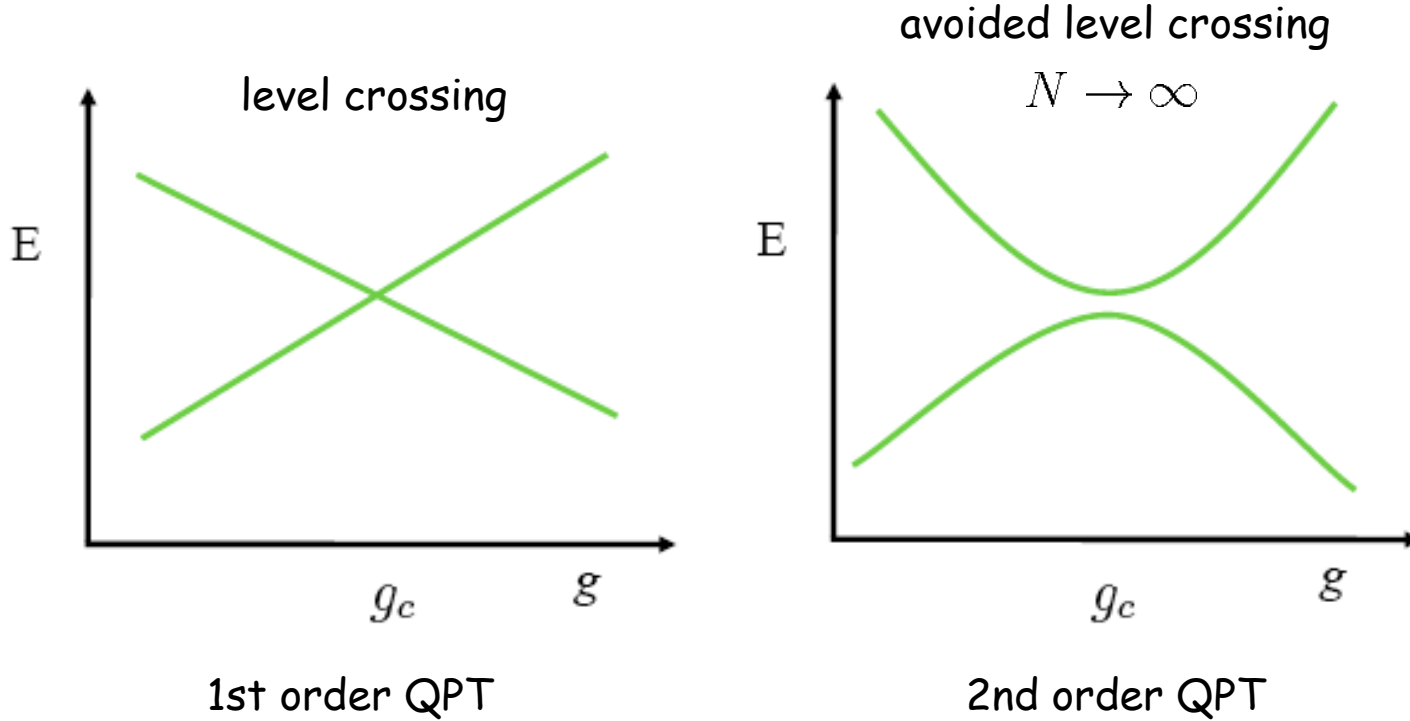


Quantum critical point in
 YbRh_2Si_2



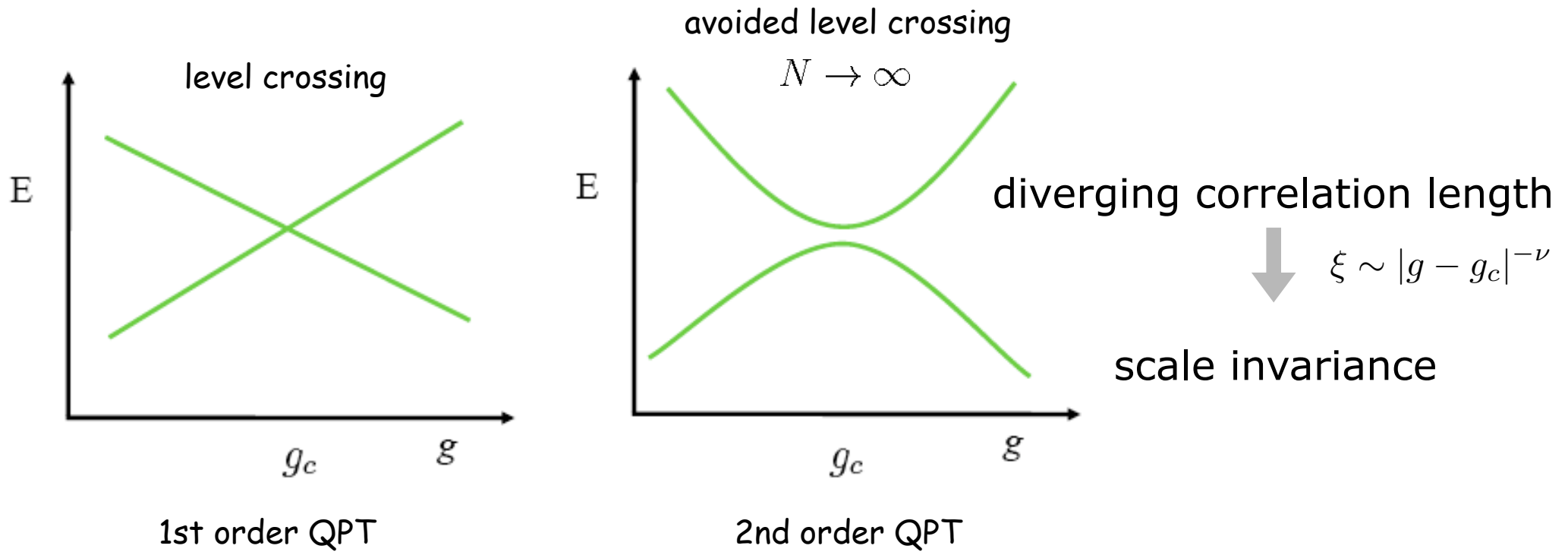
Gegenwart et al., PRL 89:56402(2002)

What is a quantum phase transition?



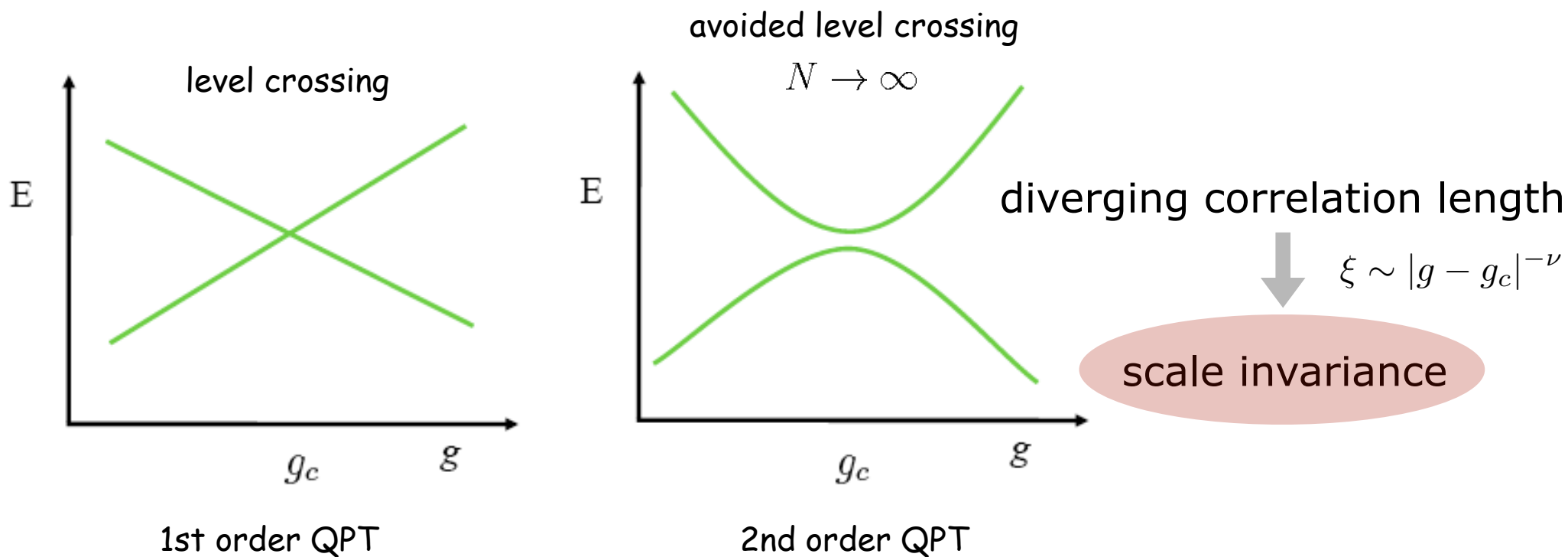
non-analytic ground state energy \rightarrow non-analytic density matrix

What is a quantum phase transition?



non-analytic ground state energy \rightarrow non-analytic density matrix

What is a quantum phase transition?



non-analytic ground state energy



non-analytic density matrix

How does this show up in the **ground state entanglement**?

