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## Outline

- Natural computing, quantum annealing, quantum spin systems
- Quantum phase transitions
- Quantum to classical mapping
- Scope: to learn an exact mapping among d-dimensional quantum systems and d+1-dimensional classical systems and universality classes; to discuss entanglement and quantum correlations in a many-body system strictly connected to qubits in quantum computers
- Supplementary material: Spectral properties: the Jordan-Wigner transformation, Entanglement and Quantum Phase Transitions

andremo quindi a studiare un modello di spin con effetti di correlazione quantistico non trascrabile

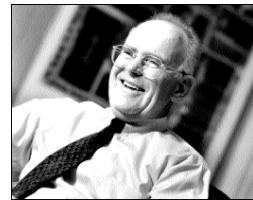
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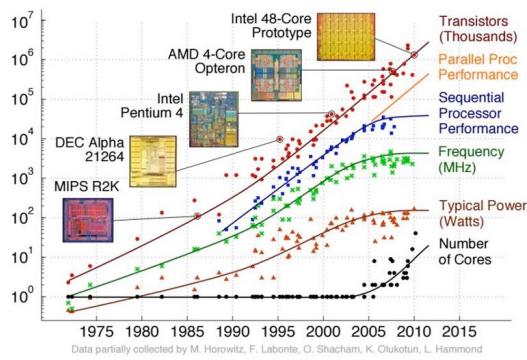
## Moore's law

- Gordon E. Moore (co-founder of Intel) predicted (Electronics, Vol. 38, 1965) that transistor density of a semiconductor chip is going to double about every 2 years ...

⇒ double performances about every 2 years



- It is not a law!  
It is a prediction on the progress of physical devices and engineering processes... but, it works!  
... since 50 years!
- But, how long? Note, that recently we had to move towards multi-core architectures
- Present: Parallel computing ..
- Future: Natural computing (e.g. Quantum computation? But it seems we are still far from a Universal Quantum computer)



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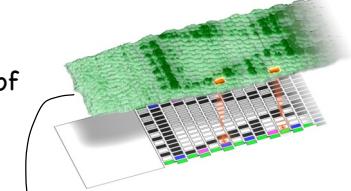
il Machine learning ha perfezionato modelli basati sul multi-core

## Natural Computation

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- Natural computing encompasses three classes of methods:
  - Methods based on the use of computers to **synthesize natural phenomena** (Computational Intelligence, Neural Networks, Genetic Algorithms, etc.) HARDWARE TRADIZIONALE
  - Methods that **employ natural materials** (electrons, atoms, molecules, DNA) to compute. HARDWARE NATURALE
  - Methods that take inspiration from nature for the development of **novel computational architectures or problem-solving techniques** (e.g. neuromorphic computing) HARDWARE TRADIZIONALE CONE MATERIAZI MA NATURALI CONCE PROGETTAZIONE
- A remarkable example of the second class is also an example of **emergence/self-organization** in a complex system is DNA computing.
- DNA computing is a form of parallel computing that uses DNA, biochemistry, and molecular biology hardware, instead of the traditional silicon-based computer technologies
- 4 key components coding: in principle 1 liter of fluid with 6 grams of DNA could memorize 3 Zbytes and perform up to 1 EFLOPS (Zetta=10<sup>21</sup>) (Exa=10<sup>18</sup>)

DNA thin slab self-assembly of a Sierpinski triangle as a Cellular Automata, *Nano Letters* (2007)



HARDWARE CONTENENTE DNA BIOLOGICO

→ POCO GENERALIZZABILE

OSS: non si ha da affermare che queste tecnologie sono generalizzabili a tutte le gerarchie

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## New computational architectures

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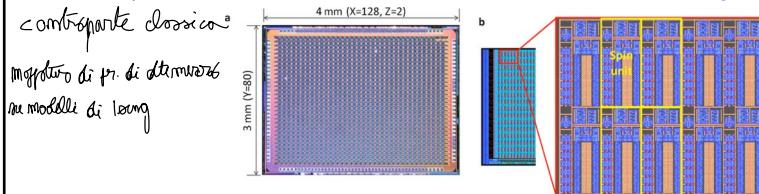
- Along the third class of Natural computing methods, recently, several special hardwares or physical systems for solving Ising models have been proposed.

### 1. D-Wave machines, based on quantum annealing

- Dwave One (2011, 128 qubits)
- Dwave Two (2013, 512 qubits)
- Dwave 2X (2015, 1152 qubits)
- Dwave 2000Q (2020, 2048 qubits)



### 1. (classical) Ising chip by Hitachi (2015) 20480 spins based on CMOS (complementary metal-oxide semiconductor) annealing



### 3. Coherent (quantum) Ising Machine (Optical/laser networks, 2011/2015)

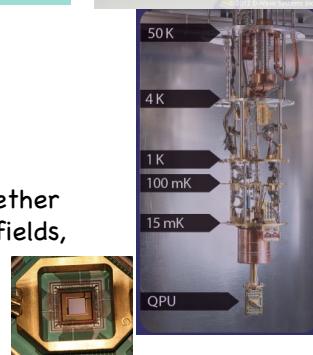
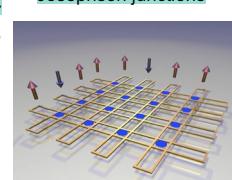
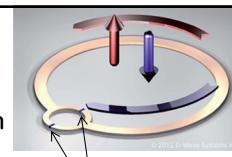
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Retiche di Nb a Loop

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## D-Wave

- The D-Wave quantum processing unit (QPU) is built from a lattice of tiny loops [Superconducting Quantum Interference Devices (SQUID)] of metal Niobium (Nb), each of which is one qubit. Below temperatures of 9.2 Kelvin, Niobium becomes a superconductor and exhibits quantum mechanical effects.
- When in a quantum state  $|\psi\rangle$ , current flows in both directions simultaneously, which means that the qubit is in superposition – that is, in both a 0 and a 1 state at the same time:  $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$   $\alpha, \beta \in \mathbb{C}$   $|\alpha|^2 + |\beta|^2 = 1$
- Going from a single qubit to a multi-qubit QPU requires that the qubits be interconnected to exchange information. Qubits are connected via couplers, which are also superconducting loops.
- The interconnection of qubits and couplers, together with control circuitry to manage the magnetic fields, creates an integrated fabric of programmable quantum devices which work as a quantum annealer



→ una specie  
di frigoriferi  
che sfrutta  $\text{He}^3$   
in fase superfluida

6

corso ms è 2  
 tecnica soluzio  
 → di Molti capi

una scorsa per parlare di open quantum

## Quantum annealing: the idea

- In **adiabatic quantum computation** the quantum evolution of a system may be used for performing computation: initialize the quantum processing unit (QPU) into a ground state of a known problem and "anneal" it toward the problem to be solved such that it remains in a low energy state throughout the process.
- At the end of the computation, each qubit ends up as either a 0 or 1. This final state is the optimal or near-optimal solution to the problem to be solved.
- More concretely, consider a **quantum system** in the state  $|\Psi(0)\rangle$  at the time  $t = 0$ , evolving according to the **Schrödinger equation**

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = \hat{H}(t) |\Psi(t)\rangle$$

governed by a **time-dependent Hamiltonian**  $H$ .  
 Suppose that:  $\hat{H}(t) = \left[1 - f\left(\frac{t}{T}\right)\right]\hat{H}_0 + f\left(\frac{t}{T}\right)\hat{H}_1$

- where  $H_0$  and  $H_1$  are time-independent Hamiltonians and  $f:[0,1] \rightarrow [0,1]$  any non-decreasing, endpoint-fixing map, and let the system evolve from  $t = 0$  to  $t = T$

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## Adiabatic theorem

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- Then, if  $|\Psi(0)\rangle$  is the eigenstate  $|n(0)\rangle$  of  $H_0$ , and if the corresponding energy level does not cross with any other one during the evolution:

$$\Delta_n := \min_{\substack{0 \leq t \leq T \\ k \neq n}} |E_n(t) - E_k(t)| > 0 \quad \text{no level-crossing}$$

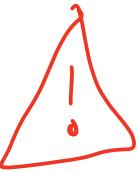
(with  $E_k(t)$  the eigenvalue corresponding to  $|k(t)\rangle$ ), then the **adiabatic theorem** [A. Messiah, *Quantum Mechanics*, Wiley (1965)] asserts that

$$\lim_{T \rightarrow \infty} \langle n(T) | T \exp \left\{ -\frac{i}{\hbar} \int_0^T \hat{H}(t) dt \right\} | n(0) \rangle = 1$$

- In other words, the eigenstate of  $H_0$  evolves under  $H$  into the corresponding eigenstate of  $H_1$  with probability going to one in the limit of infinitely slow evolution: no transitions between energy levels occur in the "adiabatic" limit.
- On the other hand, **diabatic transitions may be observed if  $T$  is kept finite**. Still, the probability for this to happen may be reduced below any desired value by taking  $T$  large enough (adiabatic approximation).
- Note that a vanishing gap (level crossing) implies that the transition probability becomes non vanishing even in the adiabatic limit.

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OSS: question si, ma nte si open follownote

sono mille lire di z

qui 1/17 1-1>

I effetti di  $\sigma_x$  è quello che fanno esistere

$\Rightarrow H_0$  è un termine "cinetico" di flip



## Quantum Ising models

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- $H_1$  encodes the problem to be solved whereas  $H_0$  is taken as an operator whose ground state is simple to prepare, and such that  $[H_0, H_1] \neq 0$  (this ensures that the dynamical evolution is nontrivial, i.e.  $H_1$  and  $H_0$  have different eigenstates).
- Typically this can be obtained with a quantum Ising model where spin variables are promoted to operators (Pauli matrices), for example:

Un po' come se  
mo qui [H<sub>0</sub>, H<sub>1</sub>] ≠ 0

$$\leftarrow \hat{H}_0 = -Jg \sum_i \hat{\sigma}_i^x \quad \hat{H}_1 = -J \sum_{\langle i,j \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z$$

tutto ancora a T=0mp=0  
in the basis where the  $\sigma_i^z$  are diagonal, these matrices have the well-known form on each site i:

$$\hat{\sigma}^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \hat{\sigma}^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \hat{\sigma}^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- The matrices on different sites act on different spin states, and so matrices with  $i \neq j$  commute with each other.
- At  $g = 0$ , when  $H$  involves only the  $\sigma_i^z$ ,  $H$  will be diagonal in the basis of eigenvalues of  $\sigma_i^z$ , and it reduces simply to the familiar classical Ising model. However, the  $\sigma_i^x$  are off-diagonal in the basis of these states, and therefore they induce quantum-mechanical tunneling events that flip the orientation of the Ising spin on a site.

