

## 1.1 cellular automata

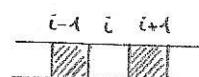
motivation: why start with cellular automata (CA)?

- 'simple' many-particle systems  
→ the models are defined by a small number of simple rules
- despite this simplicity: interesting 'many-particle' physics emerges which cannot be explained on a single-particle level ( $\hat{=}$  'mean-field')
- analytical solutions exist for some of the models (at least for certain parameters)  
but: numerical calculations are required for the general case!

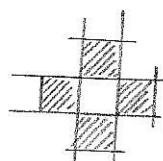
## basic features of cellular automata

- a discrete model defined on a regular grid of cells ( $\hat{=}$  sites), typically in dimension  $d=1$  or  $d=2$ 
  - $i = 1 \quad 2 \quad 3 \quad 4 \quad 5 \quad 6 \quad 7 \quad \dots$
  -
- state of cell  $i$  at time  $t$ :  
 $z_i(t) \in \{q_1, \dots, q_L\}$  → discrete and finite set of states
  - example:  $q_1 = 0$
  - $q_2 = 1$
- dynamics defined for discrete time:  
 $t = 0, 1, 2, \dots$
- $z_i(t+1)$  determined by the state of the cell at time  $t$  ( $z_i(t)$ ) and the states of the cells in its neighbourhood at time  $t$

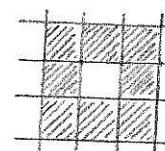
examples:  $d=1 \rightarrow z_i(t+1) = f(z_{i-1}(t), z_i(t), z_{i+1}(t))$



$d=2$



von Neumann  
neighbourhood



Moore neighbourhood

→ two types of CA:

- deterministic CA → a, rule N  
b, game of life

- probabilistic CA → c, ASEP  
d, Nagel-Schreckenberg model

} to be discussed in  
the following

### a, rule N

also: elementary cellular automata

$$\rightarrow d=1; \text{ as above: } z_i(t+1) = f(z_{i-1}(t), z_i(t), z_{i+1}(t))$$

$$\rightarrow z_i(t) \in \{0,1\}$$

example: "rule 30"

→  $f(a,b,c)$  given by the following table

$(a,b,c)$	111	110	101	100	011	010	001	000
$f(a,b,c)$	0	0	0	1	1	1	1	0

 $\rightarrow n_r = [00011110]_2 = [30]_{10}$ 

→ there are  $2^8 = 256$  such rules

⇒ use an integer  $n_r$  to label the rules

$$n_r = \sum_{i=0}^7 a_i 2^i \quad a_i: \text{the digits of the corresponding binary number}$$

$$n_r = 0, 1, \dots, 255$$

→ "Wolfram code"

→ start with the following initial configuration:

$$z_i(t=0) = \begin{cases} 1 & : i=0 \\ 0 & : i \neq 0 \end{cases} \quad \text{here: } i = \dots -3, -2, -1, 0, 1, \dots$$

$$\Rightarrow \begin{matrix} i = & -3 & -2 & -1 & 0 & 1 & 2 & 3 \\ t=0 & \square & \square & \square & \blacksquare & \square & \square & \square \\ t=1 & \square & \square & \blacksquare & \blacksquare & \square & \square & \square \\ t=2 & \blacksquare & \blacksquare & \square & \square & \blacksquare & \square & \square \end{matrix}$$

$$\blacksquare \stackrel{\wedge}{=} 1$$

$$\square \stackrel{\wedge}{=} 0$$

depending on the value of  $N$ , the initial pattern evolves into

- stable homogeneous or oscillating structures
- pseudo-random / chaotic structures (e.g. rule 30)
- structures that interact in complex and interesting ways (e.g. rule 110)

## b) Game of Life

→ or: Conway's Game of Life

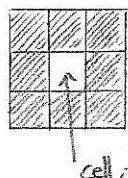
↳ invented by J.H. Conway in 1970

→ deterministic CA on a 2d grid of cells

→  $z_i(t) \in \{0, 1\}$

- $0 \hat{=} \text{dead}$
- $1 \hat{=} \text{alive}$

→ define the neighbourhood  $X(i)$  of cell  $i$ :



■ : the eight neighbours of  $i$  (Moore neighbourhood)  
 $\rightarrow X(i)$

$\Rightarrow$  number of live cells in the neighbourhood:

$$u_i(t) = \sum_{j \in X(i)} z_j(t), \quad u_i(t) \in \{0, 1, \dots, 8\}$$

the update rule:

$$z_i(t+1) = f(z_i(t), u_i(t))$$

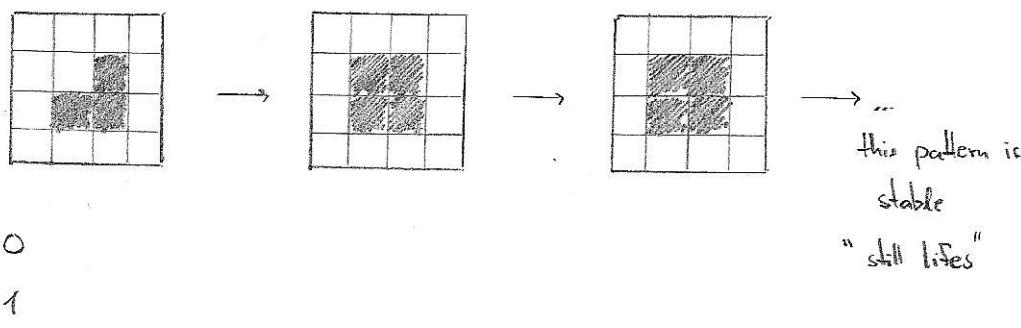
with the function  $f$  given by the following table:

$z_i \backslash u_i$	0	1	2	3	4	5	6	7	8
0	0	0	0	0	1	0	0	0	0
1	0	0	1	1	0	0	0	0	0
2	0	1	0	1	1	0	0	0	0
3	1	0	1	0	0	1	0	0	0
4	0	1	1	0	0	0	1	0	0
5	1	0	0	1	0	0	0	1	0
6	0	0	0	0	1	0	0	0	1
7	0	0	0	0	0	1	0	0	0
8	0	0	0	0	0	0	1	0	0

↓                    ↓                    ↓

"underpopulation"      "reproduction"      "overpopulation"

example:



### c) ASEP

"asymmetric simple exclusion process"  $\rightarrow$  probabilistic ca

state of cell  $i$  :  $z_i(t) \in \{0, 1\}$



cell is empty

the cell is occupied by a single 'particle'

$$\rightarrow d=1 \quad i = 1 \ 2 \ \dots \ N$$

$$\sum_{i=1}^N z_i(t) = M \rightarrow \text{number of particles (conserved)}$$

density  
 $\rho = \frac{M}{N}$

$\rightarrow$  update rules describe the hopping of particles along the 1d system

$p_r$  := probability for a particle to hop from  $i$  to  $i+1$



$$p_e = 1 - p_r$$

there are various possibilities to define the update rules!

example 1 : random sequential update (with periodic boundary conditions)

- start with a random configuration of  $M$  particles on  $N$  sites

- choose randomly one of the particles (\*)

$$\rightarrow k \in \{1, \dots, N\} \text{ with } z_k(t) = 1$$

- random number  $\gamma \in [0, 1]$

$$\text{if } p_r > \gamma \text{ and } z_{k+1}(t) = 0 \rightarrow \begin{cases} z_k(t+1) = 0 \\ z_{k+1}(t+1) = 1 \end{cases}$$

particle hops  
to the right

$$\text{if } p_r \leq \gamma \text{ and } z_{k-1}(t) = 0 \rightarrow \begin{cases} z_k(t+1) = 0 \\ z_{k-1}(t+1) = 1 \end{cases}$$

... to the left

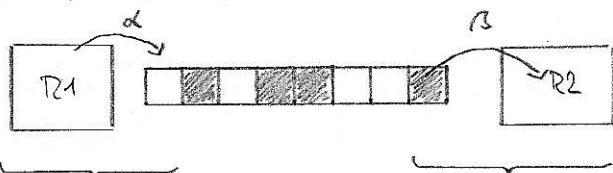
in all other cases:  $z_i(t+1) = z_i(t)$  for all  $i = 1, \dots, N$