What can we learn from it?

Spin-1/2 models (interacting qubits on a lattice)

Large body of (mostly numerical) results on spin chains and spin ladders (with or without frustration):



“A discontinuity [divergence] in the [first derivative of the] ground state **concurrence** between neighboring spins is associated with a first [second] order QPT.”

L.-A. Wu et al., PRL 93, 250404 (2004)

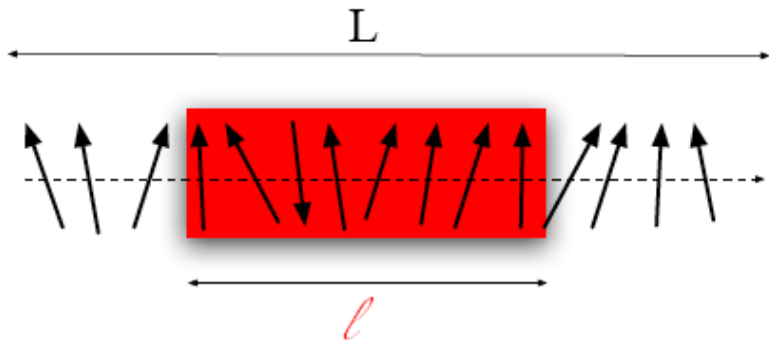
Expected from the theory of critical phenomena!
L. Campos Venuti et al., PRA 73, R010303 (2006)

Spin-1/2 models

Large body of results...



Scale invariance at criticality is reflected in the **block (von Neumann) entropy**



Example: $\Delta = 1$ transition in the XXZ chain

$$\mathcal{H} = \sum_i S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z$$

$$S_\ell = \frac{c}{3} \log_2 \left[\frac{L}{\pi a} \sin \left(\frac{\pi}{L} \ell \right) \right] + A$$

J.I. Latorre et al., Quant. Inf. and Comp. 4, 48 (2004)

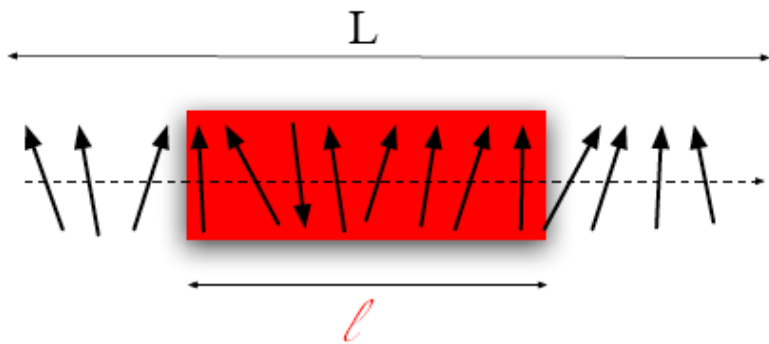
General CFT setting:

P. Calabrese and J. Cardy, J. Stat. Mech., P06002 (2004)

V.E. Korepin, PRL 92, 096402 (2004)

Spin-1/2 models

Scale invariance at criticality is reflected in the **block (von Neumann) entropy**



c-number labels the “universality class” to which the critical theory belongs

$$S_\ell = \frac{c}{3} \log_2 \left[\frac{L}{\pi a} \sin \left(\frac{\pi}{L} \ell \right) \right] + A$$

J.I. Latorre et al., Quant. Inf. and Comp. 4, 48 (2004)

General CFT setting:

P. Calabrese and J. Cardy, J. Stat. Mech., P06002 (2004)

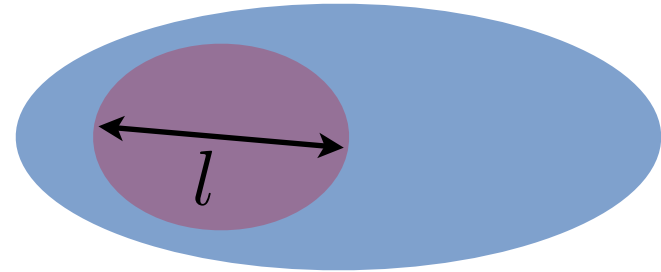
V.E. Korepin, PRL 92, 096402 (2004)

Spin-1/2 models

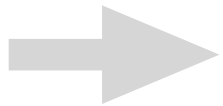
$$S_\ell = \frac{c}{3} \log_2 \left[\frac{L}{\pi a} \sin \left(\frac{\pi}{L} \ell \right) \right] + A$$

The logarithmic scaling of the block entanglement in 1D critical spin systems violates the expected “area law” for entanglement

$$S_l \sim (l/a)^{d-1}$$



L. Bombelli et al. (1986)
M. Srednicki (1993)



“strong” entanglement in 1D critical systems!

Spin-1/2 models

Many other results for entanglement in spin-1/2 systems in 1D (***and*** 2D!)

- *effect of boundaries*
- *"topological states" on spin lattices*
(Kitaev model, quantum dimer model,...)
- *impurities*
- *"quantum quenches"*
- *disorder*
- *.....*

For a review, see the special issue of J. Phys. A, soon to appear

Entanglement of itinerant particles?

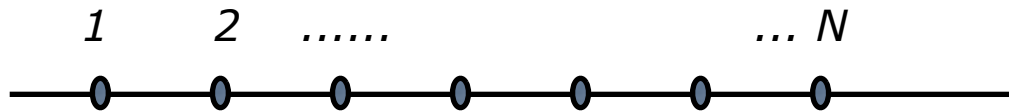
What about interacting **fermions** on a (1D) lattice?

Anti-symmetrization of fermion states:
physical Hilbert space lacks a direct product structure

How to define *entanglement*?

Use an occupation number representation!

P. Zanardi, PRA 65, 042101 (2002)



$$\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \dots \otimes \mathcal{H}_N$$

$$|n\rangle_j = |0\rangle_j, |\uparrow\rangle_j, |\downarrow\rangle_j, |\uparrow\downarrow\rangle_j \quad j=1, \dots, N$$

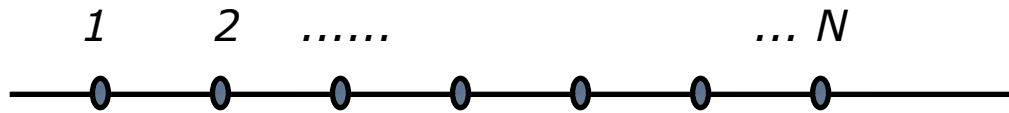
What about interacting **fermions** on a (1D) lattice?

Anti-symmetrization of fermion states:
physical Hilbert space lacks a direct product structure

How to define *entanglement*?

Use an occupation number representation!

P. Zanardi, PRA 65, 042101 (2002)



$$\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \dots \otimes \mathcal{H}_N$$

$$|n\rangle_j = |0\rangle_j, |\uparrow\rangle_j, |\downarrow\rangle_j, |\uparrow\downarrow\rangle_j \quad j=1, \dots, N$$

Entanglement of Fermions at Quantum Criticality

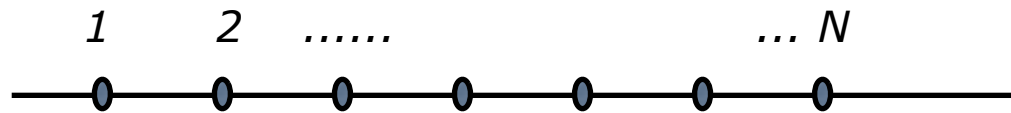
What about interacting **fermions** on a (1D) lattice?

Anti-symmetrization of fermion states:
physical Hilbert space lacks a direct product structure

How to define *entanglement*?

Use an occupation number representation!