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$\rightarrow$  se  $H=H_1$  bis il modello di Ising classico con g.s tutte up/tutte down  
se ho anche  $H_0$   $\sigma_x$  fa flippe gli spin

10

- $H_0$  so represent a T=0 analogue of a kinetic term
- The ground state of  $H$  can depend only upon the value of the dimensionless coupling  $g$ , and so it pays to consider the two opposing limits  $g \gg 1$  and  $g \ll 1$ .
- First consider  $g \gg 1$ . In this case  $H_0$  dominates, and, to leading order in  $1/g$ , the ground state is simply

\*  $|0\rangle = \prod_i |\rightarrow\rangle_i$       where  $|\rightarrow\rangle_i = (|\uparrow\rangle_i + |\downarrow\rangle_i)/\sqrt{2}; |\leftarrow\rangle_i = (|\uparrow\rangle_i - |\downarrow\rangle_i)/\sqrt{2}$

are the two eigenstates of  $\sigma_i^x$  with eigenvalues  $\pm 1$ .

- The values of  $\sigma_i^z$  on different sites are totally uncorrelated in this state, and so

$$\langle 0 | \hat{\sigma}_i^z \hat{\sigma}_j^z | 0 \rangle = \delta_{ij} \quad \text{Ripetere per tutti i } \sigma_i^z$$

- Perturbative corrections in  $1/g$  will build in correlations in  $\sigma_i^z$  that increase in range at each order in  $1/g$ ; for  $g$  large enough these correlations are expected to remain short-ranged, and we expect in general that

$$\langle 0 | \hat{\sigma}_i^z \hat{\sigma}_j^z | 0 \rangle \underset{d_{ij} \gg 1}{\approx} e^{-d_{ij}/\xi} \quad \begin{array}{l} \text{Ripetere per tutti i } \sigma_i^z \\ \rightarrow \text{di p. ordine } g^n \text{ una power-law} \end{array}$$

being  $d_{ij}$  the spatial distance among i & j sites,  $|0\rangle$  the exact ground state for large-g, and  $\xi$  a suitable "correlation length"

hanno da f quadratino  
non effetti termici  
ma effetti quantitativi  
 $\uparrow$   
di ordine  $g^n$   $\rightarrow$  di ordine di  $g$

10

\* è solo per  $g \gg 1$  che il g.s. è l'uno solo

$g \ll 1$  fattoriando si fa per le molte state con open follownote  $|0\rangle = |\uparrow\rangle \otimes |\downarrow\rangle \dots$

no

$|0\rangle$  genericus

5

\* è diversi punti di config ferromagnetiche dove ferri si staccano ferri & merce cioè il concetto di

merce



11

- Next we consider the **opposing limit**  $g \ll 1$ . The nature of the ground state is qualitatively different from the large- $g$  limit above, and we argue that there must be a **quantum phase transition** between the two limiting cases at a *critical*  $g = g_c$  of order unity.
- For  $g \ll 1$ , the term  $H_1$ , coupling neighboring sites **dominates**; at  $g = 0$  the spins are either all up or all down (in eigenstates of  $\sigma_z^i$ ):

$$\star |0\rangle = \prod_i |\uparrow\rangle_i \quad \text{or} \quad |0\rangle = \prod_i |\downarrow\rangle_i$$

- Turning on a small- $g$  will mix in a small fraction of spins of the opposite orientation. We will have:

$$\langle 0 | \hat{\sigma}_i^z | 0 \rangle = \pm N_0$$

with  $N_0 = 1$  for  $g = 0$ , but **quantum fluctuations at small- $g$**  reduce  $N_0$  to a **smaller, but nonzero, value**.

- Then, by initializing the system in the ground state of  $H_0$  and letting it evolve adiabatically, the final system will likely be in the ground state of the “problem Hamiltonian”  $H_1$ .
- A **readout** of the state then allows one to obtain the optimal configuration, thus **solving the problem** of optimizing the cost function.
- This is, in essence, the quantum adiabatic algorithm.

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## Quantum spin models

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- Like for the Ising model also the other spin models have a quantum version and a slightly different nomenclature is in use

| Number of components  | Hamiltonian   | nomenclature                     |
|-----------------------|---|----------------------------------|
| Heisenberg<br>$n = 3$ | $\hat{H} = -\sum_{\langle i,j \rangle} (J_x \hat{\sigma}_i^x \hat{\sigma}_j^x + J_y \hat{\sigma}_i^y \hat{\sigma}_j^y + J_z \hat{\sigma}_i^z \hat{\sigma}_j^z) - h \sum_i \hat{\sigma}_i^z$ | XYZ                              |
| Heisenberg<br>$n = 3$ | $\hat{H} = -\sum_{\langle i,j \rangle} (J \hat{\sigma}_i^x \hat{\sigma}_j^x + J \hat{\sigma}_i^y \hat{\sigma}_j^y + J \hat{\sigma}_i^z \hat{\sigma}_j^z) - h \sum_i \hat{\sigma}_i^z$       | XXZ<br>( $J_x = J_y = J$ )       |
| Heisenberg<br>$n = 3$ | $\hat{H} = -J \sum_{\langle i,j \rangle} (\hat{\sigma}_i^x \hat{\sigma}_j^x + \hat{\sigma}_i^y \hat{\sigma}_j^y + \hat{\sigma}_i^z \hat{\sigma}_j^z) - h \sum_i \hat{\sigma}_i^z$           | XXX<br>( $J_x = J_y = J_z = J$ ) |
| XY<br>$n = 2$         | $\hat{H} = -J \sum_{\langle i,j \rangle} (\hat{\sigma}_i^x \hat{\sigma}_j^x + \hat{\sigma}_i^y \hat{\sigma}_j^y) - h \sum_i \hat{\sigma}_i^z$   | XY                               |
| Ising<br>$n = 1$      | $\hat{H} = -J \sum_{\langle i,j \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - h \sum_i \hat{\sigma}_i^x$   | Transverse-field Ising model     |

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## Quantum phase transitions

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| Classical Ising $H$   | Quantum Ising $\hat{H}$  |
|---|--|
| $-J \sum_{i < j} \sigma_i \sigma_j - h \sum_i \sigma_i$<br>$\sigma_i = \pm 1 \forall i$ | $-J \sum_{i < j} \hat{\sigma}_i^z \hat{\sigma}_j^z - g J \sum_i \hat{\sigma}_i^x$<br>$\hat{\sigma}^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \hat{\sigma}^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \hat{\sigma}^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ |

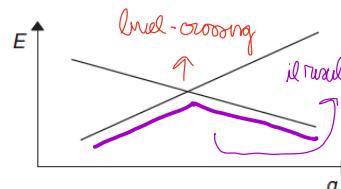
- Quantum phase transitions (QPT) are zero temperature phase transitions which are driven by quantum fluctuations and are usually associated with a non-analyticity in the ground state energy density of a quantum many-body Hamiltonian. One can extend the previous classification of phase transitions also to QPT:
  - First order QPT are characterized by a finite discontinuity in the first derivative of the ground state energy density *forts, anghos*
  - A continuous QPT is similarly characterized by a finite discontinuity, or divergence, in the second derivative of the ground state energy density, assuming that the first derivative is continuous.
  - QPT are usually accompanied by a qualitative change in the nature of the quantum correlations in the ground state; how this can emerge?

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## Trivial first order quantum phase transition

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- Consider a Hamiltonian,  $H(g)$ , whose degrees of freedom reside on the sites of a lattice, and which varies as a function of the coupling,  $g$
- For the case of a **finite lattice**, this ground state energy will generically be a smooth, analytic function of  $g$
- The main possibility of an exception comes from the case when  $g$  couples only to a conserved quantity (i.e.  $H(g) = H_0 + gH_1$ , where  $[H_0, H_1] = 0$ ).  
*↳ für exzess*
- In this case  $H_0$  and  $H_1$  can be simultaneously diagonalized and so the eigenfunctions are independent of  $g$  even though the eigenvalues vary with  $g$ .
- Then there can be a level-crossing where an excited level becomes the ground state at  $g = g_c$ , creating a point of non-analyticity of the ground state energy as a function of  $g$
- From our discussion on quantum annealing this is the less interesting case



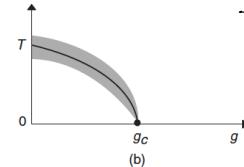
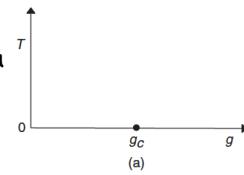
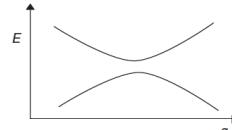
durchaus  
ist ein fortw. unkl.

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## Non trivial quantum phase transitions

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- The possibilities for an infinite lattice are richer. *(quindi livello termoformico)*
- An avoided level-crossing between the ground and an excited state in a finite lattice could become progressively sharper as the lattice size increases, leading to a non-analyticity at  $g = g_c$  in the infinite lattice limit.
- We shall identify **any point of non-analyticity** in the ground state energy of the infinite lattice system as a **quantum phase transition**, which can be first or second order
- Two possible phase diagrams**; in both cases there is a quantum critical point at  $g = g_c$  and  $T = 0$ .
- In (a) the thermodynamic singularity is present only at  $T = 0$ , and all  $T > 0$  properties are analytic as a function of  $g$  near  $g = g_c$
- In (b), there is a line of  $T > 0$  phase transitions terminating at  $g = g_c$ . The theory of phase transitions in classical systems driven by thermal fluctuations can be applied within the shaded region



→ così in cui  $g_c$  sarebbe solo a  $T=0 \Rightarrow$  la termodinamica di transizione di fase quantistica