- continue with (\*)

### other variants of the update rules

- continuous instead of discrete time  
→ not a ca as defined above
- $p_r = 1, p_e = 0 \rightarrow$  TASEP  
↳ "totally..."
- boundary conditions → infinite system  
→ periodic bc :  $z_{N+1}(t) \doteq z_1(t)$

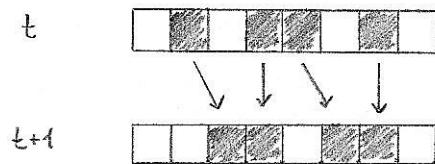
or → open system with reservoirs:



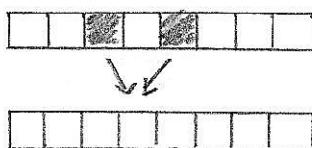
particles hop from R1 to site 1 (if  $z_1=0$ ) with probability  $\alpha$

particle hop from site N (if  $z_N=1$ ) to R2 with probability  $\beta$

- sequential vs. parallel update



note that an additional rule is required for  $p_r \neq 0, p_e \neq 0$

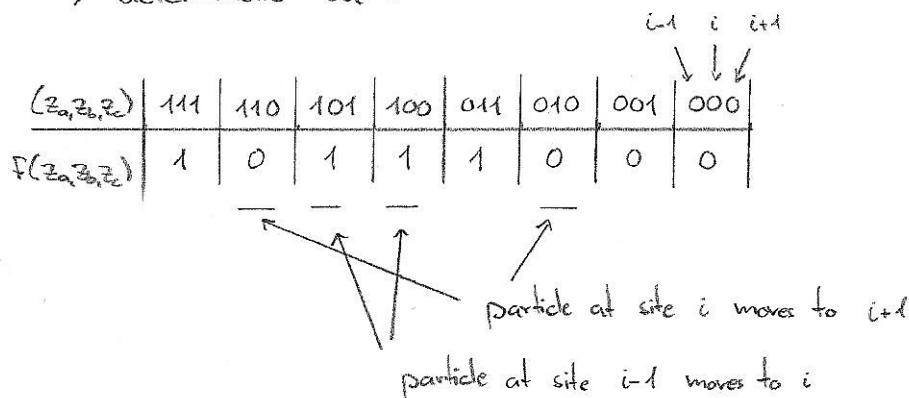


→ this has to be avoided!

example 2: TASEP with parallel update

(infinite system or pbc)

→ deterministic ca !  $\triangleq$  rule 184



$$\Rightarrow n_r = 8 + 16 + 32 + 128 = 184$$

d, Nagel-Schreckenberg model

→ K. Nagel, M. Schreckenberg (1992)

"A cellular automaton model for freeway traffic"

→ simulation of traffic flow and traffic jam

→ a collective phenomenon due to the interaction  
between the cars

→ probabilistic ca, d=1

state of cell i :  $z_i(t) \in \{0, 1\}$

cell is empty  $\downarrow$  cell is occupied by a car with velocity  
 $v \in \{0, 1, \dots, v_{\max}\}$

alternative description

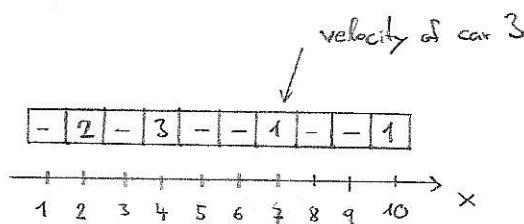
→ label the cars ( $j=1, \dots, M$ ) not the cells ( $i=1, \dots, N$ )

$x_j(t) : \text{position}$  } of car  $j$  at time  $t$   
 $v_j(t) : \text{velocity}$  }

example:

j	1	2	3	4
$x_j(0)$	2	4	7	10
$v_j(0)$	2	3	1	1

$\triangleq$



each time step ( $t \rightarrow t+1$ ) is divided into four basic steps:

### a, acceleration

→ each car attempts to accelerate up to  $v_{\max}$  (here:  $v_{\max} = 3$ )

$$v_j^a = \min(v_{\max}, v_j(t) + 1)$$

j	1	2	3
$v_j$	2	3	1
$v_j^a$	3	3	2

### b, slowing down

→ reduce the velocity of car j to avoid collisions with car  $j+1$

$$v_j^b = \min(v_j^a, x_{j+1}(t) - x_j(t) - 1)$$

j	1	2	3	4
$x_j$	2	4	7	10
$v_j^a$	3	3	2	-
$v_j^b$	1	2	2	-

### c, randomization

→ each car slows down with probability p

- random number  $\alpha \in [0,1]$

- if  $v_j^b > 0$  and  $\alpha < p$  :  $v_j^c = v_j^b - 1$
- else :  $v_j^c = v_j^b$

example:  $p = \frac{1}{2}$

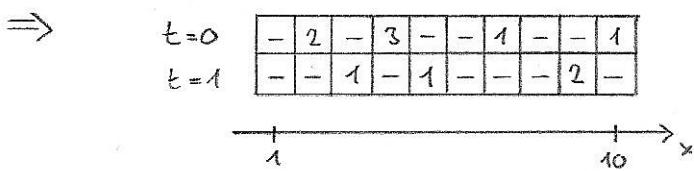
j	1	2	3
$\alpha$	0.6	0.2	0.9
$v_j^b$	1	2	2
$v_j^c$	1	1	2

### d, car motion

$$\rightarrow x_j(t+1) = x_j(t) + v_j^c$$

$$\text{and } v_j(t+1) = v_j^c$$

j	1	2	3
$x_j(t)$	2	4	7
$v_j^c$	1	1	2
$x_j(t+1)$	3	5	9



## 1.2 Statistical physics of classical many-particle systems

here: the classical Ising model as a special case of the

quantum Heisenberg model

$$H = - \sum_{ij\alpha} J_{ij}^{\alpha} S_i^{\alpha} S_j^{\alpha}$$

$i, j = 1, \dots, N$      $N$ : number of sites/spins

$\alpha = x, y, z$

(for more details, see Sec. 2)

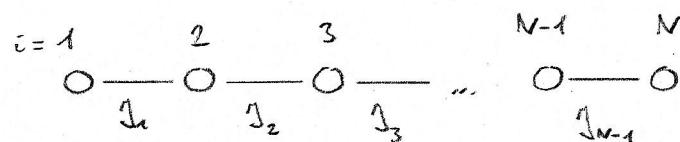
→ the isotropic Heisenberg model:  $J_{ij}^{\alpha} = J_{ij}$ ,  $\alpha = x, y, z$

→ the Ising model corresponds to the anisotropic Heisenberg model

with  $J_{ii}^x = J_{ii}^y = 0$ ,  $J_{ij}^z = J_{ij}$  ( $\neq 0$ )

$$\Rightarrow H_{\text{Ising}} = - \sum_{ij} J_{ij} S_i^z S_j^z$$

example:  $\left. \begin{array}{l} \text{- dimension} = 1 \\ \text{- nearest-neighbour interaction} \\ \text{- open boundary conditions} \end{array} \right\} H = - \sum_{i=1}^{N-1} J_i S_i^z S_{i+1}^z$



basis of the Hilbert space:

$$\{|n\rangle\} = \{|1\rangle_1, |1\rangle_1\} \otimes \{|1\rangle_2, |1\rangle_2\} \otimes \dots \otimes \{|1\rangle_N, |1\rangle_N\}$$

$$= \{|S_1 S_2 S_3 \dots S_N\rangle\} \quad \text{with } S_i = \uparrow/\downarrow$$

→ this gives  $2^N$  states    ( $n = 0, 1, \dots, 2^N - 1$ )

the  $|S_i\rangle$  are eigenstates of  $S_i^z$

$$\rightarrow S_i^z |S_i\rangle = S_i^z |S_i\rangle \quad \text{with } S_i^z = \pm \frac{k_B}{2} \quad \text{for } S_i = \uparrow/\downarrow$$