P. Zanardi, PRA 65, 042101 (2002)



$$\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \dots \otimes \mathcal{H}_N$$

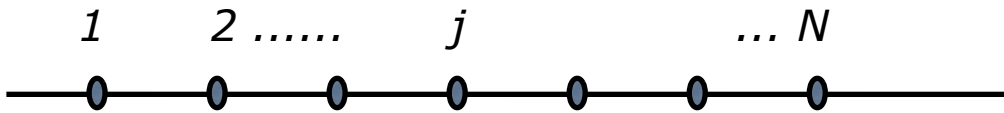
$$|n\rangle_j = |0\rangle_j, |\uparrow\rangle_j, |\downarrow\rangle_j, |\uparrow\downarrow\rangle_j \quad j=1, \dots, N$$

states describing the fermionic
occupancies of the sites on a lattice

~~Entanglement of Fermions
at Quantum Criticality~~

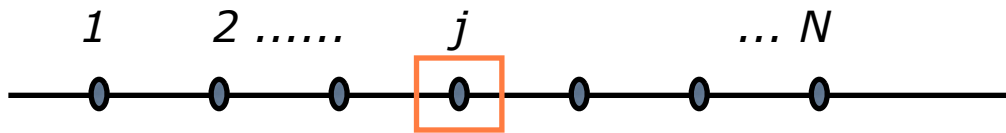
Fermionic entanglement

Introduce a translationally invariant Hamiltonian $\mathcal{H}(g) = \mathcal{H}_0 + g\Lambda$ that *conserves total spin and particle number*



Fermionic entanglement

Introduce a translationally invariant Hamiltonian $\mathcal{H}(g) = \mathcal{H}_0 + g\Lambda$ that *conserves total spin and particle number*



diagonal reduced density matrix

$$\rho_j = \sum_{\alpha=0,\uparrow,\downarrow} w_\alpha |\alpha\rangle_j \langle \alpha|_j + w_2 |\uparrow\downarrow\rangle_j \langle \uparrow\downarrow|_j$$

expectation value of double occupancy $\rightarrow w_2 = \langle \psi_0 | \hat{n}_{j\uparrow} \hat{n}_{j\downarrow} | \psi_0 \rangle$, average single-site occupation

$$w_\uparrow = \langle \psi_0 | \hat{n}_{j\uparrow} | \psi_0 \rangle - w_2 = \frac{n}{2} + m - w_2,$$

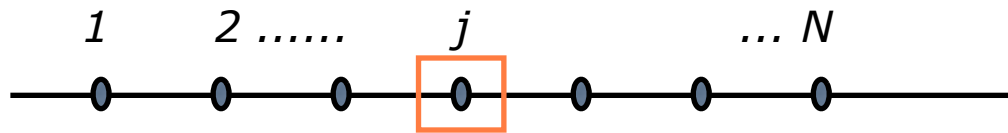
average magnetization

$$w_\downarrow = \langle \psi_0 | \hat{n}_{j\downarrow} | \psi_0 \rangle - w_2 = \frac{n}{2} - m - w_2,$$

$$w_0 = 1 - n + w_2,$$

Fermionic entanglement

Introduce a translationally invariant Hamiltonian $\mathcal{H}(g) = \mathcal{H}_0 + g\Lambda$ that *conserves total spin and particle number*



diagonal reduced density matrix

$$\rho_j = \sum_{\alpha=0,\uparrow,\downarrow} w_\alpha |\alpha\rangle_j \langle \alpha|_j + w_2 |\uparrow\downarrow\rangle_j \langle \uparrow\downarrow|_j$$



single-site entanglement

$$\mathcal{E} = -w_0 \log_2 w_0 - w_\uparrow \log_2 w_\uparrow - w_\downarrow \log_2 w_\downarrow - w_2 \log_2 w_2$$

A rectangular box containing the text m, n, w_2 . Three grey arrows originate from the box: one points to the w_0 term, one to the w_\uparrow term, and one to the w_2 term in the equation above.

Fermionic entanglement

$$\mathcal{H}(g) = \mathcal{H}_0 + g\Lambda$$

Suppose that

$\partial^{k-1} \mathcal{E} / \partial g^{k-1}$ is singular at $g = g_c$



**g = magnetic field
chemical potential
local interaction**

Fermionic entanglement

$$\mathcal{H}(g) = \mathcal{H}_0 + g\Lambda$$

Suppose that

$\partial^{k-1} \mathcal{E} / \partial g^{k-1}$ is singular at $g = g_c$



$g =$ magnetic field
chemical potential
local interaction

m

n

w_2

Fermionic entanglement

$$\mathcal{H}(g) = \mathcal{H}_0 + g\Lambda$$

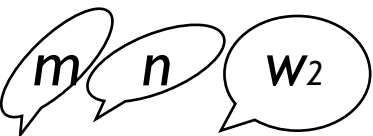
Suppose that

$$\partial^{k-1} \mathcal{E} / \partial g^{k-1} \text{ is singular at } g = g_C$$



**g = magnetic field
chemical potential
local interaction**

$$\partial^{k-1} \mathcal{O}_g / \partial g^{k-1} \text{ singular at } g = g_C$$


$$\mathcal{O}_g \equiv [\langle \psi_0 | \Lambda | \psi_0 \rangle - \text{regular terms}]$$

Fermionic entanglement

$$\mathcal{H}(g) = \mathcal{H}_0 + g\Lambda$$

Suppose that

$$\partial^{k-1} \mathcal{E} / \partial g^{k-1} \text{ is singular at } g = g_C$$



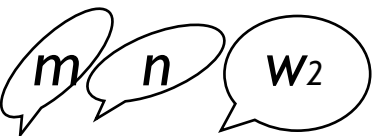
**g = magnetic field
chemical potential
local interaction**

$$\partial^{k-1} \mathcal{O}_g / \partial g^{k-1} \text{ singular at } g = g_C$$



Hellman-Feynman theorem

$$\partial^k e_0 / \partial g^k \text{ singular at } g = g_C$$


$$\mathcal{O}_g \equiv [\langle \psi_0 | \Lambda | \psi_0 \rangle - \text{regular terms}]$$

$$e_0 = \langle \psi_0 | \mathcal{H}(g) | \psi_0 \rangle$$

Fermionic entanglement

$$\mathcal{H}(g) = \mathcal{H}_0 + g\Lambda$$

Suppose that

$$\partial^{k-1} \mathcal{E} / \partial g^{k-1} \text{ is singular at } g = g_c$$



**g = magnetic field
chemical potential
local interaction**

$$\partial^{k-1} \mathcal{O}_g / \partial g^{k-1} \text{ singular at } g = g_c$$

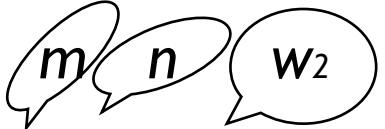


Hellman-Feynman theorem

$$\partial^k e_0 / \partial g^k \text{ singular at } g = g_c$$



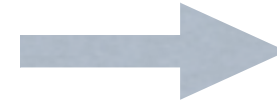
k:th order QPT at $g = g_c$


$$\mathcal{O}_g \equiv [\langle \psi_0 | \Lambda | \psi_0 \rangle - \text{regular terms}]$$

$$e_0 = \langle \psi_0 | \mathcal{H}(g) | \psi_0 \rangle$$

Fermionic entanglement

Divergence/discontinuity in the $k-1$:st derivative of the single-site entanglement

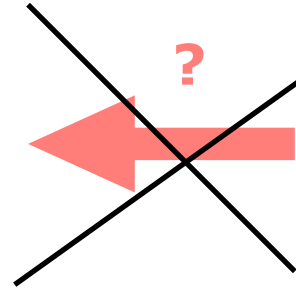


k :th order QPT

D. Larsson and H. Johannesson, PRA 73, 042320 (2006)

Fermionic entanglement

Divergence/discontinuity in the $k-1$:st derivative of the single-site entanglement



k :th order QPT

doesn't apply to

D. Larsson and H. Johannesson, PRA 73, 042320 (2006)

- Kosterlitz-Thouless type transitions (essential singularities!)
- QPTs out of topologically ordered phases (no local order parameters!)

X.-G. Wen, PRB 65, 165113 (2002)

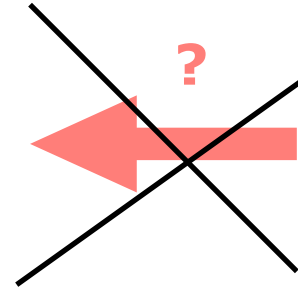
- QPTs with equal weight of the available local states

D. Larsson and H. Johannesson, PRA 73, 042320 (2006)

kills off the non-analyticity in the single-site entanglement!

Fermionic entanglement

Divergence/discontinuity in the $k-1$:st derivative of the single-site entanglement



k :th order QPT

D. Larsson and H. Johannesson, PRA 73, 042320 (2006)

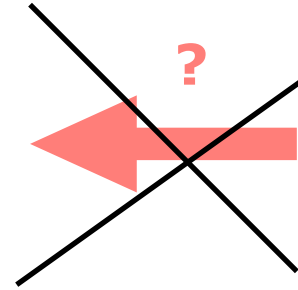
equal weight of the available local states
kills off the non-analyticity

$$\begin{aligned}\frac{\partial^{k-1} \mathcal{E}}{\partial g^{k-1}} = & - \left(\frac{\partial^{k-1}}{\partial g^{k-1}} \left[\frac{n}{2} + m - w_2 \right] \right) \log_2 \left(\frac{n}{2} + m - w_2 \right) \\ & - \left(\frac{\partial^{k-1}}{\partial g^{k-1}} \left[\frac{n}{2} - m - w_2 \right] \right) \log_2 \left(\frac{n}{2} - m - w_2 \right) \\ & + \left(\frac{\partial^{k-1}}{\partial g^{k-1}} [n - w_2] \right) \log_2 (1 - n + w_2) \\ & - \frac{\partial^{k-1} w_2}{\partial g^{k-1}} \log_2 (w_2)\end{aligned}$$