→ transizione di fase anche a  $T \neq 0$  che si chiude a  $g_c$  per  $T=0$

lo fanno con il Path-Integral

## From d-dim. quantum to d+1-dim. classical systems

- Consider now **zero temperature phase transitions** which are **driven by quantum fluctuations** arising due to the Heisenberg uncertainty principle or, equivalently, phase transitions in which the **ground state energy of the system shows anomalies in the first or high order derivatives** at some value of the parameters which define the Hamiltonian
- Here I discuss a fairly general procedure allowing one to **map the partition function of a d-dimensional quantum system to the partition function of a d+1-dimensional classical system**
- This procedure, known as the **quantum-to-classical (QC) mapping**, can be used to gain insight into quantum phase transitions from their classical counterparts or understand new quantum universality classes from Monte Carlo simulations of the appropriate classical d+1-dimensional systems.
- The main idea behind QC mapping starts from the evidence that the properties of a d-dimensional quantum system can be evaluated using **path integration**. Let's go back to the 1D quantum Ising model in a transverse field:

$$\hat{H} = \hat{H}_0 + \hat{H}_1 = -Jg \sum_i \hat{\sigma}_i^x - J \sum_i \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z$$

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- The Hilbert space  $\mathcal{H}_N$  is simply the  $N^{\text{th}}$  tensor product of the single-spin Hilbert space  $\mathcal{H}$ :

$$\mathcal{H}_N = \mathcal{H} \otimes \mathcal{H} \otimes \mathcal{H} \otimes \dots \otimes \mathcal{H} \quad \begin{matrix} \text{mon suc. d'una} \\ \text{fattori per fattori} \end{matrix}$$

- Since the Pauli matrix  $\hat{\sigma}^z$  define in  $\mathcal{H}$  an orthonormal basis  $\{|S^z\rangle\}$ , the orthonormal basis of  $\mathcal{H}_N$  is constructed from the tensor product

$$|\{S^z\}\rangle = |S_1^z \dots S_N^z\rangle = \otimes_{i=1}^N |S_i^z\rangle = |S_1^z\rangle \otimes \dots \otimes |S_N^z\rangle$$

- The partition function is:

$$Z = \text{Tr}(e^{-\beta \hat{H}}) = \text{Tr}(e^{-\beta(\hat{H}_0 + \hat{H}_1)}) = \sum_{\{S^z\}} \langle \{S^z\} | e^{\beta J g \sum_i \hat{\sigma}_i^x + \beta J \sum_i \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z} | \{S^z\} \rangle$$

- $H_0$  and  $H_1$  do not commute; anyway, by applying the Trotter formula to the partition function, we get

$$Z = \sum_{\{S^z\}} \langle \{S^z\} | e^{-\beta(\hat{H}_0 + \hat{H}_1)} | \{S^z\} \rangle = \sum_{\{S^z\}} \langle \{S^z\} | \left[ e^{\frac{\beta}{M}(\hat{H}_0 + \hat{H}_1)} \right]_M | \{S^z\} \rangle \underset{M \gg 1}{\cong} \sum_{\{S^z\}} \langle \{S^z\} | \prod_{i=1}^M e^{\frac{\beta}{M} \hat{H}_0} e^{\frac{\beta}{M} \hat{H}_1} | \{S^z\} \rangle$$

- This approximation, called the Trotter-Suzuki approximation, is controlled in the sense that one can get as close to the exact result as one desires by requiring that  $(\beta/M)^2 J h = (\beta J/M)^2 g \ll 1 \Rightarrow M \gg \beta J \sqrt{g}$

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OSS: mon poco mandare  $M \rightarrow \infty$  a cost, altrimenti succede  $e^{-\beta/M H} \rightarrow$  bronzo

quindi  $M \rightarrow \infty \frac{\beta}{M} = \text{cost}$

quindi le forze fare se mon sono raffreddati (quello che voglio fare)

- We can insert now  $M-1$  completeness:

$$1 = \otimes_{i=1}^N \left[ \sum_{S_i^z=\pm 1} |S_i^z\rangle \langle S_i^z| \right] = \sum_{\{S^z\}} |\{S^z\}\rangle \langle \{S^z\}| = \sum_{S_1^z, \dots, S_N^z=\pm 1} |S_1^z, \dots, S_N^z\rangle \langle S_1^z, \dots, S_N^z|$$

- Hence:

$$Z \underset{M \gg 1}{=} \sum_{\{S^z\}_1, \dots, \{S^z\}_M} \prod_{l=1}^M \langle \{S^z\}_l | e^{-\frac{\beta}{M} \hat{H}_0} e^{-\frac{\beta}{M} \hat{H}_1} | \{S^z\}_{l+1} \rangle$$

$$\text{with } |\{S^z\}_1\rangle = |\{S^z\}_{M+1}\rangle = |\{S^z\}\rangle$$

- Let's focus on the matrix element:  $\langle \{S^z\}_l | e^{-\frac{\beta}{M} \hat{H}_0} e^{-\frac{\beta}{M} \hat{H}_1} | \{S^z\}_{l+1} \rangle = \dots$

- $H_1$  is diagonal in the chosen basis:

$$\dots = \langle \{S^z\}_l | e^{-\frac{\beta}{M} \hat{H}_0} | \{S^z\}_{l+1} \rangle e^{\frac{\beta}{M} J \sum_i S_{i,l+1}^z S_{i+1,l+1}^z}$$

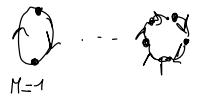
where we have added an index,  $i$ , to the variable  $S_{i,l}^z$  to indicate the  $z$ -component of the  $i$ -th spin at the  $l$ -th position in the path integration

- The remaining matrix element is

$$\langle \{S^z\}_l | e^{-\frac{\beta}{M} \hat{H}_0} | \{S^z\}_{l+1} \rangle = \langle \{S^z\}_l | e^{\frac{\beta}{M} J g \sum_i \hat{\sigma}_i^x} | \{S^z\}_{l+1} \rangle = \prod_{i=1}^N \langle S_{i,l}^z | e^{\frac{\beta}{M} J g \hat{\sigma}_i^x} | S_{i,l+1}^z \rangle$$

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apri completezza  
è una fattorizzazione



18

- One can use that  $(\hat{\sigma}^x)^2 = \hat{1}$  to write:

$$e^{\frac{\beta Jg\hat{\sigma}_i^x}{M}} = \hat{1} \cdot \cosh\left(\frac{\beta Jg}{M}\right) + \hat{\sigma}_i^x \cdot \sinh\left(\frac{\beta Jg}{M}\right)$$

- In fact:

$$e^{\frac{\beta Jg\hat{\sigma}_i^x}{M}} = \hat{1} + \left(\beta Jg/M\right)\hat{\sigma}_i^x + \frac{\left(\beta Jg/M\right)^2}{2!}(\hat{\sigma}_i^x)^2 + \frac{\left(\beta Jg/M\right)^3}{3!}(\hat{\sigma}_i^x)^3 + \frac{\left(\beta Jg/M\right)^4}{4!}(\hat{\sigma}_i^x)^4 + \dots$$

$$e^{\frac{\beta Jg\hat{\sigma}_i^x}{M}} = \hat{1} \left[ 1 + \frac{\left(\beta Jg/M\right)^2}{2!} + \frac{\left(\beta Jg/M\right)^4}{4!} + \dots \right] + \hat{\sigma}_i^x \left[ \left(\beta Jg/M\right) + \frac{\left(\beta Jg/M\right)^3}{3!} + \dots \right]$$

$$\Rightarrow e^{\frac{\beta Jg\hat{\sigma}_i^x}{M}} = \hat{1} \cosh\left(\beta Jg/M\right) + \hat{\sigma}_i^x \sinh\left(\beta Jg/M\right)$$

- Thus we obtain:

$$\prod_{i=1}^N \langle S_{i,l}^z | e^{\frac{\beta Jg\hat{\sigma}_i^x}{M}} | S_{i,l+1}^z \rangle = \prod_{i=1}^N \left[ \cosh\left(\beta Jg/M\right) \langle S_{i,l}^z | S_{i,l+1}^z \rangle + \sinh\left(\beta Jg/M\right) \langle S_{i,l}^z | \hat{\sigma}_i^x | S_{i,l+1}^z \rangle \right]$$

- To relate the quantum mechanical matrix element to a **classical Hamiltonian**, it should be required that the former matrix element be expressed in the form:

$$\langle S_{i,l}^z | e^{\frac{\beta Jg\hat{\sigma}_i^x}{M}} | S_{i,l+1}^z \rangle = \Lambda e^{\gamma S_{i,l}^z S_{i,l+1}^z} \quad \begin{matrix} \text{form nello} \\ \text{indice} \\ \text{e (nella) indice delle identità} \end{matrix}$$

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- This expression implicitly defines the variables  $\Lambda$  and  $\gamma$ , which can be determined simply by plugging in the two eigenstates  $|\uparrow\rangle$  and  $|\downarrow\rangle$ , and noting that the action of the Pauli matrix  $x$  along the  $x$ -direction reverses the spin eigenstate along the  $z$ -direction:

$$\hat{\sigma}_i^x |\uparrow\rangle_i = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_i \begin{pmatrix} 1 \\ 0 \end{pmatrix}_i = \begin{pmatrix} 0 \\ 1 \end{pmatrix}_i = |\downarrow\rangle_i \quad \hat{\sigma}_i^x |\downarrow\rangle_i = |\uparrow\rangle_i$$

- Thus we obtain:

$$\Lambda e^\gamma = \langle \uparrow | e^{\frac{\beta Jg\hat{\sigma}_i^x}{M}} | \uparrow \rangle = \left[ \cosh\left(\beta Jg/M\right) \langle \uparrow | \uparrow \rangle + \sinh\left(\beta Jg/M\right) \langle \uparrow | \downarrow \rangle \right]^0 = \cosh\left(\beta Jg/M\right)$$

$$\Lambda e^{-\gamma} = \langle \uparrow | e^{\frac{\beta Jg\hat{\sigma}_i^x}{M}} | \downarrow \rangle = \left[ \cosh\left(\beta Jg/M\right) \langle \downarrow | \uparrow \rangle + \sinh\left(\beta Jg/M\right) \langle \downarrow | \downarrow \rangle \right]^0 = \sinh\left(\beta Jg/M\right)$$

- From the product and the ratio of the previous two equations the parameters  $\Lambda$  and  $\gamma$  can be obtained explicitly:

$$\Lambda^2 = \sinh(\beta Jg/M) \cosh(\beta Jg/M)$$

$$\gamma = -\frac{1}{2} \ln [\tanh(\beta Jg/M)]$$

- We can now put back all these relation into the **quantum partition function  $Z$**  ...