→ the basis states  $|n\rangle$  are eigenstates of  $H_{\text{Ising}}$ !

$$\begin{aligned}
 \underline{\text{Proof:}} \quad H_{\text{Ising}} |n\rangle &= - \sum_{ij} J_{ij} S_i^z S_j^z |S_1 S_2 \dots S_N\rangle = \\
 &\quad \underbrace{\phantom{- \sum_{ij} J_{ij} S_i^z S_j^z} \quad}_{=} \\
 &= S_i^z |S_1 S_2 \dots S_N\rangle \\
 &= - \sum_{ij} J_{ij} S_i^z \underbrace{S_j^z |S_1 S_2 \dots S_N\rangle}_{=} = \\
 &= S_i^z |S_1 S_2 \dots S_N\rangle \\
 &= E_n |n\rangle \quad \text{with} \quad \boxed{E_n = - \sum_{ij} J_{ij} S_i^z S_j^z}
 \end{aligned}$$

note: this does not hold for the general Heisenberg model (see Sec. 2)

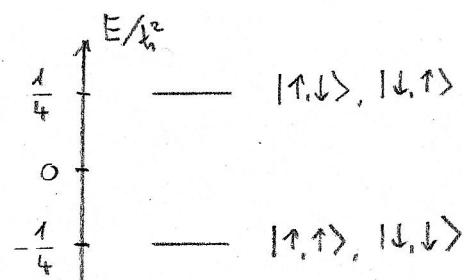
→ example No. 1 :  $N=2, J=1$

$$\Rightarrow \boxed{H = - S_1^z S_2^z} \quad \begin{matrix} i=1 & 2 \\ \bullet & \bullet \\ J=1 & \end{matrix}$$

→ we have  $2^2 = 4$  basis states :  $\{|n\rangle\} = \{|1,1\rangle, |1,1\rangle, |1,1\rangle, |1,1\rangle\}$

spectrum of eigenenergies:

$$E_n = - S_1^z S_2^z = \pm \frac{1}{4} h^2$$



Is the Ising model a classical or a quantum model?

→ it depends on the perspective!

the quantum perspective

→ we can still form linear combinations such as (for example No. 1) :

$$|4\rangle = \frac{1}{\sqrt{2}} (|1,1\rangle + |1,1\rangle) \quad \text{and we have:}$$

$$H|4\rangle = -\frac{1}{4} h^2 |4\rangle$$

→ in this sense, the Ising model can be viewed as a quantum model

### the classical perspective

instead of an operator (the Hamiltonian  $H_{\text{Ising}}$ , see p1), consider a classical Hamiltonian function defined as:

$$H(\{S_i^z\}) = - \sum_{ij} J_{ij} S_i^z S_j^z$$

with the spin configuration

$$\{S_i^z\} = (S_1^z, S_2^z, \dots, S_N^z)$$

→ the  $S_i^z$  now take the values  $S_i^z = \pm \frac{1}{2}$  ( $t_0$  can be set to 1)

→  $H(\{S_i^z\})$  corresponds to the energy  $E(\{S_i^z\})$  for a given spin configuration  $\{S_i^z\}$

from now on → use the notation for the classical Ising model

→ example No. 2:

find the spin configurations with the lowest energy for

$$H(\{S_i^z\}) = - J \sum_{i=1}^{N-1} S_i^z S_{i+1}^z \quad \hat{=} \quad \begin{array}{ccccccc} & i=1 & 2 & 3 & \dots & N-1 & N \\ & \textcircled{0} & \textcircled{0} & \textcircled{0} & \dots & \textcircled{0} & \textcircled{0} \\ & \downarrow & \downarrow & \downarrow & & \downarrow & \downarrow \end{array}$$

and  $J = 1$

⇒ neighbouring spins are parallel:  $S_i^z S_{i+1}^z = \frac{1}{4}$

and the ground-state energy is given by

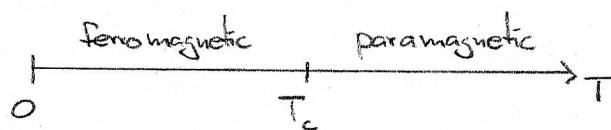
$$E_g = - \frac{1}{4} (N-1)$$

this means: the ground state is ferromagnetic with

$$\{S_i^z\} = (\uparrow, \uparrow, \uparrow, \dots, \uparrow) \text{ or } (\downarrow, \downarrow, \downarrow, \dots, \downarrow)$$

→ the Ising model is used as a model to describe magnetism and magnetic phase transitions!

phase diagram (simplified)



$T_c$ : critical temperature of the phase transition

now: calculate physical properties of the Ising model for a given temperature  $T$

→ this is a problem of statistical physics (canonical ensemble)

in the following, we focus on the (average) magnetization  $\langle m \rangle$

→ given by:

$$\langle m \rangle = \sum_{\{S_e^z\}} \frac{1}{Z} e^{-\beta H(\{S_e^z\})} m(\{S_e^z\})$$

→  $\sum_{\{S_e^z\}} \dots$  : sum over all spin configurations ( $\hat{=}$  microstates)  
 $\hookrightarrow = 2^N$

→  $m(\{S_e^z\}) = \sum_{i=1}^N S_i^z$  : magnetization of the spin configuration  $\{S_e^z\}$

→  $\beta = \frac{1}{k_B T}$  with  $k_B$ : Boltzmann constant

→ the probability for the spin configuration  $\{S_e^z\}$  being realized at temperature  $T$  is given by:

$$w(\{S_e^z\}) = \frac{1}{Z} e^{-\beta H(\{S_e^z\})}$$

with  $Z = \sum_{\{S_e^z\}} e^{-\beta H(\{S_e^z\})}$

$\hookrightarrow$  partition function

How to calculate  $\langle m \rangle$ ?

→ analytical solutions are only available for (a few) special cases!

⇒ what about numerical solutions?

the general problem:

the number of spin configurations grows exponentially with the number of sites.

therefore : use Monte-Carlo methods

in particular → Metropolis algorithm

### 1.3 Newtonian dynamics of classical many-particle systems

Newton's equation of motion:  $\vec{F} = m\vec{a}$

For a many-particle system  $\rightarrow$   $m_i \ddot{\vec{r}}_i = \sum_{j \neq i} \vec{F}_{ij} \quad i=1, \dots, N$

$\rightarrow$  this is a set of coupled ordinary differential equations of 2nd order

- can be reduced to a set of 1st order diff. eq. } see bachelor course
- 'standard' methods: Euler, Runge-Kutta } "Computerphysik"

two examples for non-trivial dynamics:

a) harmonic chain + anharmonic potential ("Fermi-Pasta-Ulam problem")

start with the harmonic chain  $\rightarrow$  masses  $m_i$  connected with springs

$$i=1 \quad 2 \quad 3 \\ \text{O-mm-O-mm-O-...} \quad \text{harmonic potential} \quad V_{ij} = \frac{1}{2} k (\xi_i - \xi_j)^2$$

and add an anharmonic potential of the form:

$$\bar{V}_{ij} = \alpha (\xi_i - \xi_j)^4$$

displacement of particle  $i$

possible questions:

starting from specific initial displacements  $\rightarrow$  How does the energy dissipate in the system?

b)  $N$ -body gravitational systems

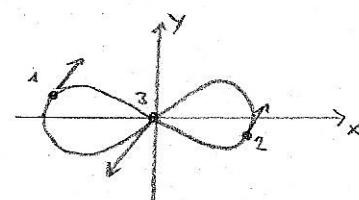
$$V_{ij} = -G m_i m_j \frac{1}{|\vec{r}_i - \vec{r}_j|} \quad G: \text{gravitational constant}$$

$N = 2$   $\rightarrow$  Kepler problem (elliptic orbits, etc.)