+ terms containing lower-order derivatives

Fermionic entanglement

Divergence/discontinuity in the $k-1$:st derivative of the single-site entanglement



k :th order QPT

equal weight of the available local states
kills off the non-analyticity

$$\begin{aligned}\frac{\partial^{k-1} \mathcal{E}}{\partial g^{k-1}} = & - \left(\frac{\partial^{k-1}}{\partial g^{k-1}} \left[\frac{n}{2} + m - w_2 \right] \right) \log_2 \left(\frac{n}{2} + m - w_2 \right) \\ & - \left(\frac{\partial^{k-1}}{\partial g^{k-1}} \left[\frac{n}{2} - m - w_2 \right] \right) \log_2 \left(\frac{n}{2} - m - w_2 \right) \\ & + \left(\frac{\partial^{k-1}}{\partial g^{k-1}} [n - w_2] \right) \log_2 (1 - n + w_2) \\ & - \frac{\partial^{k-1} w_2}{\partial g^{k-1}} \log_2 (w_2)\end{aligned}$$

+ terms containing lower-order derivatives



$$\partial \mathcal{E} / \partial g = 0$$

extremum of the
single-site entanglement

A case study: the 1D Hubbard model

$$\mathcal{H} = -t \sum_{\substack{j=1 \\ \delta=\pm 1}}^L c_{j\alpha}^\dagger c_{j+\delta\alpha} + U \sum_{j=1}^L n_{j\uparrow} n_{j\downarrow} - \mu_B H \sum_{j=1}^L S_j^z - \mu \sum_{j=1}^L (n_{j\uparrow} + n_{j\downarrow})$$

- minimal model for correlated fermions
- exactly solvable by *Bethe Ansatz*
- exhibits QPTs controlled by U , H , and μ
- realized in optical lattices of ultracold fermionic gases

Moritz et al., PRL 94, 210401 (2005)

Jördens et al., Nature 455, 204 (2008)

A case study: the 1D Hubbard model

$$\mathcal{H} = -t \sum_{\substack{j=1 \\ \delta=\pm 1}}^L c_{j\alpha}^\dagger c_{j+\delta\alpha} + U \sum_{j=1}^L n_{j\uparrow} n_{j\downarrow} - \mu_B H \sum_{j=1}^L S_j^z - \mu \sum_{j=1}^L (n_{j\uparrow} + n_{j\downarrow})$$

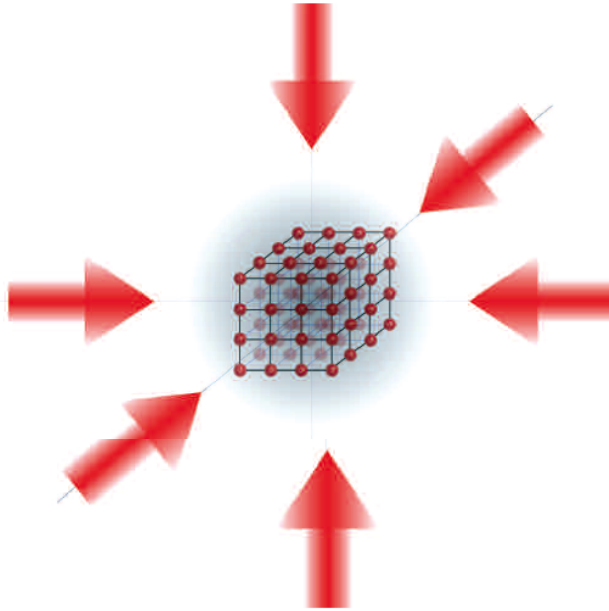
- minimal model for correlated fermions
- exactly solvable by *Bethe Ansatz*
- exhibits QPTs controlled by U , H , and μ
- realized in optical lattices of ultracold fermionic gases

Lieb and Wu, PRL 20, 1445 (1968)

Moritz et al., PRL 94, 210401 (2005)

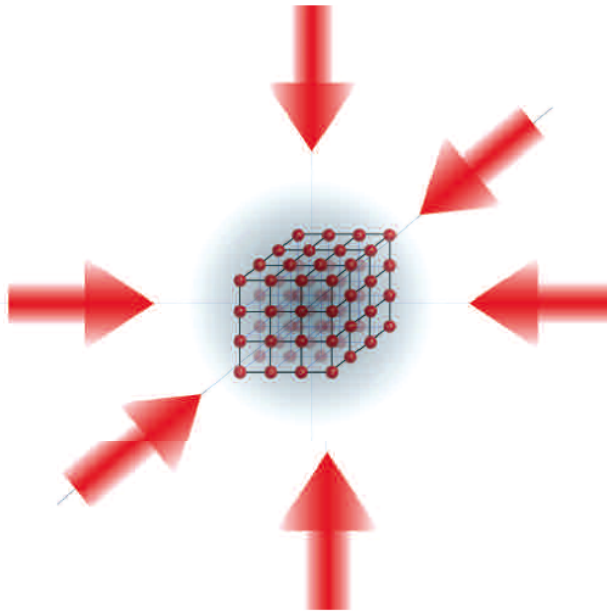
Jördens et al., Nature 455, 204 (2008)

A case study: the 1D Hubbard model



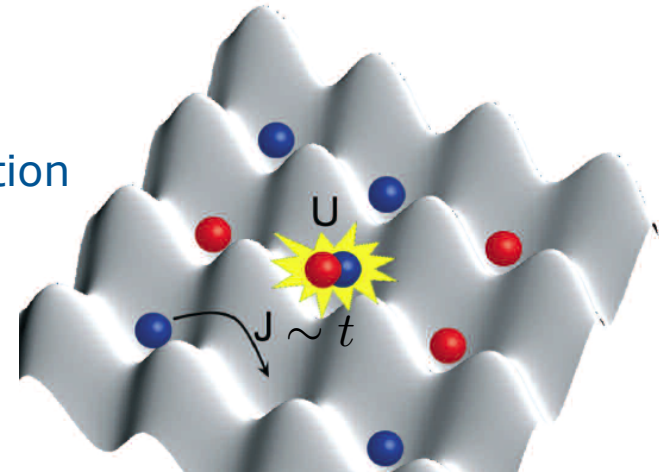
ultracold gas of fermionic atoms (^{40}K)
trapped in an optical lattice produced
by pairs of opposite laser beams

A case study: the 1D Hubbard model



ultracold gas of fermionic atoms (^{40}K)
trapped in an optical lattice produced
by pairs of opposite laser beams

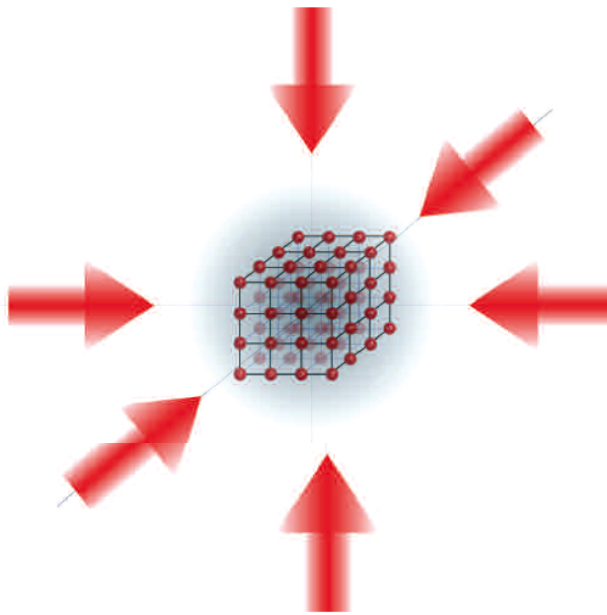
2D intersection
→



$$\mathcal{H} = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \sum_i \mu_i (n_{i\uparrow} + n_{i\downarrow})$$

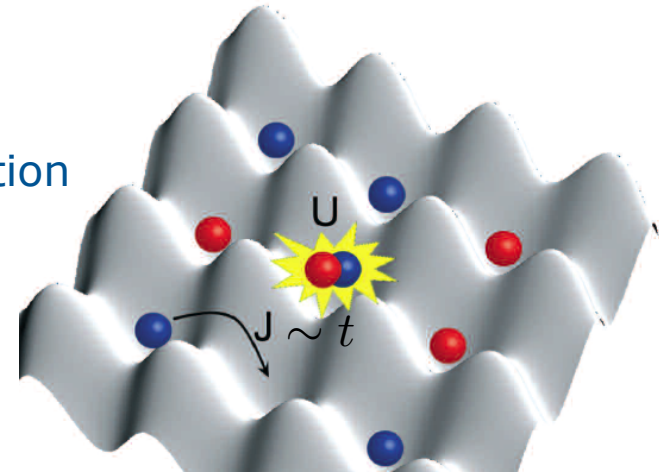
tunneling t and interaction U (determined
by a Feshbach resonance) can be tuned!

A case study: the 1D Hubbard model



ultracold gas of fermionic atoms (^{40}K)
trapped in an optical lattice produced
by pairs of opposite laser beams

2D intersection
→



$$\mathcal{H} = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \sum_i \mu_i (n_{i\uparrow} + n_{i\downarrow})$$

tunneling t and interaction U (determined
by a Feshbach resonance) can be tuned!