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In questo modo tutti gli errori introvare i primi numeri

→ quindi un modello di Ising

1+1 dimensionale 1 colonna di spin

1 dom del ferroso di fotor

è molto simile all'analogo classico Boltz-McLorin con  $e^{-\beta H}$  ma le potenze di  $\tau$  hanno  $\beta$

ed è  $M = \tau$  il numero di intervale  $\Delta\tau$

• ... to obtain:

$$\left\langle \left\{ S^z \right\}_I \middle| e^{-\frac{\beta}{M} \hat{H}_0} e^{-\frac{\beta}{M} \hat{H}_1} \left| \left\{ S^z \right\}_{I+1} \right\rangle = \dots = \Lambda^N e^{\frac{\beta}{M} J \sum_{i=1}^N S_{i,I+1}^z S_{i,I+1}^z + \gamma \sum_{i=1}^N S_{i,I}^z S_{i,I+1}^z}$$

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• It is interesting to note that the interaction term of the Hamiltonian  $H_1$  led to Ising spin couplings at the same (imaginary time) slice ( $I+1$ ), but between neighboring spatial sites ( $i$  and  $i+1$ ), while the "kinetic" term  $H_0$  led to couplings between Ising spins on the same spatial site ( $i$ ) but at different/consecutive (imaginary time) slices ( $I$  and  $I+1$ ).

$\gamma S_{i,I}^z S_{i,I+1}^z$

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↳ Trasformo questo 2-dimensionale modello  
↳ di cui ho la natura

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$$Z \underset{M \gg 1}{\cong} \Lambda^{M \times N} \sum_{\{S^z\}_1, \dots, \{S^z\}_M} e^{\frac{\beta}{M} J \sum_{i=1}^N \sum_{l=1}^M S_{i,l}^z S_{i+1,l}^z + \gamma \sum_{i=1}^N \sum_{l=1}^M S_{i,l}^z S_{i,l+1}^z}$$

- The result obtained for the partition function seems very complicated indeed and one might wonder why going through so much trouble to arrive at a form involving sums of exponentials of double sums.
- The reason appears evident if the  $z$  superscripts of the spins are dropped and if one realizes that the prefactor  $\Lambda^{NM}$  carries no physical significance since it does not affect the spins
- Thus the obtained expression for  $Z$  equation is nothing but the classical two-dimensional Ising model at zero field with different couplings in the  $i$  and  $l$  directions, i.e. an **anisotropic two-dimensional classical Ising model!**

$$Z_{classical} = \Lambda^{N_x N_y} \sum_{\{s_{i,l} = \pm 1\}} e^{\beta^* J_x \sum_{i=1}^{N_x} \sum_{l=1}^{N_y} s_{i,l} s_{i+1,l} + \beta^* J_y \sum_{i=1}^{N_y} \sum_{l=1}^{N_x} s_{i,l} s_{i,l+1}}$$

- The spatial and imaginary time direction are identified with the classical  $x$  and  $y$  directions, thus the degrees of freedom of the system are identified as  $(N_x N_y)$  where  $N_x = N$  and  $N_y = M$

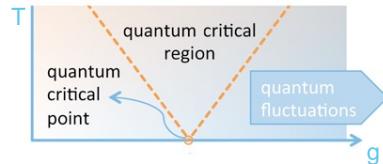
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fatto il punto terminazione 26 quale mostra  $N, M \rightarrow \infty$   
ma queste anche  $\beta \rightarrow \infty, T \rightarrow 0$  quindi la sequenza  $T=0$

- Furthermore, the classical inverse temperature  $\beta^*$  together with the classical couplings  $J_x$  and  $J_y$  are identified as  $\beta^* J_x = \beta J/M$  and  $\beta^* J_y = \gamma$ , i.e.<sup>23</sup>

$$\beta^* J_y = \gamma = -\frac{1}{2} \ln [\tanh(\beta J g/M)]$$

- With the identifications above, the 1D quantum Ising model in a transverse field can be mapped onto a classical two-dimensional Ising model with anisotropic couplings.
- It is interesting how the quantum effect of the transverse field is transmuted through imaginary time-slicing into an additional classical spatial dimension, leaving the resulting classical two-dimensional Ising model field-free.
- The results derived here for the quantum Ising chain and the classical two-dimensional Ising lattice do not hold only for these specific cases, but can in fact be generalized to arbitrary dimensions: a quantum d-dimensional Ising model can be mapped to a classical (d+1)-dimensional Ising model and vice versa.
- Concerning the 1D transverse field quantum Ising model, the obtained QC mapping indicates the existence of a quantum critical point?



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### Quantum critical point

- We know that the classical two dimensional Ising model can be solved exactly in the absence of an external magnetic field (Onsager, 1944; Baxter, 1982).
- It is known that in the thermodynamic limit,  $N_x \rightarrow \infty$  and  $N_y \rightarrow \infty$ , this system has a critical point given by the relation

$$\sinh(2J_x \beta_{cl}^c) \sinh(2J_y \beta_{cl}^c) = 1 \rightarrow \text{così doce}$$

where  $\beta_{cl}^c$  is the critical inverse temperature for the classical system.

- For low temperature the system is ordered (magnetized) while for high temperature the system is disordered. While the value of  $\beta_{cl}^c$  depends on the relative values of  $J_x$  and  $J_y$ , i.e. on the anisotropy; the critical exponents themselves do not (Onsager, 1944)
- With the mapping of the 1D quantum system to the (1+1) classical system, the obtained classical partition function  $Z_{\text{classical}}$  and its parameter identification in term of the quantum parameters, we, therefore, see that as  $N \rightarrow \infty$  and  $M \rightarrow \infty$  the quantum system will exhibit a critical point given by the conditions:

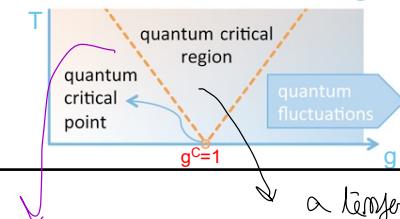
$$\sinh(2\beta J^c/M) \sinh(2\gamma^c) = 1 \quad \gamma^c = -\frac{1}{2} \ln [\tanh(\beta J^c g^c/M)]$$

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- This, however, is not a thermal phase transition since it takes place when the quantum system is at zero temperature. We see this by noting that for the transition to take place, both  $N \rightarrow \infty$  and  $M \rightarrow \infty$ . But when  $M \rightarrow \infty$  at fixed  $\beta/M$ , which is the case here, it means that  $\beta \rightarrow \infty$  and thus the system is at  $T=0$
- We have here, therefore, a quantum phase transition reached by tuning  $J$  and  $h=gJ$ , the coupling parameters while the system is at  $T=0$ . We now get the critical point. Substituting the expression for  $\gamma^c$  in the condition for criticality yields

$$\begin{aligned} 1 = \sinh\left(2\beta J^c/M\right) \sinh\left(-\ln\left[\tanh\left(\beta J^c g^c/M\right)\right]\right) &= \sinh\left(2\beta J^c/M\right) \frac{e^{-\ln\left[\tanh\left(\beta J^c g^c/M\right)\right]} - e^{+\ln\left[\tanh\left(\beta J^c g^c/M\right)\right]}}{2} = \\ &= \frac{1}{2} \sinh\left(2\beta J^c/M\right) \left[ \frac{\cosh\left(\beta J^c g^c/M\right)}{\sinh\left(\beta J^c g^c/M\right)} - \frac{\sinh\left(\beta J^c g^c/M\right)}{\cosh\left(\beta J^c g^c/M\right)} \right] = \\ &= \frac{\sinh\left(2\beta J^c/M\right)}{2} \frac{\cosh^2\left(\beta J^c g^c/M\right) - \sinh^2\left(\beta J^c g^c/M\right)}{\sinh\left(\beta J^c g^c/M\right) \cosh\left(\beta J^c g^c/M\right)} = \frac{\sinh\left(2\beta J^c/M\right)}{\sinh\left(2\beta J^c g^c/M\right)} = 1 \Rightarrow g^c = 1 \forall J \end{aligned}$$

- We therefore conclude that the 1D quantum Ising model in a transverse field, undergoes a quantum phase transition at the critical coupling  $g^c=1$

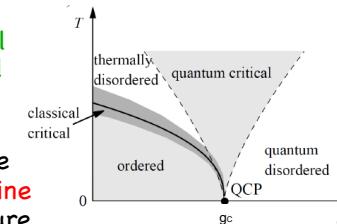
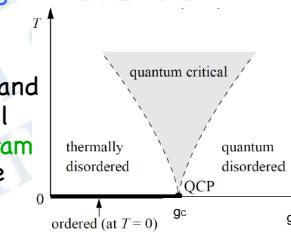


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Que secede se allenes la linea trazogate?

a temperatura finita non ha limite  
termodynamico → non ha frontiera di  
fase quantistica

- The QC mapping is rather general. Details of the mapping will depend on the model but the approach is the same: d-dimensional quantum systems can be mapped onto an equivalent (d+1)-dimensional classical models (quite often not a trivial one!).
- What happens to the QPT at finite  $T$ ? When  $h=0$  (and therefore  $g=0$ ), the 1D Ising model is simply the classical 1D Ising chain which exhibits no phase transition at any  $T$
- At finite  $T$ ,  $M$  is finite and therefore when  $N \rightarrow \infty$ , the partition function describes an infinite strip and consequently the system is effectively 1D and will not exhibit any phase transitions. Its phase diagram will, therefore, be like the one in the next figure
- Now consider the quantum 2D Ising model in a transverse field. When  $T=0$ , there is a QPT at a given  $g^c$ . In addition, however, when  $h=0$  (i.e.  $g=0$ ) the system becomes the two-dimensional classical Ising model which exhibits a thermal second order phase transition.
- So, there is a quantum phase transition at  $(g^c; T=0)$  and a thermal one at  $(g=0; T_c)$ . These two transitions are typically connected by a line of thermal critical points as illustrated in figure