$N = 3$   $\rightarrow$  "three-body problem"

chaotic dynamics

periodic orbits  
e.g. "figure eight"



## 2 quantum mechanical spin models - introduction

### 2.1 quantum spin models

consider a model of  $N$  quantum mechanical spins (here: spin- $\frac{1}{2}$  particles)

in  $d=1$  :  $i = 1 \quad 2 \quad 3 \quad \dots \quad N$   
 $0 - 0 - 0 - \dots - 0$

spin operator for site  $i$

$$\vec{S}_i = \begin{pmatrix} S_i^x \\ S_i^y \\ S_i^z \end{pmatrix} \quad \rightarrow \text{commutation relations:}$$

$$[S_i^x, S_j^x] = i\hbar S_i^z S_{ij} \quad \text{etc.}$$

interaction between neighbouring spins:

$$-\beta \vec{S}_i \cdot \vec{S}_{i+1} = -\beta (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z)$$

$\Rightarrow$  the Hamiltonian is of the following form:

$$H = -\beta \sum_{i=1}^{N-1} \vec{S}_i \cdot \vec{S}_{i+1} \quad \text{Heisenberg model}$$

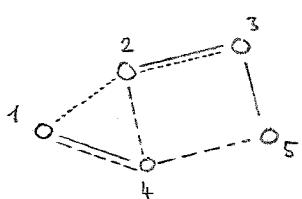
- $\hookrightarrow$  here:
- $d=1$ , open boundary conditions
  - interaction between nearest neighbours only
  - homogeneous:  $J_i = J$
  - isotropic:  $J_i^\alpha = J_i \quad \alpha = x, y, z$

$\rightarrow$  we now consider the following generalization:

$$H = - \sum_{i,j,\alpha} J_{ij}^\alpha S_i^\alpha S_j^\alpha \quad (*) \quad \begin{aligned} i, j &= 1, \dots, N \\ \alpha &= x, y, z \end{aligned}$$

$\rightarrow$  the model is defined on a finite cluster with  $N$  sites

example:



- : x
- - - : y
- .... : z

- further generalizations are possible:
- (not considered here)
  - magnetic field  $\rightarrow h S_i^z$
  - couplings between different spin components  $\rightarrow S_i^\alpha S_j^\beta$
  - higher order terms  $\rightarrow S_i^\alpha S_j^\beta S_k^\gamma$  etc.

basis of the Hilbert space

$$\{|n\rangle\} = \{|\uparrow\rangle_1, |\downarrow\rangle_1\} \otimes \{|\uparrow\rangle_2, |\downarrow\rangle_2\} \otimes \dots \otimes \{|\uparrow\rangle_N, |\downarrow\rangle_N\}$$

→ this gives  $2^N$  states such as  $|\uparrow\downarrow\uparrow\uparrow\dots\downarrow\rangle$   
 ↓      ↓      ↓  
 site 1 site 2 ... site N

the basis for each site  $i$ :  $\{|\uparrow\rangle_i, |\downarrow\rangle_i\}$  is chosen as a basis of eigenstates of the operator  $S_i^z$ :  $S_i^z |\uparrow\rangle_i = +\frac{\hbar}{2} |\uparrow\rangle_i$  (we set  $\hbar=1$  in the following)  
 $S_i^z |\downarrow\rangle_i = -\frac{\hbar}{2} |\downarrow\rangle_i$

it is convenient (for the numerics) to write:

$$\begin{aligned} |\uparrow\rangle_i &\hat{=} |\uparrow\rangle_i \rightarrow z_i = 1 \\ |\downarrow\rangle_i &\hat{=} |0\rangle_i \rightarrow z_i = 0 \end{aligned} \quad \left. \right\} |\uparrow\downarrow\uparrow\uparrow\dots\rangle \hat{=} |1011\dots\rangle$$

now identify the  $z_i$  as the digits of the binary number  $[z_N \dots z_2 z_1]_2$

⇒ we can label the basis with a single integer number  $n$ ,

$$\text{with } [n]_{10} = [z_N \dots z_2 z_1]_2$$

$$\rightarrow n = \sum_{i=1}^N z_i 2^{i-1} \quad \text{with } n = 0, 1, \dots, 2^N - 1$$

→ introduce the operators  $S_i^\pm = S_i^x \pm i S_i^y$  with the properties:

$$S_i^+ |\uparrow\rangle_i = 0, \quad S_i^- |\uparrow\rangle_i = |\downarrow\rangle_i$$

$$S_i^+ |\downarrow\rangle_i = |\uparrow\rangle_i, \quad S_i^- |\downarrow\rangle_i = 0$$

$$\rightarrow \text{rewrite the Hamiltonian } (\ast) : \quad S_i^x = \frac{1}{2} (S_i^+ + S_i^-)$$

$$S_i^y = \frac{1}{2i} (S_i^+ - S_i^-)$$

$$\begin{aligned} \Rightarrow \sum_{\alpha} J_{ij}^{\alpha} S_i^{\alpha} S_j^{\alpha} &= J_{ij}^x S_i^x S_j^x + J_{ij}^y S_i^y S_j^y + J_{ij}^z S_i^z S_j^z \\ &= \frac{1}{4} J_{ij}^x (S_i^+ S_i^+ + S_i^+ S_i^- + S_i^- S_i^+ + S_i^- S_i^-) \\ &- \frac{1}{4} J_{ij}^y (S_i^+ S_i^+ - S_i^+ S_i^- - S_i^- S_i^+ + S_i^- S_i^-) \\ &+ J_{ij}^z S_i^z S_j^z \end{aligned}$$

special case  $\rightarrow J_{ij}^x = J_{ij}$  (Heisenberg model)

$$\Rightarrow \underbrace{\sum_{\alpha} J_{ij} S_i^{\alpha} S_j^{\alpha}}_{= J_{ij} \vec{S}_i \cdot \vec{S}_j} = J_{ij} \left[ \frac{1}{2} (S_i^z S_j^z + S_i^- S_j^+) + S_i^2 S_j^2 \right]$$

example: Heisenberg model for two sites ( $N=2$ )

$$\begin{array}{c} 1 \\ 0 - 0 \\ 0 \end{array} \quad H = - J \vec{S}_1 \cdot \vec{S}_2$$

$\rightarrow$  the basis consists of four states ( $2^2 = 4$ ):

$$|\downarrow\downarrow\rangle = |00\rangle = |0\rangle, \quad [0]_{10} = [00]_2$$

$$|\uparrow\downarrow\rangle = |10\rangle = |1\rangle, \quad [1]_{10} = [01]_2$$

$$|\downarrow\uparrow\rangle = |01\rangle = |2\rangle, \quad [2]_{10} = [10]_2$$

$$|\uparrow\uparrow\rangle = |11\rangle = |3\rangle, \quad [3]_{10} = [11]_2$$

### eigenstates of the two-site model

$$|4_1\rangle = \frac{1}{\sqrt{2}} (|1\downarrow\rangle - |\downarrow 1\rangle), \quad E_1 = \frac{3}{4} J \quad \rightarrow \text{singlet state}$$

$$\left. \begin{aligned} |4_2\rangle &= \frac{1}{\sqrt{2}} (|1\downarrow\rangle + |\downarrow 1\rangle) \\ |4_3\rangle &= |\uparrow\uparrow\rangle \\ |4_4\rangle &= |\downarrow\downarrow\rangle \end{aligned} \right\} \quad \begin{aligned} E_i &= -\frac{3}{4}, \quad i=2,3,4 \\ &\rightarrow \text{three triplet states} \end{aligned}$$

a)  $J < 0$   $\rightarrow$  the anti-ferromagnetic case

$$\rightarrow \text{ground state } |4_3\rangle = |4_1\rangle, \quad E_g = \frac{3}{4} J$$

b)  $J > 0$   $\rightarrow$  the ferromagnetic case

$\rightarrow$  the ground state is three-fold degenerate with  $E_g = -\frac{1}{4}$

note the difference to the Ising model (for two sites)

$$H = - J S_i^z S_j^z \quad |4_1\rangle = |\downarrow\downarrow\rangle, \quad |4_2\rangle = |\uparrow\downarrow\rangle, \quad |4_3\rangle = |\downarrow\uparrow\rangle, \quad |4_4\rangle = |\uparrow\uparrow\rangle \quad : \quad E_{12} = \frac{3}{4}$$

$$|4_3\rangle = |\uparrow\uparrow\rangle, \quad |4_4\rangle = |\downarrow\downarrow\rangle \quad : \quad E_{34} = -\frac{3}{4}$$