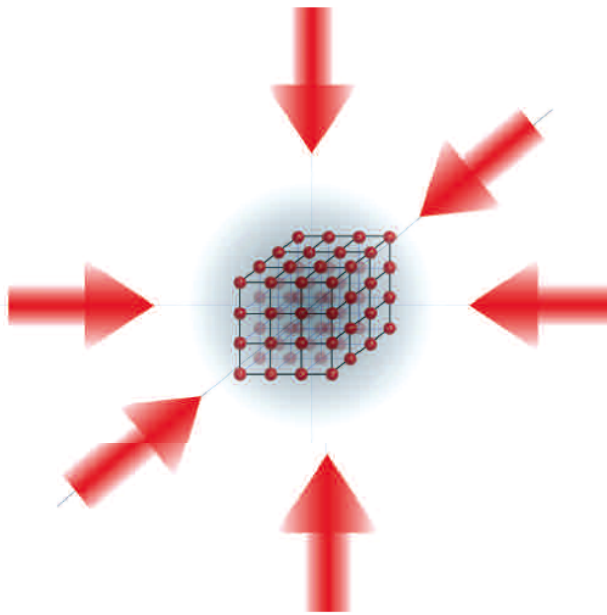
1D geometry created when two pairs of
the laser beams have very high intensity
(suppresses tunneling along these beam
directions)



1D Hubbard model

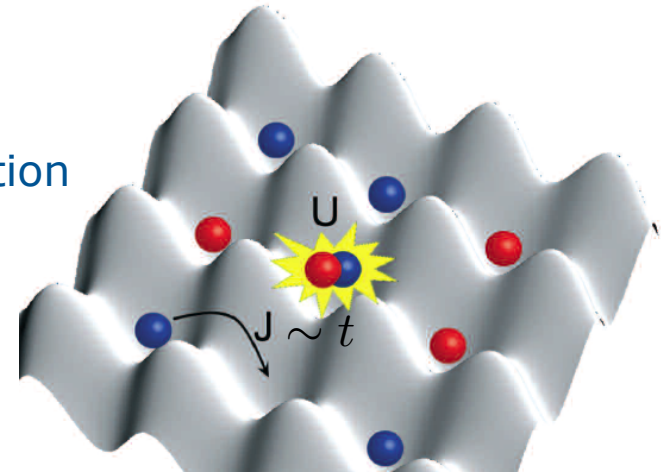
For a review, see
M. Köhl and T. Esslinger, *Europhysics News* 37/2, 18 (2006)

A case study: the 1D Hubbard model



ultracold gas of fermionic atoms (^{40}K)
trapped in an optical lattice produced
by pairs of opposite laser beams

2D intersection



$$\mathcal{H} = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \sum_i \mu_i (n_{i\uparrow} + n_{i\downarrow})$$

tunneling t and interaction U (determined
by a Feshbach resonance) can be tuned!

1D geometry created when two pairs of
the laser beams have very high intensity
(suppresses tunneling along these beam
directions)



1D Hubbard model (with a confining potential)

For a review, see
M. Köhl and T. Esslinger, *Europhysics News* 37/2, 18 (2006)

A case study: the 1D Hubbard model

$$\mathcal{H} = -t \sum_{j=1}^L \sum_{\delta=\pm 1} c_{j\alpha}^\dagger c_{j+\delta\alpha} + U \sum_{j=1}^L n_{j\uparrow} n_{j\downarrow} - \mu_B H \sum_{j=1}^L S_j^z - \mu \sum_{j=1}^L (n_{j\uparrow} + n_{j\downarrow})$$

QPTs at $U = U_c$, $H = H_c$ and $\mu = \mu_c$

How to extract the single-site entanglement?

Recipe:

write $\mathcal{E} = -w_0 \log_2 w_0 - w_\uparrow \log_2 w_\uparrow - w_\downarrow \log_2 w_\downarrow - w_2 \log_2 w_2$

calculate $w_0, w_\uparrow, w_\downarrow, w_2$ from the groundstate energy using the Hellman-Feynman theorem

A case study: the 1D Hubbard model

$$\mathcal{H} = -t \sum_{j=1}^L \sum_{\delta=\pm 1} c_{j\alpha}^\dagger c_{j+\delta\alpha} + U \sum_{j=1}^L n_{j\uparrow} n_{j\downarrow} - \mu_B H \sum_{j=1}^L S_j^z - \mu \sum_{j=1}^L (n_{j\uparrow} + n_{j\downarrow})$$

QPTs at $U = U_c$, $H = H_c$ and $\mu = \mu_c$

How to extract the single-site entanglement?

Recipe:

write $\mathcal{E} = -w_0 \log_2 w_0 - w_\uparrow \log_2 w_\uparrow - w_\downarrow \log_2 w_\downarrow - w_2 \log_2 w_2$

calculate $w_0, w_\uparrow, w_\downarrow, w_2$ from the groundstate energy using the Hellman-Feynman theorem

from the Bethe Ansatz solution of the Hubbard model

E.H. Lieb and F.Y. Wu, PRL 20, 1445 (1968)

A case study: the 1D Hubbard model

Mott-Hubbard transition at half-filling ($n=1$)

$U > 0, H = 0$, control parameter: μ

$$\mathcal{H} = -t \sum_{j=1}^L \sum_{\delta=\pm 1} c_{j\alpha}^\dagger c_{j+\delta\alpha} + U \sum_{j=1}^L n_{j\uparrow} n_{j\downarrow} - \mu_B H \sum_{j=1}^L S_j^z - \mu \sum_{j=1}^L (n_{j\uparrow} + n_{j\downarrow})$$

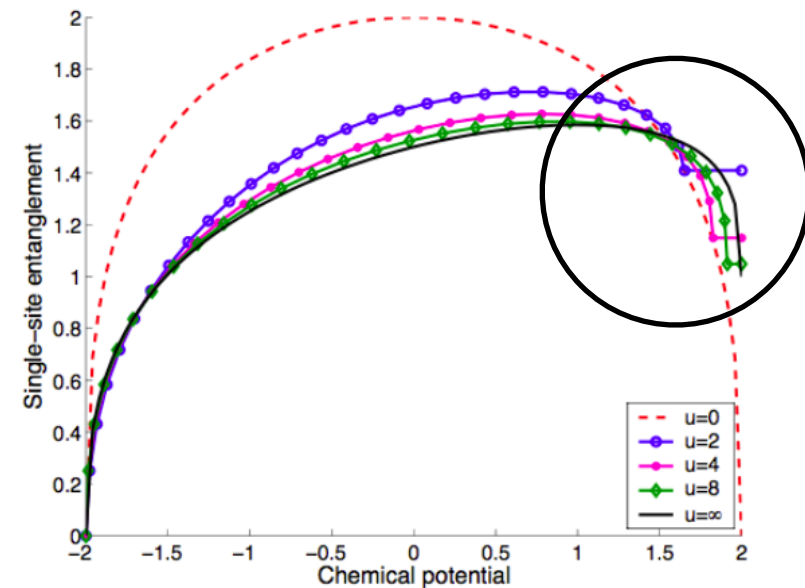
$u \rightarrow \infty$ limit

$$\partial \mathcal{E} / \partial \mu = \chi_c (\ln |\mu - \mu_c| + \text{const.}) / (2 \ln 2)$$

$$\chi_c = \partial n / \partial \mu \sim |\mu - \mu_c|^{-1/2}$$

finite u

$$\partial \mathcal{E} / \partial \mu = \chi_c C(u)$$



D. Larsson and H. Johannesson
PRL 95, 196406 (2005);
ibid. 96, 169906(E) (2006)

A case study: the 1D Hubbard model

Mott-Hubbard transition at half-filling ($n=1$)

$U > 0, H = 0$, control parameter: μ

$$\mathcal{H} = -t \sum_{j=1}^L \sum_{\delta=\pm 1} c_{j\alpha}^\dagger c_{j+\delta\alpha} + U \sum_{j=1}^L n_{j\uparrow} n_{j\downarrow} - \mu_B H \sum_{j=1}^L S_j^z - \mu \sum_{j=1}^L (n_{j\uparrow} + n_{j\downarrow})$$