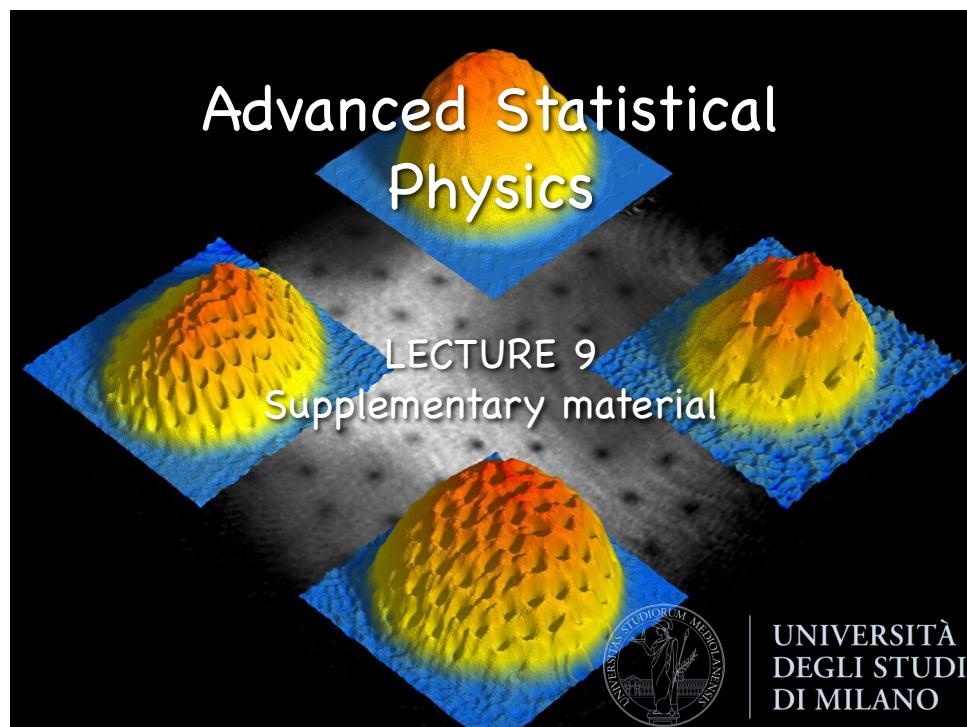
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## Lecture 9: Suggested books

- H. Nishimori and G. Ortiz, *Elements of Phase Transitions and Critical Phenomena*, Oxford
- S. Suzuki, Jun-ichi Inoue, B. K. Chakrabarti, *Quantum Ising Phases and Transitions in Transverse Ising Models*, Springer
- S. Sachdev, *Quantum Phase Transitions*, Cambridge
- J. Ignacio Cirac, *Entanglement in many-body quantum systems*, in Many-Body Physics with Ultracold Gases (Ecole de Physique des Houches, 2010), Oxford

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## Transverse-field Ising chain: exact spectrum

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- We now take a different route and set up a formalism that eventually leads to an exact determination of the excitation spectrum for the Transverse-field Ising chain but also for other quantum spin lattices.
- The essential tool is the **Jordan-Wigner transformation**. This is a very powerful mapping between models with spin-1/2 degrees of freedom and spinless fermions. The central observation is that there is a simple **mapping between the Hilbert space of a system with a spin-1/2 degree of freedom per site and that of spinless fermions hopping between sites with single orbitals**.
- We may associate the **spin-down state** with an **empty orbital** on the site and a **spin-up state** with an **occupied orbital**.
- If the **canonical fermion operator**  $a_j$  annihilates a spinless fermion on site  $j$ , then this simple mapping immediately implies the operator relation  $\hat{\sigma}_j^z = 2\hat{n}_j - 1 = 2\hat{a}_j^\dagger \hat{a}_j - 1$

In fact:

$$\left\{ \begin{array}{l} \hat{\sigma}_j^z |\uparrow\rangle_j = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_j \begin{pmatrix} 1 \\ 0 \end{pmatrix}_j = \begin{pmatrix} 1 \\ 0 \end{pmatrix}_j = |\uparrow\rangle_j = |1\rangle_j \Rightarrow (2\hat{n}_j - 1)|1\rangle_j = 2|1\rangle_j - |1\rangle_j = |1\rangle_j \quad c.v.d. \\ \hat{\sigma}_j^z |\downarrow\rangle_j = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_j \begin{pmatrix} 0 \\ 1 \end{pmatrix}_j = -\begin{pmatrix} 0 \\ 1 \end{pmatrix}_j = -|\downarrow\rangle_j = -|0\rangle_j \Rightarrow (2\hat{n}_j - 1)|0\rangle_j = -|0\rangle_j \quad c.v.d. \end{array} \right.$$

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## The Jordan-Wigner transformation

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- It is also clear that the operation of  $a_j^\dagger$ , i.e. the creation of a fermion, is equivalent to flipping the spin from down to up, which can be accomplished with the rising operator

$$\hat{s}_j^+ = \frac{1}{2} [\hat{\sigma}_j^x + i\hat{\sigma}_j^y] = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_j + \frac{i}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}_j = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}_j$$

- Note, in fact, that

$$\hat{s}_j^+ |\downarrow\rangle_j = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}_j \begin{pmatrix} 0 \\ 1 \end{pmatrix}_j = \begin{pmatrix} 1 \\ 0 \end{pmatrix}_j = |\uparrow\rangle_j = |1\rangle_j$$

- similarly, **destroying a fermion by  $a_j$  is equivalent to lowering the spin**

$$\hat{s}_j^- = \frac{1}{2} [\hat{\sigma}_j^x - i\hat{\sigma}_j^y] = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_j - \frac{i}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}_j = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}_j$$

$$\hat{s}_j^- |\uparrow\rangle_j = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}_j \begin{pmatrix} 1 \\ 0 \end{pmatrix}_j = \begin{pmatrix} 0 \\ 1 \end{pmatrix}_j = |\downarrow\rangle_j = |0\rangle_j$$

- Although this equivalence works for a single site, we cannot yet equate the fermion operators with the corresponding rising and lowering spin operators for the many-site problem; this is because **while two fermionic operators on different sites anticommute, two spin operators commute**.

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- In fact, let me take for example **only 2 sites**, for spin rising operators, if we start from the state that both spins are pointing down,  $| \downarrow, \downarrow \rangle$ , we can rise the spin on site 1 first, and then the spin on site 2, which is

$$\hat{S}_2^+ \hat{S}_1^+ | \downarrow, \downarrow \rangle_{1,2} = \hat{S}_2^+ | \uparrow, \downarrow \rangle_{1,2} = | \uparrow, \uparrow \rangle_{1,2}$$

- or, we can rise the two spins in opposite ordering, i.e. rise the spin on site 2 first, and then the spin on site 1, which is

$$\hat{S}_1^+ \hat{S}_2^+ | \downarrow, \downarrow \rangle_{1,2} = \hat{S}_1^+ | \downarrow, \uparrow \rangle_{1,2} = | \uparrow, \uparrow \rangle_{1,2}$$

- Regardless the ordering, we have the same final state.
- However, for **fermionic operators**, we know that starting from the double empty state, and creating a particle on site 1 and then on site 2 we obtain a result which is **different** when the creation operators are applied in the opposite order:

$$\hat{a}_2^+ \hat{a}_1^+ | 0 \rangle = \hat{a}_2^+ | 1_1 \rangle = | 1_2 1_1 \rangle = -| 1_1 1_2 \rangle = -\hat{a}_1^+ | 1_2 \rangle = -\hat{a}_1^+ \hat{a}_2^+ | 0 \rangle$$

- The correct mapping for a system with 2 sites is

$$\hat{S}_1^+ = \hat{a}_1^+ \quad \hat{S}_2^+ = \hat{a}_2^+ (-1)^{\hat{n}_1}$$

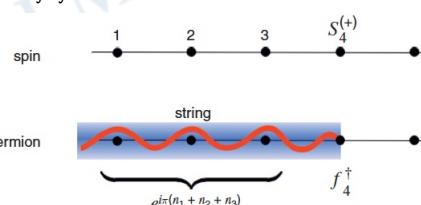
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- In fact, for example  $\hat{S}_2^+ \hat{S}_1^+ | \downarrow, \downarrow \rangle_{1,2} = \hat{a}_2^+ (-1)^{\hat{n}_1} \hat{a}_1^+ | 0 \rangle = \hat{a}_2^+ (-1)^{\hat{n}_1} | 1_1 \rangle = -\hat{a}_2^+ | 1_1 \rangle = -| 1_2 1_1 \rangle$
- Now, for  $\hat{S}_1^+ \hat{S}_2^+ | \downarrow, \downarrow \rangle_{1,2} = \hat{a}_1^+ \hat{a}_2^+ (-1)^{\hat{n}_1} | 0 \rangle = \hat{a}_1^+ \hat{a}_2^+ | 0 \rangle = \hat{a}_1^+ | 1_2 \rangle = | 1_1 1_2 \rangle = -| 1_2 1_1 \rangle$
- Using this mapping, we find that indeed  $\hat{S}_1^+ \hat{S}_2^+ = \hat{S}_2^+ \hat{S}_1^+$  as it should be
- If we have many sites  $j=1,2,3\dots N$ , the correct mapping is

$$\begin{cases} \hat{S}_j^+ = \hat{a}_j^+ \prod_{l=1}^{j-1} (1 - 2\hat{n}_l) = \hat{a}_j^+ \prod_{l=1}^{j-1} (-1)^{\hat{n}_l} = \hat{a}_j^+ (-1)^{\sum_{l=1}^{j-1} \hat{n}_l} = \hat{a}_j^+ e^{-i\pi \sum_{l=1}^{j-1} \hat{n}_l} \\ \hat{S}_j^- = \prod_{l=1}^{j-1} (1 - 2\hat{n}_l) \hat{a}_j^- = \prod_{l=1}^{j-1} (-1)^{\hat{n}_l} \hat{a}_j^- = (-1)^{\sum_{l=1}^{j-1} \hat{n}_l} \hat{a}_j^- = e^{i\pi \sum_{l=1}^{j-1} \hat{n}_l} \hat{a}_j^- \\ \hat{\sigma}_j^z = 2\hat{n}_j - 1 = 2\hat{a}_j^+ \hat{a}_j^- - 1 \end{cases}$$

This is the **Jordan-Wigner transformation**. The naive single-site correspondence has been modified by a "string" of operators, whose value is +1 fermion (-1) if the total number of fermions on the sites to the left of site  $j$  are even (odd). Note that the spin operators have a highly nonlocal representation in terms of the fermion operators.