## Kitaev model

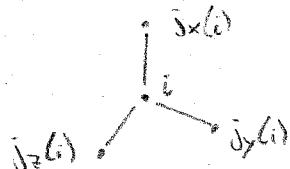
back to the general form (see page 1)

$$H = - \sum_{i,j} J_{ij}^{\alpha} S_i^{\alpha} S_j^{\alpha}$$

$$i,j = 1,..N, \alpha = x,y,z$$

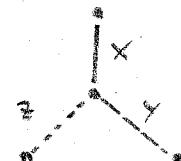
→ the following rules define a Kitaev cluster:

- each spin  $i$  is connected to exactly three spins:  $j_x(i), j_y(i), j_z(i)$



- the couplings between  $i$  and  $j_{\alpha}(i)$  are of the form  $J_{ij_{\alpha}}^{\alpha} S_i^{\alpha} S_{j_{\alpha}}^{\alpha}$

this means: only one type of coupling  
for each of the three neighbours

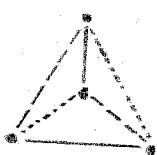


⇒ for a cluster of  $N$  spins we have  $\frac{3N}{2}$  couplings

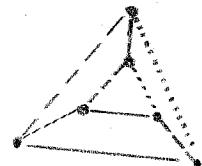
→  $N$  must be even (and  $\geq 4$ )

examples:

$N=4$

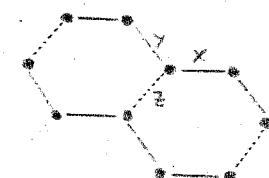


$N=6$



## the (original) Kitaev model

→ defined on an infinite honeycomb lattice



this model can be solved exactly using a representation of the spin operators in terms of Majorana Fermions

→ spin-liquid ground state with short-range spin correlations

already present in small Kitaev clusters

→ "fractionalization" of the spin

## 2.2 diagonalization of small clusters

given → a time-independent Hamiltonian  $\underline{H}$   
 such as the quantum spin models of Sec. 2.1

→ a complete basis  $\{|n\rangle\}$  of the Hilbert space

↳ define the unit operator  $\underline{1} = \sum_n |n\rangle \langle n|$

⇒ the stationary Schrödinger equation,  $\underline{H}|\psi\rangle = E|\psi\rangle$ , can be written  
 as a matrix-eigenvalue problem:

→ insert  $\underline{1}$ :  $\underline{H}\underline{1}|\psi\rangle = E|\psi\rangle$

$$\sum_n \underline{H}|n\rangle \langle n|\psi\rangle = E|\psi\rangle \quad | \text{ from the left: } \langle n| -$$

$$\begin{aligned} \sum_n \underbrace{\langle m|\underline{H}|n\rangle}_{= (\bar{H})_{mn}} \underbrace{\langle n|\psi\rangle}_{= (\bar{\psi})_n} &= E \underbrace{\langle m|\psi\rangle}_{= (\bar{\psi})_m} \quad (*) \\ &= (\bar{H})_{mm} = (\bar{\psi})_m = (\bar{\psi})_m \end{aligned}$$

This defines the Hamilton matrix  $\bar{H}$  with matrix elements

$$(\bar{H})_{mn} = \langle m|\underline{H}|n\rangle$$

and the vector  $\bar{\psi}$  with  $(\bar{\psi})_n = \langle n|\psi\rangle$

→ eq. (\*) can be written as

$$\bar{H} \bar{\psi} = E \bar{\psi}$$

this means: the solution of the Schrödinger equation is reduced to a  
 problem in linear algebra → determine the eigenvectors  
 $\bar{\psi}_k$  and the corresponding eigenvalues  $E_k$

⇒ How to set up the Hamilton matrix?

either by hand for very small clusters, such as  $\begin{smallmatrix} 1 & 2 \\ 0 & 0 \end{smallmatrix}$  ( $N=2$ )

$H = -J \vec{S}_1 \cdot \vec{S}_2 \quad \sim \text{calculate the } 4 \times 4 \text{ matrix } \bar{H}$

→ there are various approaches to set up the Hamilton matrix numerically  
 i, rewrite each spin operator appearing in the Hamiltonian ( $\rightarrow$  the operators  $S_i^x, S_i^y, S_i^z$ ) as matrices  $\tilde{S}_i^z$ , etc. with matrix elements

$$\langle \tilde{S}_i^z \rangle_{mn} = \langle m | S_i^z | n \rangle$$

→ the Hamilton matrix can then be constructed as (for example)

$$H = - \sum_{ijkl} J_{ij}^z \tilde{S}_i^z \tilde{S}_j^z$$

↓ calculate the matrix products

→ here we focus on the following approach

ii, consider the action of each term in the Hamiltonian

on each of the basis states  $|n\rangle$       ↳ each link  $J_{pq}^z \tilde{S}_p^z \tilde{S}_q^z$

with       $|n\rangle = |10 \dots 1 \dots 0 \dots \rangle$   
               ↓                          ↓  
                $z_p$                            $z_q$

x-link:       $J_{pq}^x \tilde{S}_p^x \tilde{S}_q^x |n\rangle =$

$$\frac{1}{4} J_{pq}^x (S_p^+ S_q^- + S_p^- S_q^+ + S_p^+ S_q^- + S_p^- S_q^+) |10 \dots z_p \dots z_q \dots \rangle = \dots$$

only one of these four terms gives a non-zero contribution!

→ the resulting state is the one with both spins flipped

example:  $N=4, n=13$

$$\rightarrow [13]_{10} = [\langle 01 \rangle_2 \rightarrow |13\rangle = |1\bar{1}\bar{1}\bar{1}\rangle$$

apply the operator       $J_{23}^x \tilde{S}_2^x \tilde{S}_3^x \rightarrow p=2, q=3$

$$\rightarrow J_{23}^x \tilde{S}_2^x \tilde{S}_3^x = \frac{1}{4} J_{23}^x (S_2^+ S_3^- + S_2^- S_3^+ + S_2^+ S_3^- + S_2^- S_3^+) |1\bar{1}\bar{1}\bar{1}\rangle = \frac{1}{4} J_{23}^x \underbrace{|1\bar{1}\bar{1}\bar{1}\rangle}_{=|10\rangle}$$

only one term  
 gives a contribution

the spins 2 and 3 are flipped

now: calculate the label  $\ell$  of the resulting state

$$\text{remember that } n = \sum_{i=1}^N z_i 2^{i-1}$$

$$\text{in this example: } n = 1 + 0 + 4 + 8 = 13$$

$$\rightarrow \ell = 1 + 2 + 0 + 8 = 11$$

$$\Rightarrow \ell = n + 2^1 - 2^2 =$$

$$= n + 2^{p-1} - 2^{q-1} \quad (p=2, q=3)$$

$$= n + (1 - 2 \cdot 0) 2^{p-1} + (1 - 2 \cdot 1) 2^{q-1}$$

$$\downarrow \\ = z_p$$

$$\downarrow \\ = z_q$$

$$(z_2=0, z_3=1)$$

$\rightarrow$  the terms  $(1 - 2 z_{p/q})$  give either  $+1$  or  $-1$

$$z_p = 0 \text{ gives } +1 \rightarrow \text{add } 2^{p-1} \stackrel{+}{=} \downarrow \rightarrow 1$$

$$z_p = 1 \text{ gives } -1 \rightarrow \text{subtract } 2^{p-1} \stackrel{-}{=} 1 \rightarrow 0$$

( $z_q$ -according)

this gives the following expression for  $\ell$ :

$$\boxed{\ell = n + (1 - 2 z_p) 2^{p-1} + (1 - 2 z_q) 2^{q-1}} \quad (*)$$

$$\Rightarrow J_{pq}^x S_p^x S_q^x |n\rangle = \frac{1}{4} J_{pq}^x |l\rangle \quad \text{with } l \text{ given by eq. (*)}$$