$u \rightarrow \infty$ limit

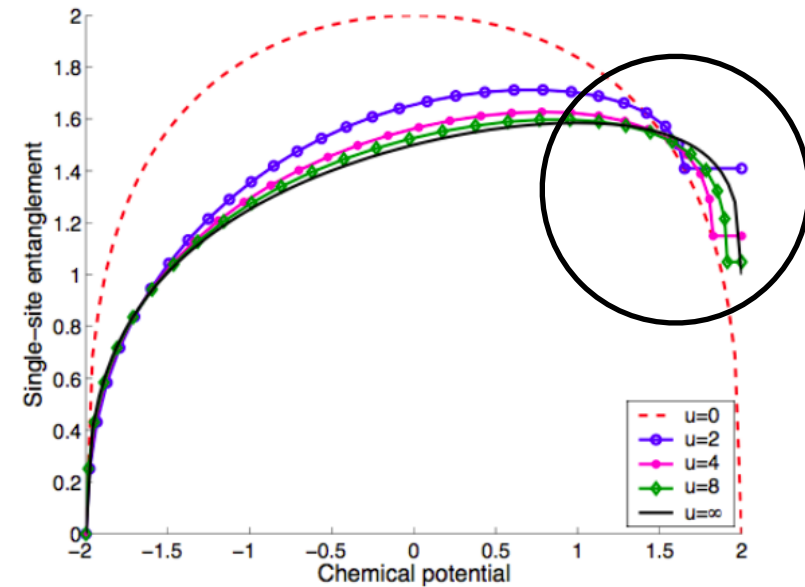
$$\partial \mathcal{E} / \partial \mu = \chi_c (\ln |\mu - \mu_c| + \text{const.}) / (2 \ln 2)$$

$$\chi_c = \partial n / \partial \mu \sim |\mu - \mu_c|^{-1/2}$$

1/u-expansion of the ground state energy
 J. Carmelo and D. Baeriswyl,
 Phys. Rev. B 37, 7541 (1988)

finite u

$$\partial \mathcal{E} / \partial \mu = \chi_c C(u)$$



D. Larsson and H. Johannesson
 PRL 95, 196406 (2005);
 ibid. 96, 169906(E) (2006)

A case study: the 1D Hubbard model

Mott-Hubbard transition at half-filling ($n=1$)

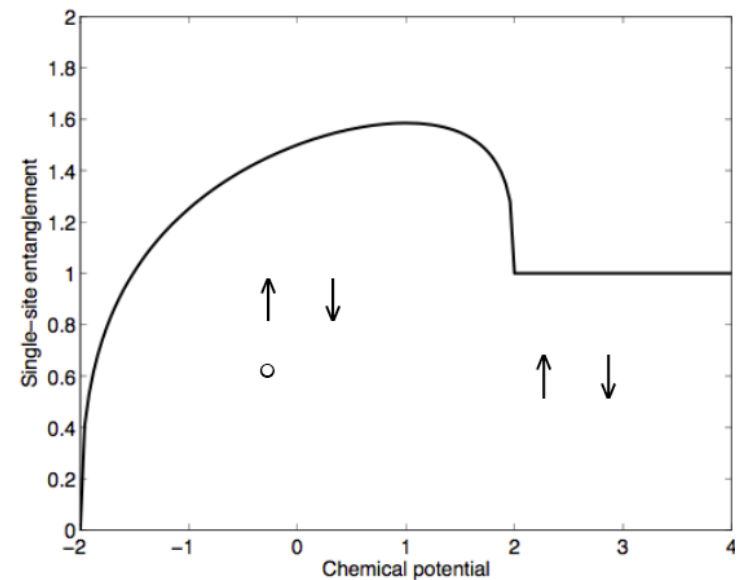
$U > 0$, $H = 0$, control parameter: μ

$$\mathcal{H} = -t \sum_{j=1}^L \sum_{\delta=\pm 1} c_{j\alpha}^\dagger c_{j+\delta\alpha} + U \sum_{j=1}^L n_{j\uparrow} n_{j\downarrow} - \mu_B H \sum_{j=1}^L S_j^z - \mu \sum_{j=1}^L (n_{j\uparrow} + n_{j\downarrow})$$

$u \rightarrow \infty$ limit

$$\partial \mathcal{E} / \partial \mu = \chi_c (\ln |\mu - \mu_c| + \text{const.}) / (2 \ln 2)$$

logarithmic correction
change of "effective"
local dimension



D. Larsson and H. Johannesson
PRL 95, 196406 (2005);
ibid. 96, 169906(E) (2006)

A case study: the 1D Hubbard model

Mott-Hubbard transition at half-filling ($n=1$)

$U > 0, H = 0$, control parameter: μ

$$\mathcal{H} = -t \sum_{j=1}^L \sum_{\delta=\pm 1} c_{j\alpha}^\dagger c_{j+\delta\alpha} + U \sum_{j=1}^L n_{j\uparrow} n_{j\downarrow} - \mu_B H \sum_{j=1}^L S_j^z - \mu \sum_{j=1}^L (n_{j\uparrow} + n_{j\downarrow})$$

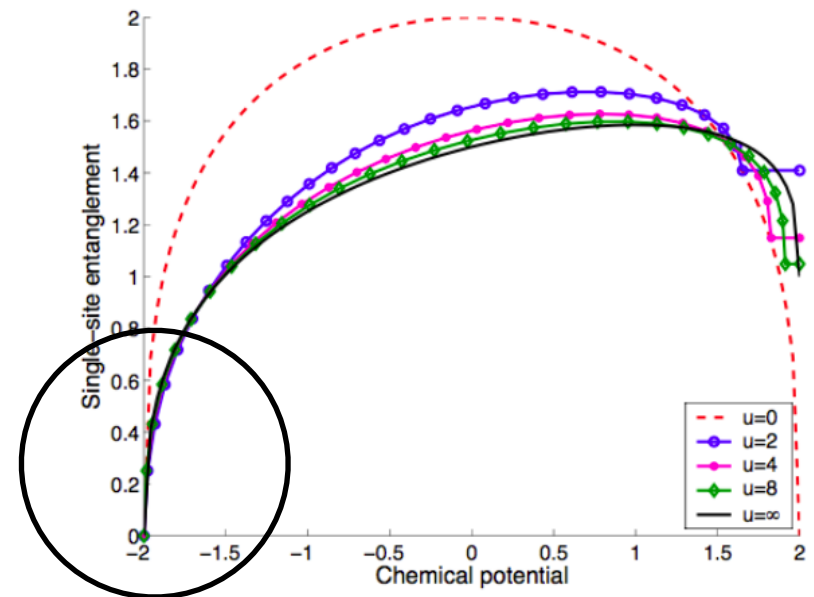
$u \rightarrow \infty$ limit

$$\partial \mathcal{E} / \partial \mu = \chi_c (\ln |\mu - \mu_c| + \text{const.}) / (2 \ln 2)$$

$$\chi_c = \partial n / \partial \mu \sim |\mu - \mu_c|^{-1/2}$$

finite u

$$\partial \mathcal{E} / \partial \mu = \chi_c C(u)$$



empty lattice transition

same scaling as Mott-Hubbard in $u \rightarrow \infty$ limit

D. Larsson and H. Johannesson
PRL 95, 196406 (2005);
ibid. 96, 169906(E) (2006)

A case study: the 1D Hubbard model

repulsive
interaction

Magnetic transitions at half-filling ($n=1$, μ fixed)
 $U > 0$, control parameter: H

$$\mathcal{H} = -t \sum_{j=1}^L \sum_{\delta=\pm 1} c_{j\alpha}^\dagger c_{j+\delta\alpha} + U \sum_{j=1}^L n_{j\uparrow} n_{j\downarrow} - \mu_B H \sum_{j=1}^L S_j^z - \mu \sum_{j=1}^L (n_{j\uparrow} + n_{j\downarrow})$$

saturation at $H = h_{c2}$

any $u > 0$

$$\frac{\partial \mathcal{E}}{\partial h} = \frac{C}{2 \ln(2)} \chi_S (\ln|h - h_{c2}| + \text{const}).$$

$$h \rightarrow h_{c2-} \quad h_{c2} = 4(\sqrt{1+u^2} - u)$$

$$2\pi\chi_S = (4 + 4u^2)^{1/4} |h - h_{c2}|^{-1/2}$$

$$C = 2 - u/\sqrt{1+u^2},$$

A case study: the 1D Hubbard model

attractive
interaction

Magnetic transitions at half-filling ($n=1$, μ fixed)
 $U < 0$, control parameter: H

$$\mathcal{H} = -t \sum_{j=1}^L \sum_{\delta=\pm 1} c_{j\alpha}^\dagger c_{j+\delta\alpha} + U \sum_{j=1}^L n_{j\uparrow} n_{j\downarrow} - \mu_B H \sum_{j=1}^L S_j^z - \mu \sum_{j=1}^L (n_{j\uparrow} + n_{j\downarrow})$$