Illustrating the Jordan-Wigner transformation:  
The spin-raising operator at site  $j=4$  is decomposed into a product of a fermion operator and a string operator

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## The Jordan-Wigner transformation

- Let's check the Jordan-Wigner transformation:

$$\begin{aligned}\hat{\sigma}_j^z &= 2\hat{a}_j^+\hat{a}_j - 1 = 2\hat{S}_j^+e^{-i\pi\sum_{l=1}^{j-1}\hat{S}_l^+\hat{S}_l^-}e^{i\pi\sum_{l=1}^{j-1}\hat{S}_l^-\hat{S}_l^+}\hat{S}_j^- - \hat{1} = 2\hat{S}_j^+\hat{S}_j^- - \hat{1} = \\ &= 2\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}_j \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}_j - \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}_j = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_j \text{ c.v.d.}\end{aligned}$$

- To check that the operators  $a_j$  and  $a_j^\dagger$  satisfy fermionic anti-commutation relations

$$[\hat{a}_i^\dagger, \hat{a}_k]_{+1} = \delta_{ik} \quad [\hat{a}_i, \hat{a}_k]_{+1} = 0 \quad [\hat{a}_i^\dagger, \hat{a}_k^\dagger]_{+1} = 0$$

- one uses the simple relations obeyed by Pauli spin operators

$$\hat{S}_j^+\hat{S}_j^- = \frac{1}{2}(1 + \hat{\sigma}_j^z) \quad \hat{S}_j^-\hat{S}_j^+ = \frac{1}{2}(1 - \hat{\sigma}_j^z) \quad e^{i\frac{\pi}{2}\hat{\sigma}_j^z} = i\hat{\sigma}_j^z$$

- So that, the Jordan-Wigner transformation can be rewritten as

$$\begin{cases} \hat{a}_j^\dagger = \hat{S}_j^+ \prod_{l=1}^{j-1} (-\hat{\sigma}_l^z) \\ \hat{a}_j = \prod_{l=1}^{j-1} (-\hat{\sigma}_l^z) \hat{S}_j^- \end{cases} \Rightarrow [\hat{a}_j^\dagger, \hat{a}_j] = \hat{a}_j^\dagger \hat{a}_j + \hat{a}_j \hat{a}_j^\dagger = \hat{S}_j^+ \hat{S}_j^- + \hat{S}_j^- \hat{S}_j^+ = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}_j + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}_j = \hat{1}$$

- To prove  $[\hat{a}_j^\dagger, \hat{a}_k]_+ = 0$ , for  $j \neq k$ , without loss of generality we assume  $j < k$ . Now

$$\begin{aligned}[\hat{a}_j^\dagger, \hat{a}_k]_+ &= \hat{a}_j^\dagger \hat{a}_k + \hat{a}_k \hat{a}_j^\dagger = \hat{S}_j^+ \prod_{l=1}^{j-1} (-\hat{\sigma}_l^z) \prod_{l=1}^{k-1} (-\hat{\sigma}_l^z) \hat{S}_k^- + \prod_{l=1}^{k-1} (-\hat{\sigma}_l^z) \hat{S}_k^- \hat{S}_j^+ \prod_{l=1}^{j-1} (-\hat{\sigma}_l^z) = \\ &= \hat{S}_j^+ \prod_{l=k}^{j-1} (-\hat{\sigma}_l^z) \hat{S}_k^- + \hat{S}_k^- \prod_{l=k}^{j-1} (-\hat{\sigma}_l^z) \hat{S}_j^+ = \dots\end{aligned}$$

- If one now uses the fact

$$\hat{S}_n^- \hat{\sigma}_n^z = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}_n \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_n = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}_n = -\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_n \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}_n = -\hat{\sigma}_n^z \hat{S}_n^-$$

- It follows that:

$$\dots = -\hat{S}_j^+ \hat{S}_k^- \prod_{l=k}^{j-1} (-\hat{\sigma}_l^z) + \hat{S}_k^- \hat{S}_j^+ \prod_{l=k}^{j-1} (-\hat{\sigma}_l^z) = -\hat{S}_j^+ \hat{S}_k^- \prod_{l=k}^{j-1} (-\hat{\sigma}_l^z) + \hat{S}_j^+ \hat{S}_k^- \prod_{l=k}^{j-1} (-\hat{\sigma}_l^z) = 0$$

- Similarly, one can derive the other anti-commutation relations.

- This feature is also found in the inverse transformation:

$$\begin{cases} \hat{a}_j^+ = \hat{S}_j^+ \prod_{l=1}^{j-1} (1 - 2\hat{S}_l^+ \hat{S}_l^-) = \hat{S}_j^+ \prod_{l=1}^{j-1} (-1)^{\hat{S}_l^+ \hat{S}_l^-} = \hat{S}_j^+ (-1)^{\sum_{l=1}^{j-1} \hat{S}_l^+ \hat{S}_l^-} = \hat{S}_j^+ e^{-i\pi \sum_{l=1}^{j-1} \hat{S}_l^+ \hat{S}_l^-} \\ \hat{a}_j^- = \prod_{l=1}^{j-1} (1 - 2\hat{S}_l^+ \hat{S}_l^-) \hat{S}_j^- = \prod_{l=1}^{j-1} (-1)^{\hat{S}_l^+ \hat{S}_l^-} \hat{S}_j^- = (-1)^{\sum_{l=1}^{j-1} \hat{S}_l^+ \hat{S}_l^-} \hat{S}_j^- = e^{i\pi \sum_{l=1}^{j-1} \hat{S}_l^+ \hat{S}_l^-} \hat{S}_j^- \end{cases}$$

- Let's start from the transverse-field open chain Ising Hamiltonian:

$$\hat{H} = -J \sum_{i=1}^{N-1} \hat{\sigma}_i^x \hat{\sigma}_{i+1}^x - g J \sum_{i=1}^N \hat{\sigma}_i^z$$

- To express the spin Hamiltonian in terms of the fermion operators, for the transverse field we use the relation,

$$\hat{\sigma}_j^z = 2\hat{n}_j - 1 = 2\hat{a}_j^+ \hat{a}_j^- - 1$$

- For the coupling term

$$\begin{aligned} \hat{\sigma}_i^x &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_i = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}_i + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}_i = [\hat{S}_i^+ + \hat{S}_i^-] \Rightarrow \hat{\sigma}_i^x \hat{\sigma}_{i+1}^x = [\hat{S}_i^+ + \hat{S}_i^-][\hat{S}_{i+1}^+ + \hat{S}_{i+1}^-] \\ \hat{S}_i^+ \hat{S}_{i+1}^- &= \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}_i \hat{S}_{i+1}^- = - \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}_i \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_i \hat{S}_{i+1}^- = -\hat{S}_i^+ \hat{\sigma}_i^z \hat{S}_{i+1}^- = \\ &= -\hat{a}_i^+ e^{-i\pi \sum_{l=1}^{i-1} \hat{n}_l} (2\hat{n}_i - 1) e^{i\pi \sum_{l=i}^i \hat{n}_l} \hat{a}_{i+1}^- = \hat{a}_i^+ e^{-i\pi \sum_{l=1}^{i-1} \hat{n}_l} e^{i\pi \sum_{l=i}^i \hat{n}_l} \hat{a}_{i+1}^- = \hat{a}_i^+ \hat{a}_{i+1}^- \end{aligned} \quad 35$$

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- Similarly one can derive the following relations

$$\hat{S}_i^- \hat{S}_{i+1}^+ = -\hat{a}_i^- \hat{a}_{i+1}^+ \quad \hat{S}_i^+ \hat{S}_{i+1}^+ = \hat{a}_i^+ \hat{a}_{i+1}^+ \quad \hat{S}_i^- \hat{S}_{i+1}^- = -\hat{a}_i^- \hat{a}_{i+1}^-$$

- Thus the coupling term can be written in terms of fermion operators which are also only coupled to nearest neighbours.

- Collecting all the terms we arrive at the Hamiltonian

$$\begin{aligned} \hat{H} &= -J \sum_{i=1}^{N-1} [\hat{S}_i^+ \hat{S}_{i+1}^+ + \hat{S}_i^+ \hat{S}_{i+1}^- + \hat{S}_i^- \hat{S}_{i+1}^+ + \hat{S}_i^- \hat{S}_{i+1}^-] - g J \sum_{i=1}^N \hat{\sigma}_i^z = \\ &= -J \sum_{i=1}^{N-1} [\hat{a}_i^+ \hat{a}_{i+1}^+ + \hat{a}_i^+ \hat{a}_{i+1}^- - \hat{a}_i^- \hat{a}_{i+1}^+ - \hat{a}_i^- \hat{a}_{i+1}^-] - g J \sum_{i=1}^N (2\hat{a}_i^+ \hat{a}_i^- - 1) = \\ &= NgJ - 2gJ\hat{N} - J \sum_{i=1}^{N-1} [\hat{a}_i^+ \hat{a}_{i+1}^- + \hat{a}_{i+1}^+ \hat{a}_i^-] + J \sum_{i=1}^{N-1} [\hat{a}_{i+1}^+ \hat{a}_i^+ + \hat{a}_i^- \hat{a}_{i+1}^-] \end{aligned}$$

- The first term is an irrelevant constant, in the second term  $2gJ$  can be considered as a **chemical potential**, the third term describes **nearest-neighbor hoppings**. This fermionic Hamiltonian has terms such as  $a_{j+1}^\dagger a_j^\dagger$  or  $a_j a_{j+1}$  that violate the **fermion conservation number**. Hence the eigenstates of  $H$  will not have a definite fermion number.
- The above transformed Hamiltonian is already quadratic in the fermion operators and it is diagonalizable.