### matrix elements

$$\langle m | J_{pq}^x S_p^x S_q^x | n \rangle = \quad (n, m = 0, \dots, 2^N - 1)$$

$$= \frac{1}{4} J_{pq}^x \langle m | l \rangle = \frac{1}{4} J_{pq}^x \delta_{lm} \quad \text{with } l \text{ given by eq. (*)}$$

This means:

each term in the Hamiltonian of the form  $J_{pq}^x S_p^x S_q^x$  results in  $2^N$  non-zero matrix elements of the Hamilton matrix

$\rightarrow$  only one matrix element  $\frac{1}{4} J_{pq}^x \delta_{lm}$  for each  $n = 0, \dots, 2^N - 1$

$$\underline{y\text{-link}}: \langle \hat{J}_{pq}^Y S_p^+ S_q^- | n \rangle =$$

$$-\frac{1}{4} \hat{J}_{pq}^Y (S_p^+ S_q^+ - S_p^+ S_q^- - S_p^- S_q^+ + S_p^- S_q^-) |10 \dots z_p \dots z_q \dots\rangle = \dots$$

→ the resulting state  $|l\rangle$  has the same label  $l$  as for the x-link (see eq. (\*) on page 7)

but: there is a minus sign depending on the spin configuration

$$\dots = s \frac{1}{4} \hat{J}_{pq}^Y |l\rangle \quad \text{with} \quad s = \begin{cases} +1 & : z_p \neq z_q \\ -1 & : z_p = z_q \end{cases}$$

→ the sign  $s$  can be written as:

$$s = -(2z_p - 1)(2z_q - 1)$$

matrix elements:

$$\langle m | \hat{J}_{pq}^Y S_p^+ S_q^- | n \rangle = s \frac{1}{4} \hat{J}_{pq}^Y \underbrace{\langle m | l \rangle}_{= \delta_{ml}}$$

$$\underline{z\text{-link}}: \langle \hat{J}_{pq}^Z S_p^2 S_q^2 | n \rangle =$$

$$= \hat{J}_{pq}^Z \underbrace{S_p^2 S_q^2 |10 \dots z_p \dots z_q \dots\rangle}_{\text{eigenstates of both } S_p^2 \text{ and } S_q^2} = \dots$$

eigenvalues:  $+\frac{1}{2}$  for  $z_p, z_q = 1$

$-\frac{1}{2}$  for  $z_p, z_q = -1$

$$\dots = \frac{1}{4} \hat{J}_{pq}^Z (2z_p - 1)(2z_q - 1) |n\rangle$$

matrix elements:

$$\langle m | \hat{J}_{pq}^Z S_p^2 S_q^2 | n \rangle = \frac{1}{4} \hat{J}_{pq}^Z (2z_p - 1)(2z_q - 1) \underbrace{\langle m | n \rangle}_{= \delta_{mn}}$$

⇒ z-links give diagonal matrix elements only

## Structure of the code

$N$ : number of sites/spins (= size of the cluster)

$L$ : number of links = number of terms in the Hamiltonian of the form  $\frac{1}{4} J_{pq}^{\alpha} S_p^{\alpha} S_q^{\alpha}$

the code can be set up in the following way:

for  $n=0$  to  $2^N-1$  : loop over the basis states

calculate the binary representation of  $n$  :  $[n]_{10} \rightarrow [z_N \dots z_1]_2$

for  $j=1$  to  $L$  : loop over the links

if  $\alpha=x$  or  $\alpha=y$

calculate  $l$  according to eq. (\*) on page 7

add to the matrix element  $\bar{H}_{ln}$  of the Hamilton matrix:

$$\frac{1}{4} J_{pq}^x \text{ for } \alpha=x$$

$$s \frac{1}{4} J_{pq}^y \text{ for } \alpha=y \quad \text{with the sign } s \text{ (see page 8)}$$

else ( $\hat{\alpha}=z$ )

$$\text{add to the matrix element } \bar{H}_{ln} : \frac{1}{4} J_{pq}^z (2z_p - 1)(2z_q - 1) \quad (\text{see page 8})$$

end

end

end

note: a double for-loop (over  $n$  and  $m$ ) is not required!

→ from this structure of the code, the maximum number  $z$  of non-zero matrix elements of  $\bar{H}$  can be calculated:

$$z = L \cdot 2^N$$

(the actual number of non-zero matrix elements is lower)

⇒ fraction of non-zero matrix elements of the Hamilton matrix

$$\gamma = \frac{z}{2^N \cdot 2^N} = \frac{L}{2^N}$$

example: Kitaev cluster with  $N$  sites (see Sec. 2.1)

$$L = \frac{3}{2}N \Rightarrow \boxed{\gamma = \frac{3}{2} \frac{N}{2^N}}$$

this means:  $\gamma$  falls off exponentially with increasing  $N$   
 $\rightarrow$  "sparse matrix"

for the numerics: to reduce the required memory, only store the non-zero matrix element

special case: the XXZ-model

start from the general form:  $H = - \sum_{ij\alpha} J_{ij}^{\alpha} S_i^{\alpha} S_j^{\alpha}$

and set  $J_{ij}^x = J_{ij}^y$

$$\Rightarrow \boxed{H_{xxz} = - \sum_{ij} \left[ \frac{1}{2} J_{ij}^x (S_i^+ S_j^- + S_i^- S_j^+) + J_{ij}^z S_i^z S_j^z \right]}$$

$\rightarrow$  the  $S_i^z S_j^z$ -term is treated as before (see page 8)

$\rightarrow$  the  $(S_i^+ S_j^- + S_i^- S_j^+)$  can be treated as a single link in the code

$$\frac{1}{2} J_{ij}^x (S_i^+ S_j^- + S_i^- S_j^+) |10-z_p z_q \dots\rangle =$$

$$= \begin{cases} \frac{1}{2} J_{ij}^x |ll\rangle & \text{for } z_p + z_q = 1, \text{ with } l \text{ given by eq.(6) on page 7} \\ 0 & \text{otherwise} \end{cases}$$

$\rightarrow$  the transitions  $| \dots \uparrow \dots \uparrow \dots \rangle \leftrightarrow | \dots \downarrow \dots \downarrow \dots \rangle$  are forbidden  
in the XXZ-model

some remarks on the computation time

the time consuming part in the code

$\rightarrow$  the full diagonalization of the  $\dim \times \dim$  Hamilton matrix  $\bar{H}$

computation time  $T \sim \dim^3$

For the quantum spin models discussed in this section:

$$\dim = 2^N \Rightarrow \boxed{T \sim (2^N)^3 = 2^{3N}}$$

the computation time for the full diagonalization grows exponentially with system size!

How to reduce the computation time?

(for advanced methods, see Secs. 4 & 7)

here → use the symmetries of the model

→ for a given Hamiltonian  $H$ , find a set of operators  $A_i$  with  
 $[H, A_i] = 0$  (this might be difficult in general)

example: XXZ - model

$$H_{XXZ} = - \sum_{ij} \left[ \frac{1}{2} J_{ij}^x (S_i^+ S_j^- + S_i^- S_j^+) + J_{ij}^z S_i^z S_j^z \right]$$

for this model, the z-component of the total spin

$$S_{\text{tot}}^z = \sum_{i=1}^N S_i^z \quad \text{is conserved}$$

why: → calculate  $[H_{XXZ}, S_{\text{tot}}^z]$  (this gives 0)

or → by inspection:

each term in the Hamiltonian conserves the number of  
 $\uparrow$  and  $\downarrow$  spins

How to set up the Hamilton matrix?