onset of magnetization at $H=h_{c1}$
 saturation at $H=h_{c2}$

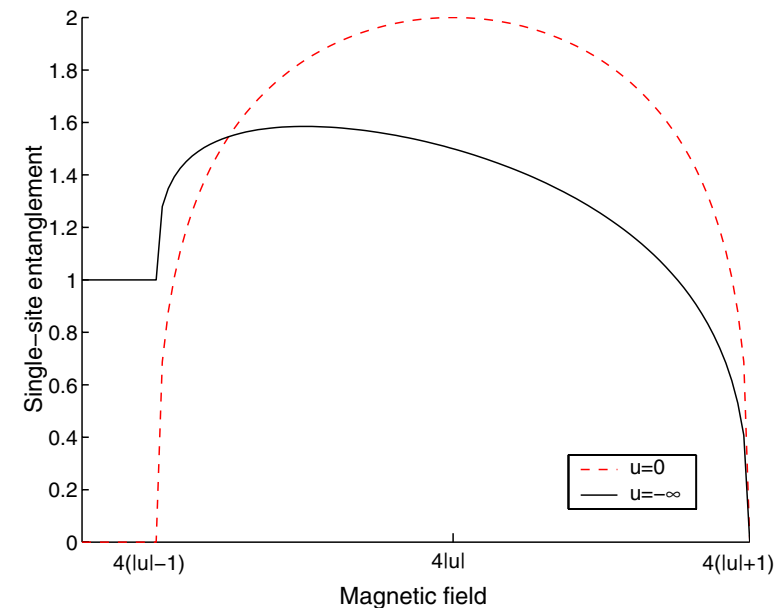
$$|u| \gg 1$$

$$\frac{\partial \mathcal{E}}{\partial h} = (-1)^i \frac{\chi_{Si}}{\ln(2)} (\ln|h - h_{ci}| + \text{const})$$

$$i = 1, 2$$

$$h \rightarrow h_{c1+} \quad h \rightarrow h_{c2-}$$

$$\chi_{Si} = (32\pi^2|h - h_{ci}|)^{-1/2}$$



D. Larsson and H. Johannesson
 PRL 95, 196406 (2005)

A case study: the 1D Hubbard model

Mott-Hubbard transition at $U=0$

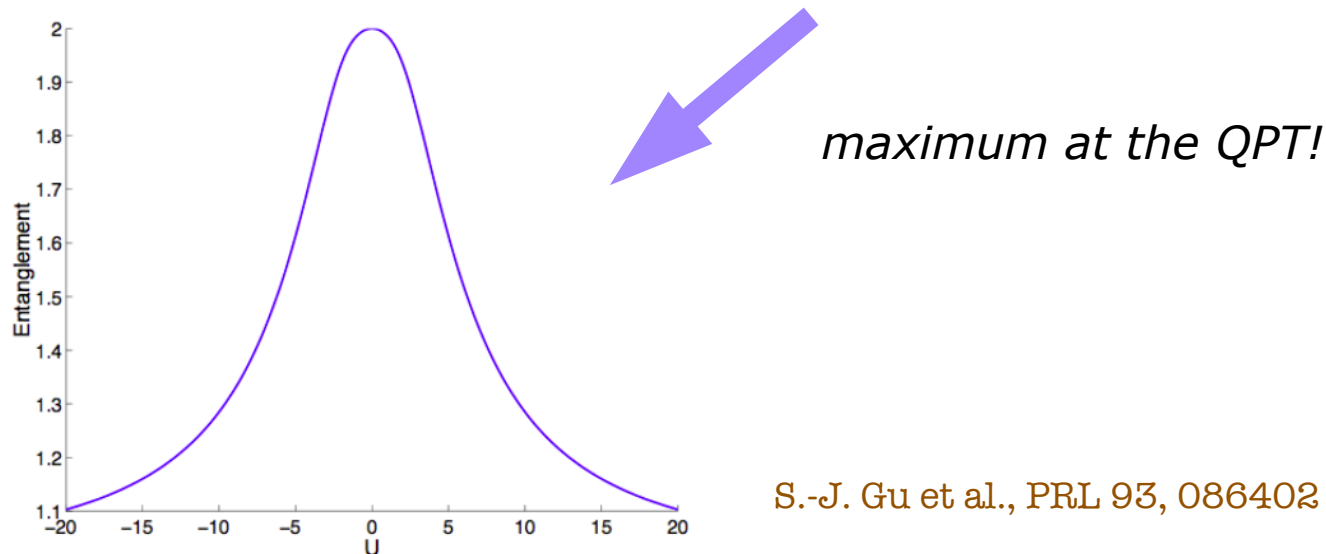
control parameter: U ($H=0$, half-filling)

$$\mathcal{H} = -t \sum_{j=1}^L \sum_{\delta=\pm 1} c_{j\alpha}^\dagger c_{j+\delta\alpha} + U \sum_{j=1}^L n_{j\uparrow} n_{j\downarrow} - \mu_B H \sum_{j=1}^L S_j^z - \mu \sum_{j=1}^L (n_{j\uparrow} + n_{j\downarrow})$$

– QPT of *infinite order* (Kosterlitz-Thouless type)

Metzner and Vollhardt, PRB 39, 4462 (1989)

– $|n\rangle_j = |0\rangle_j, |\uparrow\rangle_j, |\downarrow\rangle_j, |\uparrow\downarrow\rangle_j$ $j=1, \dots, N$ equally weighted at $U=0$



S.-J. Gu et al., PRL 93, 086402 (2004)

Another case study

Hubbard model with long-range hopping

F. Gebhard and A.E. Ruckenstein, PRL 68, 244 (1992)

$$H = \sum_{\substack{\ell \neq m=1 \\ \sigma=\uparrow,\downarrow}}^L t_{\ell m} \hat{c}_{\ell\sigma}^\dagger \hat{c}_{m\sigma} + u \sum_{l=1}^L \hat{n}_{l\uparrow} \hat{n}_{l\downarrow}$$
$$t_{\ell m} = i(-1)^{(l-m)}(l-m)^{-1}$$

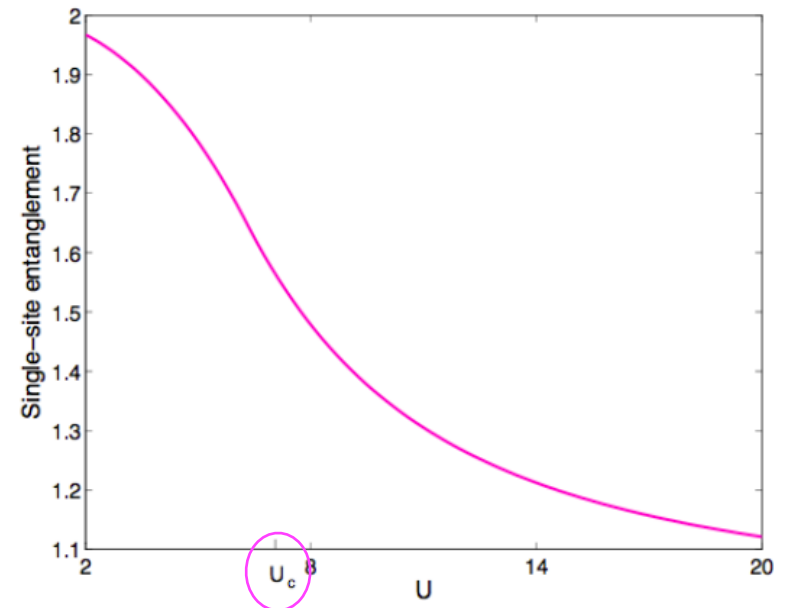
Mott-Hubbard transition

control parameter: u (half-filling)

$\partial^2 \mathcal{E} / \partial u^2$ discontinuous at $u_c = 2\pi$



third-order QPT



D. Larsson and H. Johannesson, PRA 73, 042320 (2006)

Another case study

Hubbard model with long-range hopping

F. Gebhard and A.E. Ruckenstein, PRL 68, 244 (1992)

$$H = \sum_{\substack{\ell \neq m=1 \\ \sigma=\uparrow,\downarrow}}^L t_{\ell m} \hat{c}_{\ell\sigma}^\dagger \hat{c}_{m\sigma} + u \sum_{l=1}^L \hat{n}_{l\uparrow} \hat{n}_{l\downarrow}$$
$$t_{\ell m} = i(-1)^{(l-m)}(l-m)^{-1}$$

Mott-Hubbard transition

control parameter: μ ($u > u_c$)

$\partial\mathcal{E}/\partial\mu$ discontinuous at $\mu_c = \pi$



second-order QPT

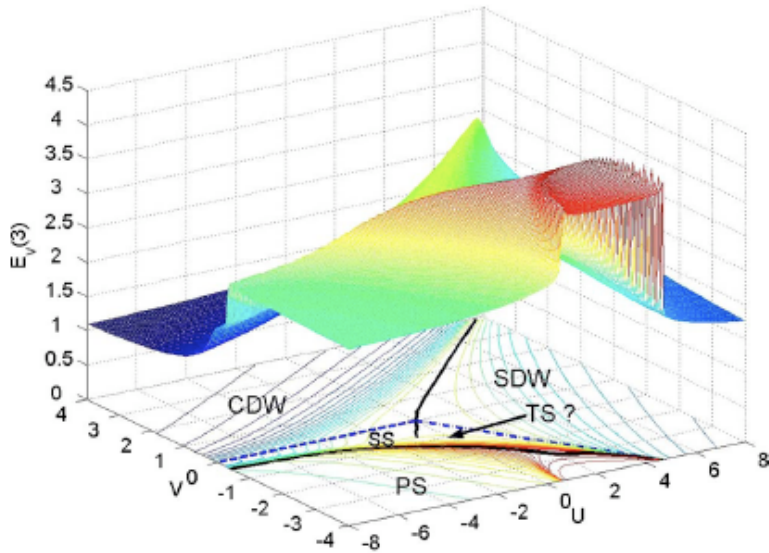
with logarithmic correction for $\mu \rightarrow \mu_{c-}$