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- To do so, let us consider fermions in **momentum space**
- The energy shifted Hamiltonian becomes:

$$\begin{aligned}
\hat{H} &= -2gJ\hat{N} - J \sum_{j=1}^{N-1} [\hat{a}_j^+ \hat{a}_{j+1} + \hat{a}_{j+1}^+ \hat{a}_j] + J \sum_{j=1}^{N-1} [\hat{a}_{j+1}^+ \hat{a}_j^+ + \hat{a}_j^+ \hat{a}_{j+1}] = \\
&= -2gJ\hat{N} - J \sum_{q,q'} \hat{a}_q^+ \hat{a}_{q'} e^{iq} \frac{1}{N} \sum_{j=1}^{N-1} e^{-i(q-q')j} - J \sum_{q,q'} \hat{a}_q^+ \hat{a}_{q'} e^{-iq} \frac{1}{N} \sum_{j=1}^{N-1} e^{-i(q-q')j} + \\
&\quad + J \sum_{q,q'} \hat{a}_q^+ \hat{a}_{q'}^+ e^{iq} \frac{1}{N} \sum_{j=1}^{N-1} e^{-i(q+q')j} + J \sum_{q,q'} \hat{a}_q^+ \hat{a}_q e^{-iq} \frac{1}{N} \sum_{j=1}^{N-1} e^{-i(q+q')j} = \\
&= -2gJ\hat{N} - J \sum_q \hat{a}_q^+ \hat{a}_q e^{iq} - J \sum_{q \neq 0} \hat{a}_q^+ \hat{a}_q e^{-iq} + J \sum_q \hat{a}_q^+ \hat{a}_{-q}^+ e^{-iq} + J \sum_q \hat{a}_{-q} \hat{a}_q e^{iq} = \\
&= -2J \sum_q \hat{a}_q^+ \hat{a}_q (\cos q + g) + J \sum_q [\hat{a}_q^+ \hat{a}_{-q}^+ e^{-iq} + \hat{a}_{-q} \hat{a}_q e^{iq}]
\end{aligned}$$

- Summing only on positive  $q$

$$\begin{aligned}
\hat{H} &= \sum_{q>0} (\hat{a}_q^+ \hat{a}_q + \hat{a}_{-q}^+ \hat{a}_{-q}) (-J \cos q - gJ) + \sum_{q>0} [(-iJ \sin q) \hat{a}_q^+ \hat{a}_{-q}^+ + (iJ \sin q) \hat{a}_{-q} \hat{a}_q] \\
\Rightarrow \hat{H} &= \sum_{q>0} (\hat{a}_q^+ \hat{a}_{-q}) \begin{pmatrix} -J \cos q - gJ & -iJ \sin q \\ iJ \sin q & J \cos q + gJ \end{pmatrix} \begin{pmatrix} \hat{a}_q \\ \hat{a}_{-q}^+ \end{pmatrix}
\end{aligned}$$

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- By diagonalising the kernel matrix, we can then find the **eigenvalues** of the Hamiltonian.

$$\begin{aligned}
0 &= \det \begin{pmatrix} -J \cos q - gJ - \lambda & -iJ \sin q \\ iJ \sin q & J \cos q + gJ - \lambda \end{pmatrix} = [\lambda^2 - (J \cos q + gJ)^2] - (J \sin q)^2 \\
\Rightarrow \lambda_{\pm}(q) &= \pm J \sqrt{(\cos q + g)^2 + \sin^2 q} = \pm J \sqrt{1 + g^2 + 2g \cos q}
\end{aligned}$$

- It is simple to see that it gives **two energy bands**. Since the Hamiltonian is diagonalizable, it shows that the initial 1D Ising model of spins can be completely described by free fermions filling the energy levels above.
- We get two bands with  $\lambda_-(q) \leq 0$  and  $\lambda_+(q) \geq 0$ . At  $T = 0$  K, the  $\lambda_-$  band is fully filled while the  $\lambda_+$  band is empty. In fact, the **ground state energy** is  $E_0 = \sum_q \lambda_-(q)$  and the diagonalized Hamiltonian (see original articles on Ariel) via a canonical transformation turns out to be:

$$\hat{H} = E_0 + 2 \sum_q \lambda_+(q) \hat{\eta}_q^+ \hat{\eta}_q$$

being  $\eta_q^+$  and  $\eta_q$  the new fermionic creation and destruction operators

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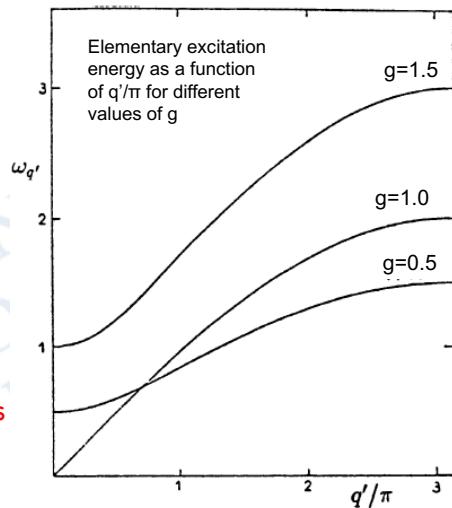
- The energy of the elementary excitations as a function of wave vector  $q' = \pi - q$ , the pseudo wave vector of the excitations, for different values of  $g$  is shown in figure. The  $q' = 0$  excitation corresponds to the excited state whose configuration is closest to the ground state configuration.

- There is an **energy gap** in the excitation spectrum of the system:

$$\Delta(q) = 2J\sqrt{1 + g^2 + 2g \cos q}$$

- The minimum of  $\Delta(q)$  is at  $q'=0$ . This **gap goes to zero** at  $q'=0$  for  $g=1$ , which is the **quantum critical point** of transverse-field Ising model.

- Note that this is somewhat what we should expect in presence of a quantum phase transition in a system with an energy gap above the ground state: a vanishing gap exactly at the quantum critical point and a transition from one type of ground state to another



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## QPT & entanglement

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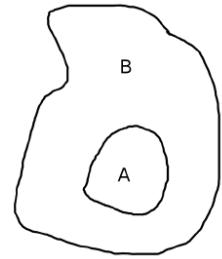
- Entanglement** is a pure quantum property that **may appear whenever we have two or more quantum objects**. It highlights the appearance of certain kind of quantum correlations which cannot appear in classical theories.
- By **object** we may mean a **particle**, a **bosonic or fermionic mode**, etc. Strictly speaking, the **Hilbert space** corresponding to the **whole system** must **decompose as a tensor product of several Hilbert space**, one for **each and every object**. **Entanglement will depend on how we understand this decomposition** and thus we must specify with respect to what (particles, modes, etc.) we refer when we discuss entanglement properties of systems.
- Given that the entanglement itself has the property of "effective" non-locality (EPR paradox, Bell's states), we may intuitively **expect** to see certain **relations between the quantum long-range correlations occurs at criticality and the entanglement of the system**
- A quantum phase transition (QPT) happens when the zero-temperature quantum fluctuations in a quantum many-particle system cause a transition from one type of ground state to another. We therefore **expect further that systems near quantum critical points can be characterized also in terms of entanglement**

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## Entanglement in many-body systems: Pure States 41

- We start out considering the simplest case, namely the entanglement present in a many-body quantum state  $|\Psi\rangle$  whenever we have a pure state. This is the case, for instance, at zero temperature, or in most applications in quantum information science
- We consider here two systems, A and B. We denote by  $\mathcal{H}_A$  and  $\mathcal{H}_B$  the corresponding Hilbert spaces, and by  $\{|n\rangle_x\}$  and orthonormal basis in  $\mathcal{H}_x$ , where  $n = 1, 2, \dots, d_x$ , with  $d_x = \dim(\mathcal{H}_x)$ .
- Most of the time we will concentrate on the simplest systems, qubits, where  $d_A = d_B = 2$ . In that case, in order to keep the standard notation, we will take as a basis  $\{|l\rangle_x, |u\rangle_x\} = \{|0\rangle_x, |1\rangle_x\}$ . Unless we state it differently, we will always work with qubits ... i.e. quantum spins
- The Hilbert space corresponding to the whole system,  $\mathcal{H}$ , is the tensor product of  $\mathcal{H}_A$  and  $\mathcal{H}_B$ , which we write  $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ .
- An orthonormal basis in  $\mathcal{H}$  is  $\{|m\rangle_A \otimes |n\rangle_B\}$ . To simplify the notation, we will typically omit the symbol " $\otimes$ ", and the sub-indices A,B whenever there is no possible confusion.



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- For instance, any state for two qubits can be written as

$$|\Psi\rangle = \sum_{n,m=0}^1 c_{n,m} |n, m\rangle \quad \sum_{n,m=0}^1 |c_{n,m}|^2 = 1$$

- We will consider observables for each of the systems, which will be represented as operators acting on the corresponding spaces. For instance,  $\sigma_A^1 \otimes \sigma_B^2$  denotes an operator  $\sigma^1$  acting in  $\mathcal{H}_A$  and  $\sigma^2$  in  $\mathcal{H}_B$ . As before, we will omit the symbol for the tensor product; additionally,  $\sigma_A^1$  will stand for  $\sigma_A^1 \otimes 1_B$ , where  $1_B$  is the identity operator in  $\mathcal{H}_B$ .
- We say that  $|\Psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$  is a product state if there exist two vectors  $|\varphi_1\rangle \in \mathcal{H}_A$  and  $|\varphi_2\rangle \in \mathcal{H}_B$  such that  $|\Psi\rangle = |\varphi_1\rangle_A \otimes |\varphi_2\rangle_B$ . Otherwise we say that is an entangled state. Examples of product states are those forming the orthonormal basis  $|m,n\rangle = |m\rangle_A \otimes |n\rangle_B$  in  $\mathcal{H}$ . Examples of entangled state are the so-called Bell states

$$|\Phi^\pm\rangle = \frac{1}{\sqrt{2}} (|l, l\rangle \pm |u, u\rangle) = \frac{1}{\sqrt{2}} (|0, 0\rangle \pm |1, 1\rangle)$$

$$|\Psi^\pm\rangle = \frac{1}{\sqrt{2}} (|l, u\rangle \pm |u, l\rangle) = \frac{1}{\sqrt{2}} (|0, 1\rangle \pm |1, 0\rangle)$$

The difference between entangled and product states is that the first ones give rise to correlations.

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- If we have a **product state**  $|\Psi\rangle = |\varphi_1\rangle_A \otimes |\varphi_2\rangle_B = |\varphi_1, \varphi_2\rangle$ , then the expectation value  $\langle \Psi | \sigma_A^i \otimes \sigma_B^j | \Psi \rangle$  factorizes into  $\langle \varphi_1 | \sigma_A^i | \varphi_1 \rangle \langle \varphi_2 | \sigma_B^j | \varphi_2 \rangle$ , and thus the results of measurements in both systems will be uncorrelated.
  - For any **entangled state**, on the contrary, there always exist observables in  $\mathcal{H}_A$  and in  $\mathcal{H}_B$  for which the expectation value does not factorize and thus for which the results of measurements will be correlated. For example, considering  $\hat{\sigma}^{\vec{n}} = n_x \hat{\sigma}^x + n_z \hat{\sigma}^z$
- we have (check!)  $\langle \Phi^+ | \hat{\sigma}_A^{\vec{n}} \otimes \hat{\sigma}_B^{\vec{m}} | \Phi^+ \rangle = n_x m_x + n_z m_z = \vec{n} \cdot \vec{m}$   
whereas (check!)  $\langle \Phi^+ | \hat{\sigma}_{A(B)}^{\vec{n}} | \Phi^+ \rangle = \langle \Phi^+ | \hat{\sigma}_{A(B)}^{\vec{n}} \otimes \hat{I}_{B(A)} | \Phi^+ \rangle = 0$
- Thus, whenever we measure the same Pauli operators in  $\mathcal{H}_A$  and  $\mathcal{H}_B$  (i.e., when  $\mathbf{n}$  and  $\mathbf{m}$  are parallel), the results are random ( $\langle \Phi^+ | \sigma_{A(B)}^i | \Phi^+ \rangle = 0$ ) but completely correlated ( $\langle \Phi^+ | \sigma_A^i \sigma_B^i | \Phi^+ \rangle = 1$ , i.e. the same outcome in A and B).
  - In order to analyze the entanglement in bipartite systems it is useful to introduce the **Schmidt decomposition (SD)**.