→ use a set of basis states  $\{|n\rangle\}$  which are eigenstates of the operators  $A_i$

in the above example:

the standard basis →  $|S_1, S_2, \dots, S_N\rangle$  (see Sec. 2.1)

these basis states are already eigenstates of  $S_{\text{tot}}^z$ !

$$S_{\text{tot}}^z |S_1, S_2, \dots, S_N\rangle = \left( \sum_i S_i \right) |S_1, S_2, \dots, S_N\rangle \quad \text{with } S_i = \pm \frac{1}{2}$$

now: relabel the basis states  $|n\rangle$

$$\{|n\rangle\} \rightarrow \{|r, m\rangle\} \quad \text{with } r = 1, \dots, \dim_m$$

$\dim_m$ : dimension of the subspace with eigenvalue  $m$

$$\rightarrow A|r, m\rangle = m|r, m\rangle$$

$$(\text{here } m = \sum_i \epsilon_i, A = S_{\text{tot}}^z)$$

example:  $N=3$

$n$	0	1	2	3	4	5	6	7
$ n\rangle$	$ 111\rangle$	$ 110\rangle$	$ 101\rangle$	$ 011\rangle$	$ 111\rangle$	$ 110\rangle$	$ 101\rangle$	$ 011\rangle$
$m$	$-\frac{3}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{3}{2}$

$\rightarrow$  four subspaces with  
 $m = -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}$

$\downarrow$  relabel the basis states

$m$	$-\frac{3}{2}$	$-\frac{1}{2}$		$\frac{1}{2}$	$\frac{3}{2}$
$r$	1	1	2	3	1
$ r, m\rangle$	$ 111\rangle$	$ 110\rangle$	$ 101\rangle$	$ 011\rangle$	$ 111\rangle$
				$ 110\rangle$	$ 101\rangle$

$\rightarrow$  set up the Hamilton matrix  $\bar{H}$  with matrix elements

$$\langle r, m | H | r', m' \rangle = \langle r, m | H | r', m' \rangle \delta_{mm'}$$

$\hookrightarrow$  there are no matrix elements between states with different  $m$ !

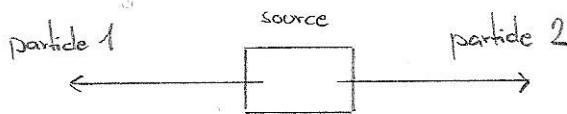
this means: we arrive at a block structure of the Hamilton matrix

$-\frac{3}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	$\frac{3}{2}$
0	0	0	0
0	0	0	0
0	0	0	0
0	0	0	0

$\Rightarrow$  each subspace can be diagonalized individually!

### 3.2 entanglement

the standard example: two particles emitted from a source



basis of the Hilbert space for each particle:  $\{|1\rangle_i, |1\rangle_i\}$   $i=1,2$

$\Rightarrow$  the state of the two-particle system can be written as:

$$|4\rangle = \alpha_1 |11\rangle + \alpha_2 |1\downarrow\rangle + \alpha_3 |\downarrow 1\rangle + \alpha_4 |\downarrow\downarrow\rangle \quad \sum_{i=1}^4 \alpha_i^2 = 1$$

important: quantum mechanics allows to form linear combinations of many-particle states!

example: the 'singlet' state

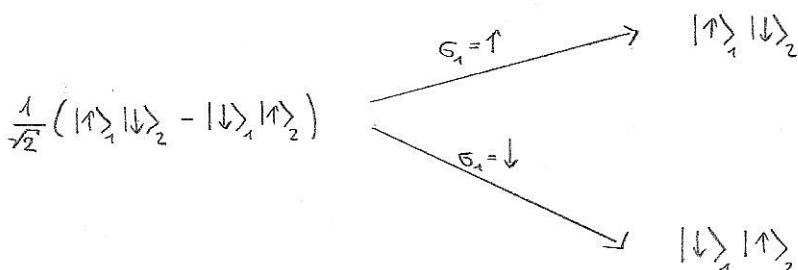
$$|4\rangle = \frac{1}{\sqrt{2}} (|1\rangle_1 |\downarrow\rangle_2 - |\downarrow\rangle_1 |1\rangle_2) \quad \rightarrow \text{case 1}$$

now  $\rightarrow$  perform a measurement on particle 1

$\hookrightarrow$  here: measure the z-component of the spin  $\rightarrow S_1$

$\Rightarrow$  the result is either  $S_1 = \uparrow$  or  $S_1 = \downarrow$ , each with probability  $\frac{1}{2}$

the measurement leads to a collapse of  
the two-particle wave function



does this 'action at a distance' lead to any effects which can be measured in experiments?

$\rightarrow$  calculate the conditional probability  $P(S_2 | S_1)$

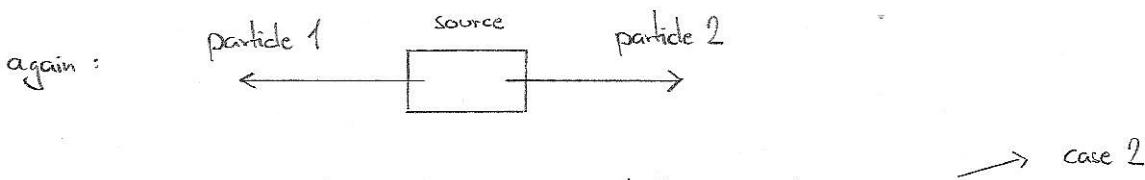
$P(\xi_2 | \xi_1)$  : probability to measure — in a subsequent measurement —  $\xi_2$  for spin 2 if the first measurement gave  $\xi_1$  for spin 1

For the singlet state we obtain:

$$\boxed{\begin{array}{ll} P(\uparrow|\uparrow) = 0, & P(\downarrow|\uparrow) = 1 \\ P(\uparrow|\downarrow) = 1, & P(\downarrow|\downarrow) = 0 \end{array}} \quad (*)$$

but: a measurement of these probabilities does not prove that the state is given by the singlet state!

⇒ consider the following set-up:



now: the source emits particle pairs, which are either in the state  $|\uparrow\rangle_1 |\downarrow\rangle_2 = |\Psi_1\rangle$  or  $|\downarrow\rangle_1 |\uparrow\rangle_2 = |\Psi_2\rangle$  each with probability  $p_i = \frac{1}{2}$  ( $i=1,2$ )

this situation can be described by a density operator  $\hat{\rho}$  for a mixed state

$$\rightarrow \hat{\rho} = \sum_{i=1}^2 p_i |\Psi_i\rangle \langle \Psi_i| \quad (\text{case 2})$$

in contrast to the density operator for the pure state  $|\Psi\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle_1 |\downarrow\rangle_2 - |\downarrow\rangle_1 |\uparrow\rangle_2)$

$$\rightarrow \hat{\rho} = |\Psi\rangle \langle \Psi| \quad (\text{case 1})$$

in case 2, we do not have a collapse of a two-particle wave function as in case 1, but: the conditional probabilities are again given by (\*)

⇒ these two scenarios cannot be distinguished (with this type of measurement)

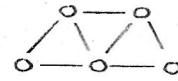
(before we deal with the modifications required to distinguish case 1 and case 2  
→ Bell inequalities)

→ what does entanglement mean?

## 1

### 4.2 iterative diagonalization

so far: Hamiltonian for a finite cluster



↓ basis  $\{|i\rangle\}$  of the whole system

Hamilton matrix, with  $(\bar{H})_{ij} = \langle i | H | j \rangle$

↪ a single matrix for the whole system

(size of the matrix can be reduced:  
- symmetries  
- Lanczos algorithm)

↓ numerical diagonalization

$E_n, |\psi_n\rangle$

in this section: "iterative" diagonalization

the general idea → set up the Hamilton matrix of  $H_{N+1}$  using the eigenstates of  $H_N$

$$\begin{array}{ccccccccc} 1 & 2 & 3 & \dots & N-1 & N & N+1 \\ \underbrace{O-O-O-\dots-O-O-O-O}_{\hat{=} H_N} & & & & & & \hat{=} H_{N+1} \end{array}$$

example → one-dimensional Heisenberg model with open boundary conditions

$$H_N = -J \sum_{i=1}^{N-1} \vec{S}_i \cdot \vec{S}_{i+1} \quad \Rightarrow \quad H_{N+1} = H_N - J \vec{S}_N \cdot \vec{S}_{N+1}$$

⇒ in each step of the iteration, one site is added to the system

$$H_2 : \quad O-O \quad \rightarrow \quad \text{set up } \bar{H}_2, \text{ diagonalize } \bar{H}_2$$



$$H_3 : \quad O-O-O \quad \rightarrow \quad \text{set up } \bar{H}_3, \text{ diagonalize } \bar{H}_3$$



etc.

etc.

start with:  $H_2 = -\frac{\hbar}{4} \vec{S}_1 \cdot \vec{S}_2 \hat{=} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$

basis:  $\{ |s\rangle \} \otimes \{ |\uparrow\rangle_2, |\downarrow\rangle_2 \}$  → use the same notation as for the iterative part already at this stage  
 $\downarrow$   
 basis of spin 1, given by  $\{ |\uparrow\rangle_1, |\downarrow\rangle_1 \}$ .