(suppression of empty local states)

D. Larsson and H. Johannesson, PRA 73, 042320 (2006)

Yet another case study: the **extended 1D Hubbard model**

$$\mathcal{H} = - \sum_{\sigma, i, \delta} c_{i, \sigma}^\dagger c_{i+\delta, \sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_i n_i n_{i+1}$$



Phase diagram from numerical study
of the block entanglement ($n=1$)

S.-J. Gu et al, Phys. Rev. Lett. 93, 086402 (2004)

S.-S. Deng et al. Phys. Rev. B 74, 045103 (2006)

Another case study: the **extended 1D Hubbard model**

$$\mathcal{H} = - \sum_{\sigma, i, \delta} c_{i, \sigma}^\dagger c_{i+\delta, \sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_i n_i n_{i+1}$$

$n=1/2, V \rightarrow \infty$ K. Penc and F. Mila, Phys. Rev. B 49, 9670 (1994)

Analytic results for entanglement scaling:

$$\frac{\partial \mathcal{E}}{\partial U} \approx \frac{1}{4\sqrt{2}\pi} \frac{1}{\sqrt{|U_c - U|}} \{\log_2(|U_c - U|)\}$$

H. Johannesson and D. Larsson, Low Temp. Phys. 33, 1232 (2007)

$U_c = -4$: *metal to superconductor transition*

$U_c = 4$: *metal-insulator transition*

Another case study: the **extended 1D Hubbard model**

$$\mathcal{H} = - \sum_{\sigma, i, \delta} c_{i, \sigma}^\dagger c_{i+\delta, \sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_i n_i n_{i+1}$$

$n=1/2, V \rightarrow \infty$ K. Penc and F. Mila, Phys. Rev. B 49, 9670 (1994)

Analytic results for entanglement scaling:

$$\frac{\partial \mathcal{E}}{\partial U} \approx \frac{1}{4\sqrt{2}\pi} \frac{1}{\sqrt{|U_c - U|}} \left\{ \log_2(|U_c - U|) \right\}$$

H. Johannesson and D. Larsson, Low Temp. Phys. 33, 1232 (2007)

$U_c = -4$: *metal to superconductor transition*

$U_c = 4$: *metal-insulator transition*

$n=1/2, U \rightarrow \infty$

Jordan-Wigner

Mott-Hubbard transition at $V = 2$  AFM Ising transition in the $s=1/2$ XXZ chain

Analytic two-site entanglement with a *maximum* at $V = 2$
due to the particular weighting of the local states!

Another case study: the **extended 1D Hubbard model**

$$\mathcal{H} = - \sum_{\sigma, i, \delta} c_{i, \sigma}^\dagger c_{i+\delta, \sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_i n_i n_{i+1}$$

$n=1/2, V \rightarrow \infty$ K. Penc and F. Mila, Phys. Rev. B 49, 9670 (1994)

Analytic results for entanglement scaling:

$$\frac{\partial \mathcal{E}}{\partial U} \approx \frac{1}{4\sqrt{2}\pi} \frac{1}{\sqrt{|U_c - U|}} \left\{ \log_2(|U_c - U|) \right\}$$

H. Johannesson and D. Larsson, Low Temp. Phys. 33, 1232 (2007)

$U_c = -4$: *metal to superconductor transition*

$U_c = 4$: *metal-insulator transition*

$n=1/2, U \rightarrow \infty$

Jordan-Wigner

Mott-Hubbard transition at $V = 2$  AFM Ising transition in the $s=1/2$ XXZ chain

D. Larsson and H. Johannesson, in progress

Analytic two-site entanglement with a *maximum* at $V = 2$
due to the particular weighting of the local states!

Entanglement in inhomogeneous fermion systems

Entanglement in **inhomogeneous** fermion systems



**boundaries, interfaces, impurities, defects,
spatial modulations of system parameters and external fields...**

Entanglement in inhomogeneous fermion systems

boundaries, interfaces, impurities, defects,
spatial modulations of system parameters and external fields...

*e.g. a **confining potential** in an optical
lattice of ultracold fermionic atoms*

Entanglement in inhomogeneous fermion systems

boundaries, interfaces, impurities, defects,
spatial modulations of system parameters and external fields...

*e.g. a **confining potential** in an optical
lattice of ultracold fermionic atoms*

If quantum information processing is ever to become reality we must be able to quantify entanglement in systems with inhomogeneities!

Entanglement in inhomogeneous fermion systems

Example: Hubbard chain with a local potential

$$\hat{H} = -t \sum_{i,\sigma} (c_{i\sigma}^\dagger c_{i+1,\sigma} + H.c.) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + \sum_{i\sigma} v_{i\sigma} \hat{n}_{i\sigma}$$

*e.g. a **confining potential** in an optical lattice of ultracold fermionic atoms*

The Hohenberg-Kohn theorem guarantees that the entanglement is a functional of the ground-state density $n[x]$

$$\mathcal{E}[n(x)]$$

Local-density approximation (LDA) for the entanglement:

V. V. Franca and K. Capelle, Phys. Rev. Lett. 100, 070403 (2008)

$$\mathcal{E}[n(x)] \approx \mathcal{E}^{LDA}[n(x)] = \int dx \mathcal{E}^{hom}(n)_{n \rightarrow n(x)}$$

Entanglement in inhomogeneous fermion systems

Example: Hubbard chain with a local potential

$$\hat{H} = -t \sum_{i,\sigma} (c_{i\sigma}^\dagger c_{i+1,\sigma} + H.c.) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + \sum_{i\sigma} v_{i\sigma} \hat{n}_{i\sigma}$$

e.g. a **confining potential** in an optical lattice of ultracold fermionic atoms

The Hohenberg-Kohn theorem guarantees that the entanglement is a functional of the ground-state density $n[x]$

$$\mathcal{E}[n(x)]$$

Local-density approximation (LDA) for the entanglement:

V. V. Franca and K. Capelle, Phys. Rev. Lett. 100, 070403 (2008)

$$\mathcal{E}[n(x)] \approx \mathcal{E}^{LDA}[n(x)] = \int dx \mathcal{E}^{hom}(n)_{n \rightarrow n(x)}$$

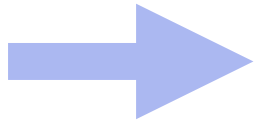
$v_{i\sigma}$ from *Bethe-Ansatz* LDA

N. A. Lima et al., Phys. Rev. Lett. 90, 146402 (2003)

Entanglement in inhomogeneous fermion systems

Example: Hubbard chain with a local potential

$$\hat{H} = -t \sum_{i,\sigma} (c_{i\sigma}^\dagger c_{i+1,\sigma} + H.c.) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + \sum_{i\sigma} v_{i\sigma} \hat{n}_{i\sigma}$$



A harmonic confining potential strongly reduces the entanglement

V. V. Franca and K. Capelle, Phys. Rev. Lett. 100, 070403 (2008)

How do *local* potentials (impurities) influence the entanglement?
Entanglement close to a *boundary*?
Entanglement scaling at criticality in the presence of *inhomogeneities*?
...and many other questions...

A rich and important field of study!

Summary

A generic finite-order QPT in a spin-1/2 fermionic lattice system driven by a change of a local interaction or an external field can be identified and characterized via the *single-site entanglement* (with some caution!)

example

second-order QPTs in the 1D Hubbard model

$$\frac{\partial \mathcal{E}}{\partial h} = \frac{C}{2 \ln(2)} \chi_S(\ln|h - h_{c2}| + \text{const}).$$

Summary

A generic finite-order QPT in a spin-1/2 fermionic lattice system driven by a change of a local interaction or an external field can be identified and characterized via the *single-site entanglement* (with some caution!)

example

second-order QPTs in the 1D Hubbard model

$$\frac{\partial \mathcal{E}}{\partial h} = \frac{C}{2 \ln(2)} \chi_s (\ln|h - h_{c2}| + \text{const}).$$

! entanglement scaling at a QPT governed by the *same* critical exponent as for the corresponding **susceptibility**

Summary

A generic finite-order QPT in a spin-1/2 fermionic lattice system driven by a change of a local interaction or an external field can be identified and characterized via the *single-site entanglement* (with some caution!)

example

second-order QPTs in the 1D Hubbard model

$$\frac{\partial \mathcal{E}}{\partial h} = \frac{C}{2 \ln(2)} \chi_s (\ln|h - h_{c2}| + \text{const}).$$

! entanglement scaling at a QPT governed by the *same* critical exponent as for the corresponding **susceptibility**

×

logarithmic correction when the **number of accessible local states change** at the transition

Summary

A generic finite-order QPT in a spin-1/2 fermionic lattice system driven by a change of a local interaction or an external field can be identified and characterized via the *single-site entanglement* (with some caution!)

Implications for the theory of QPTs / quantum information?

More work needed!