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### Schmidt decomposition

- Given the state  $|\Psi\rangle = \sum_{n,m} c_{n,m} |n, m\rangle$   $\sum_{n,m} |c_{n,m}|^2 = 1$  is always possible to find an orthonormal basis  $\{|u_n\rangle\}$  in  $\mathcal{H}_A$  and  $\{|v_m\rangle\}$  in  $\mathcal{H}_B$ , such that we can write  $|\Psi\rangle = \sum_{k \leq \min(d_A, d_B)} d_k |u_k, v_k\rangle$
- In case one of the Schmidt coefficients is one and the rest are zero, we have a product state, also called a separable state. Otherwise, our state is entangled.
- The SD is also very useful to determine the reduced density operators  $\rho_A$  and  $\rho_B$  for subsystems A and B alone:

$$\hat{\rho}_A = Tr_B(\hat{\rho}_{pure}) = Tr_B(|\Psi\rangle\langle\Psi|) = \sum_q \langle v_q | \Psi \rangle \langle \Psi | v_q \rangle = \sum_k |d_k|^2 |u_k\rangle\langle u_k|$$

$$\hat{\rho}_B = Tr_A(\hat{\rho}_{pure}) = \sum_k |d_k|^2 |v_k\rangle\langle v_k|$$

where by  $Tr_X$  we mean the trace with respect to system X.

- The reduced density operators so obtained, via SD, are automatically diagonalized, and we observe that their eigenvalues are nothing but the square modulus of the Schmidt coefficients.

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- We find out that  $\rho_B$  has the same non-zero eigenvalues of  $\rho_A$  although dimensions of  $\mathcal{H}_A$  and  $\mathcal{H}_B$  might be different, in which case the number of null eigenvalues will differ. In conclusion, The square of the Schmidt coefficients are the non-zero eigenvalues of both  $\rho_A$  and  $\rho_B$ .
  - It is important to stress the fact that if the pure state representing the whole system is separable, then the reduced density matrices  $\rho_A$  and  $\rho_B$  describe pure subsystems; if the pure state is entangled, then the reduced density matrices describe mixed subsystems
  - Consider the following example:
- $$|\Phi^\theta\rangle = \cos\theta|0,0\rangle + \sin\theta|1,1\rangle$$
- $|\Phi^\theta\rangle$  is already written in the SD form.
- The eigenvalues of the reduced density operator are  $\cos^2\theta$  and  $\sin^2\theta$ ; for  $\theta=0$  we have a product state, whereas for  $\theta=\pi/4$  we have the Bell state  $|\Phi^+\rangle$ , which is a maximally entangled state. In parallel, the reduced density operators get more and more mixed as one increases  $\theta$  from 0 to  $\pi/4$ .
  - This example shows that entanglement of a pure state is linked to the mixedness of the reduced density operators.

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## Entropy of entanglement

- As a consequence, to introduce a measure of entanglement of a pure state,  $|\Phi\rangle$ , we could use a measure of mixedness of its subsystems. Thus, we define the entropy of entanglement of a pure state as:
- $$E(\Phi) = S(\hat{\rho}_A) = -Tr_A(\hat{\rho}_A \log \hat{\rho}_A) = -\sum_k |d_k|^2 \log |d_k|^2 = S(\hat{\rho}_B)$$
- For a product state  $E(\Phi) = 0$  (since Schmidt number equals 1 and  $d=1$ ), whereas the maximum entanglement is  $E = \log[\min(d_A; d_B)]$  which is reached for the state for which all  $d_k$  are equal to  $1/[\min(d_A; d_B)]^{1/2}$ . These are thus called maximally entangled states.
  - We want to emphasize the fact that, in order to evaluate the amount of entanglement of the total pure state, we quantify the von Neumann entropy of its subsystems A and B,  $E(\Phi)=S(\rho_A)=S(\rho_B)$ , rather than the von Neumann entropy of the whole state,  $S(\rho_{AB})$ , which is always zero for pure states.
  - This because entanglement is strictly related to the correlation between the two subsystems, which can be visualized through a measure of their von Neumann entropy  $E(\Phi)=S(\rho_A)=S(\rho_B)$ .

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- One can easily verify that the Bell states are maximally entangled states, as already pointed out.
- First of all consider the Hilbert space of 2 quantum spins (qubits):  $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B = \mathcal{H}_1 \otimes \mathcal{H}_1$  with  $d_A = d_B = 2$ ; we can start working in the orthonormal basis  $\{|m\rangle_A \otimes |n\rangle_B\} = (|11\rangle, |10\rangle, |01\rangle, |00\rangle)$ ; if the density operator is diagonal in this basis

$$\hat{\rho} = \rho_1 |11\rangle\langle 11| + \rho_2 |10\rangle\langle 10| + \rho_3 |01\rangle\langle 01| + \rho_4 |00\rangle\langle 00|$$

the computation of the von Neumann entropy is straightforward

- For a **pure state** like  $|\Psi\rangle = |11\rangle$ , which is already written in the SD form, we have the density matrix, in this basis,

$$\rho_{ij} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

**von Neumann entropy:**

$$S(\hat{\rho}) = S(\hat{\rho}_{AB}) = -Tr(\hat{\rho} \log \hat{\rho}) = -\sum_{i=1}^4 \rho_i \log \rho_i = 0$$

**Entropy of entanglement:**

$$S(\hat{\rho}_A) = -Tr_A(\hat{\rho}_A \log \hat{\rho}_A) = -\sum_k |d_k|^2 \log |d_k|^2 = 0$$

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- For a **pure state** like  $|\Phi^+\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$ , which again is already written in the SD form, we have the density matrix, in this basis, which is no more diagonal

$$\rho_{ij} = \begin{pmatrix} 1/2 & 0 & 0 & 1/2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1/2 & 0 & 0 & 1/2 \end{pmatrix}$$

**Entropy of entanglement:**

$$S(\hat{\rho}_A) = -\sum_k |d_k|^2 \log |d_k|^2 = -\frac{1}{2} \log \frac{1}{2} - \frac{1}{2} \log \frac{1}{2} = \log 2$$

$|\Phi^+\rangle$  is thus a **maximally entangled** state; what is its von Neumann entropy?

- If we diagonalize  $\rho_{ij}$  we obtain in the basis  $(|\Phi^+\rangle, |\Phi^-\rangle, |\Psi^+\rangle, |\Psi^-\rangle)$

$$\rho_{ij} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

thus

**von Neumann entropy:**  $S(\hat{\rho}) = -\sum_{i=1}^4 \rho_i \log \rho_i = 0$

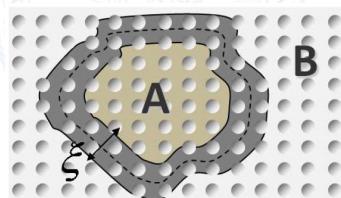
- We confirm therefore that the maximally entangled **pure state**  $|\Phi^+\rangle$  has zero von Neumann entropy.

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## Area law

- Consider a connected region A of the system with a smooth boundary and the complementary region B, and concentrate on the amount of entanglement between these two regions, and its growth as we make region A larger and larger.
- Since we are dealing with a bipartite system of a pure state  $|\Psi\rangle$ , we can evaluate such amount through the entropy of entanglement  $E(\Psi) = S(\rho_A)$ .
- In general, since entropy is an extensive quantity, one would expect that it scales with the number of spins in region A. However, for ground states of Hamiltonians as we are considering here, this seems not to be the case. Instead, the entanglement (entropy of entanglement) scales not with the volume of region A, but with its boundary area, and thus the name area law.



Only particles that are at a distance smaller than the correlation length are correlated (or entangled) to the particles in B. Thus, only they contribute to the entanglement entropy and therefore the area law

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## Entanglement & Transverse-field Ising chain

- The area law could be broken in a quantum phase transition (QPT) when the correlation length diverges
- As we know, QPT may happen when the ground state energy level cross or touch the first excited state energy level. It directly leads to non-analyticity of the energy of the system.
- However, we also know that the system sits in the ground state. We should be able to probe similar non-analyticity behavior of the state near quantum phase transition by measuring the entanglement entropy near quantum critical point.
- A non-analyticity in the ground state automatically propagates into the elements of the density matrix and hence the entanglement entropy of the system. And indeed, this conjecture has been confirmed in many one dimensional exactly solved spin chain model as in the Transverse-field Ising chain

$$\frac{\hat{H}}{h} = -\lambda \sum_{i=1}^{N-1} \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z - \sum_{i=1}^N \hat{\sigma}_i^x$$

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- The exact results for entanglement entropy are [P. Calabrese and J. Cardy, J. of Stat. Mech. P06002 (2004)]:

- $\lambda < 1$  (Paramagnetic phase):

$$S(\rho_A) = \varepsilon \sum_{j=0}^{\infty} \frac{2j+1}{1+e^{(2j+1)\varepsilon}} + \sum_{j=0}^{\infty} \log(1+e^{-(2j+1)\varepsilon})$$

$$\varepsilon = \pi \frac{K(\sqrt{1-k^2})}{K(k)} \quad k = \min(\lambda, \lambda^{-1})$$

- $\lambda > 1$  (Ferromagnetic phase)

$$S(\rho_A) = \varepsilon \sum_{j=0}^{\infty} \frac{2j}{1+e^{2j\varepsilon}} + \sum_{j=0}^{\infty} \log(1+e^{-2j\varepsilon})$$

$K(k)$  is the complete elliptic integral of the first kind

- The figure shows a plot of  $S_\lambda(\rho_A)$  as a function of  $\lambda$ . Note that  $S_{\lambda=0}=0$  and  $S_{\lambda=\infty}=\log 2$ , in agreement with the expectation that the pure ferromagnetic ground state has two possible accessible configurations with opposite sign of magnetization and the pure paramagnetic ground state has only one configuration available with all the spins aligned in the direction of the transverse field