Hamilton matrix of  $H_2$ :

$$(H_2)_{mn} = \langle n | H_2 | m \rangle \quad \text{with } |n\rangle \hat{=} |s, \epsilon_2\rangle$$

$$\rightarrow \bar{H}_2 = \frac{\hbar}{4} \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & -2 & 0 \\ 0 & -2 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \quad \begin{array}{l} \text{ordering of the states:} \\ \text{same as in Sec. 2} \end{array}$$

eigenstates of  $H_2$ :  $H_2 |\tau\rangle = E_\tau |\tau\rangle, \tau = 0, 1, 2, 3$

with  $|\tau\rangle = \sum_n U_{n\tau} |s, \epsilon_2\rangle$

the iteration

$$H_{N+1} = H_N - \frac{\hbar}{4} \vec{S}_N \cdot \vec{S}_{N+1} \quad N = 2, 3, \dots$$

basis of  $H_{N+1}$ :

$$\{ |\tau\rangle \} \otimes \{ |\uparrow\rangle_{N+1}, |\downarrow\rangle_{N+1} \} \rightarrow \text{the new basis } \{ |i\rangle \}, i = 0, 1, \dots, 2d-1$$

↳ the eigenstates of  $H_N$ ,  $\tau = 0, 1, \dots, d-1$

the states are labeled as follows:

$$i = \underbrace{0, 1, \dots, d-1}_{\hat{=} |\tau, \downarrow\rangle_{N+1}} , \underbrace{d, d+1, \dots, 2d-1}_{\hat{=} |\tau, \uparrow\rangle_{N+1}} \rightarrow |i\rangle \hat{=} |\tau, \epsilon_{N+1}\rangle$$

## Hamilton matrix of $H_{N+1}$

→ the matrix elements:

$$\langle i | H_{N+1} | j \rangle = \langle i | H_N | j \rangle - \gamma \langle i | \vec{S}_N \cdot \vec{S}_{N+1} | j \rangle$$

1st term:  $\langle i | H_N | j \rangle = \langle r, \sigma_{N+1} | H_N | r', \sigma'_{N+1} \rangle$

$$\begin{aligned} &= \underbrace{\langle r | H_N | r' \rangle}_{H_N \text{ does not act on } |\sigma_{N+1}\rangle} \underbrace{\langle \sigma_{N+1} | \sigma'_{N+1} \rangle}_{= E_{\sigma'} |r'\rangle} \\ &= E_r |r'\rangle = \delta_{\sigma_{N+1}, \sigma'_{N+1}} \end{aligned}$$

$$\Rightarrow \boxed{\langle i | H_N | j \rangle = E_r \delta_{r'r} \delta_{\sigma_{N+1}, \sigma'_{N+1}}}$$

this gives diagonal matrix elements only:

$$\begin{pmatrix} E_0 & & & & & & & \\ & E_1 & & & & & & \\ & & E_d & & & & & \\ & & & E_{d-1} & & & & \\ & & & & E_0 & & & \\ & & & & & E_1 & & \\ & & & & & & E_d & \\ & & & & & & & E_{d-1} \end{pmatrix}$$

2nd term → this is the difficult part

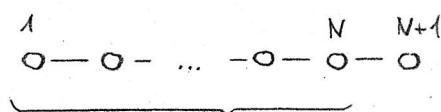
$$-\gamma \underbrace{\langle i | \vec{S}_N \cdot \vec{S}_{N+1} | j \rangle}_{}$$

$$= \frac{1}{2} \underbrace{\langle i | S_N^+ S_{N+1}^- | j \rangle}_{a)} + \frac{1}{2} \underbrace{\langle i | S_N^- S_{N+1}^+ | j \rangle}_{b)} + \underbrace{\langle i | S_N^z S_{N+1}^z | j \rangle}_{c)}$$

a)  $\langle i | S_N^+ S_{N+1}^- | j \rangle = \langle r, \sigma_{N+1} | S_N^+ S_{N+1}^- | r', \sigma'_{N+1} \rangle =$

$$\begin{aligned} &= \underbrace{\langle r | S_N^+ | r' \rangle}_{\downarrow} \underbrace{\langle \sigma_{N+1} | S_{N+1}^- | \sigma'_{N+1} \rangle}_{=} \\ &= \delta_{\sigma_{N+1}, \downarrow} \delta_{\sigma'_{N+1}, \uparrow} \end{aligned}$$

How does  $S_N^+$  act on  $|r'\rangle$ ?



$|\tau\rangle \rightarrow$  has to be expressed in a basis containing site N explicitly

$$\rightarrow |\tau'\rangle = \sum_{S, S'_N} U_{S'G_N^1, \tau'} |S', S'_N\rangle, \langle \tau| = \sum_{S, G_N} U_{SG_N, \tau} \langle S, S_N|$$

$$\Rightarrow \langle \tau | S_N^+ | \tau' \rangle = \sum_{SS'} \sum_{G_N G_N^1} U_{SG_N, \tau} U_{S'G_N^1, \tau'} \underbrace{\langle S, S_N | S_N^+ | S', S_N^1 \rangle}_{= \langle S | S' \rangle \langle S_N | S_N^+ | S' \rangle} = \dots$$

$S_N^+$  does not act on the states  $|S\rangle, |S'\rangle$

$$= \langle S | S' \rangle \langle S_N | S_N^+ | S' \rangle \\ = \delta_{SS'} \delta_{G_N, \uparrow} \delta_{G_N^1, \downarrow}$$

$$\dots = \sum_S U_{S1, \tau} U_{S1, \tau'}$$

$$\Rightarrow \boxed{\langle i | S_N^+ S_{N+1}^- | j \rangle = \delta_{G_{N+1}, \downarrow} \delta_{G_{N+1}^1, \uparrow} \sum_S U_{S1, \tau} U_{S1, \tau'}}$$

b, similar as in a) :

$$\boxed{\langle i | S_N^- S_{N+1}^+ | j \rangle = \delta_{G_{N+1}, \uparrow} \delta_{G_{N+1}^1, \downarrow} \sum_S U_{S1, \tau} U_{S1, \tau'}}$$

$$c, \langle i | S_N^z S_{N+1}^z | j \rangle = \langle \tau | S_N^z | \tau' \rangle \underbrace{\langle S_{N+1} | S_{N+1}^z | S_{N+1}^1 \rangle}_{= \delta_{G_{N+1}, \pm \frac{1}{2}}} \\ = \delta_{G_{N+1}, \pm \frac{1}{2}} \quad (G_{N+1} = \pm \frac{1}{2})$$

$$\langle \tau | S_N^z | \tau' \rangle = \sum_S \sum_{G_N G_N^1} U_{SG_N, \tau} U_{S'G_N^1, \tau'} \underbrace{\langle S_N | S_N^z | S_N^1 \rangle}_{= \delta_{G_N, G_N^1}} \\ = \delta_{G_N, G_N^1}$$

$$\Rightarrow \boxed{\langle i | S_N^z S_{N+1}^z | j \rangle = \delta_{G_{N+1}, G_{N+1}^1} \sum_S \sum_{G_N} \delta_{G_N, G_N^1} U_{SG_N, \tau} U_{S'G_N^1, \tau'}}$$