

# PHYS-E0510 – Advanced Computational Methods in Physics D

Lecture Notes

Sessions 1 to 5

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The title box of each session gives its Jupyter notebook and its prerequisites.

## How this course is organized

Every session of this course has five pieces, and we should use them together, not one instead of another. The recording is the lecture itself, with the derivations done live and with the questions that came up during the lecture. The slides show the definitions, figures and equations in the order of the lecture, so they are the fastest way to find a point in a recording or to review a session before the exam. These lecture notes follow the same sessions in the same order. The difference is that they write the physics as a connected text, and they do step by step what a slide does in one line. So we can read them instead of watching a session a second time, or next to the slides, to fill in what a bullet point skips.

The Jupyter notebook of each session is named in the box under the session title, and the *Computational companion* boxes inside the text point to it again. The notebooks are the place where the physics is computed. Nothing there is a fixed figure, and you are meant to run the cells, change the parameters and see what happens. Finally, every session has four exercise shorts, which are short silent films of one to two minutes each, and they are at [https://joselado.github.io/Advanced\\_Computational\\_Methods\\_Physics\\_2026/exercise\\_shorts/](https://joselado.github.io/Advanced_Computational_Methods_Physics_2026/exercise_shorts/). Each film shows one idea of the session, and every number on the screen is computed with the same codes as the notebooks.

None of these pieces is complete alone. The recordings and the slides give the story and the intuition, the notes give derivations that we can check line by line, and the notebooks give the numerics, which build a kind of intuition that the other pieces cannot give. A good way to work on a session is to watch the recording once, and then read the notes with the notebook open next to them. After this, we go back to the notebook and change things, until the results feel like our own calculation and not like something that happened on the screen of someone else.

## The computational libraries

All the numerics of the course are done with two Python libraries, and not with code written from zero inside the notebooks. Both libraries have to be installed before the notebooks can run, and the first cell of each notebook says which environment variables they need.

- `pyqula`, at <https://github.com/joselado/pyqula>, does single-particle and mean-field electronic structure. This means tight-binding Hamiltonians, band structures, and the self-consistent Hubbard and charge-density-wave calculations of Session 1. The notebook of Session 1, `classical_magnetism.ipynb`, uses it.
- `dmrgpy`, at <https://github.com/joselado/dmrgpy>, does the quantum many-body calculations. These are the exact diagonalization of spin and fermionic Hamiltonians, and the matrix-product-state and DMRG calculations of the later sessions. The notebooks of Sessions 2 to 5 use it.

We use both libraries as tools. To follow the course you do not need to read their source code, and it is enough to call the functions that the notebooks show.

# Contents

|                                                                         |          |
|-------------------------------------------------------------------------|----------|
| <b>How this course is organized</b>                                     | <b>1</b> |
| <b>1 Classical Magnetism and Mean-Field Theory</b>                      | <b>8</b> |
| 1.1 Single-particle versus many-body Hamiltonians . . . . .             | 8        |
| 1.1.1 Single-particle Hamiltonians . . . . .                            | 8        |
| 1.1.2 The quartic interaction term . . . . .                            | 9        |
| 1.1.3 The size of the many-body problem . . . . .                       | 9        |
| 1.2 Second quantization . . . . .                                       | 9        |
| 1.2.1 Creation and annihilation operators . . . . .                     | 10       |
| 1.2.2 Anticommutation and local degrees of freedom . . . . .            | 10       |
| 1.3 The tight-binding dimer as a worked example . . . . .               | 10       |
| 1.3.1 Bonding and antibonding orbitals . . . . .                        | 10       |
| 1.3.2 The two-electron many-body basis . . . . .                        | 11       |
| 1.4 Two microscopic interactions, two broken symmetries . . . . .       | 11       |
| 1.4.1 The Hubbard model of spinful fermions . . . . .                   | 11       |
| 1.4.2 The spinless nearest-neighbor model . . . . .                     | 12       |
| 1.4.3 Where do $U$ and $V$ come from physically? . . . . .              | 12       |
| 1.5 Mean-field theory . . . . .                                         | 13       |
| 1.5.1 A single-particle approximation . . . . .                         | 13       |
| 1.5.2 Decoupling the interaction . . . . .                              | 13       |
| 1.5.3 The self-consistency loop in practice . . . . .                   | 13       |
| 1.5.4 Mean-field theory as a variational method . . . . .               | 14       |
| 1.5.5 Gap opening at half filling . . . . .                             | 15       |
| 1.5.6 Multiple self-consistent solutions and their energetics . . . . . | 15       |
| 1.6 From electrons to spins at strong coupling . . . . .                | 15       |
| 1.6.1 Saturation of the local moment . . . . .                          | 15       |
| 1.6.2 The Hubbard dimer and its low-energy manifold . . . . .           | 16       |
| 1.6.3 Superexchange and the coupling $J = 4t^2/U$ . . . . .             | 16       |
| 1.7 Classical magnetic order and frustration . . . . .                  | 18       |
| 1.7.1 Bipartite lattices . . . . .                                      | 18       |

|          |                                                              |           |
|----------|--------------------------------------------------------------|-----------|
| 1.7.2    | Frustration . . . . .                                        | 18        |
| 1.7.3    | Anisotropic exchange . . . . .                               | 19        |
| 1.8      | Charge density waves as a mean-field problem . . . . .       | 20        |
| 1.8.1    | Mean-field decoupling of the spinless model . . . . .        | 20        |
| 1.8.2    | The charge imbalance as order parameter . . . . .            | 20        |
| 1.9      | Where mean-field theory breaks down . . . . .                | 20        |
| 1.9.1    | The mean-field solution of the dimer . . . . .               | 20        |
| 1.9.2    | The exact singlet ground state . . . . .                     | 20        |
| 1.9.3    | Why this matters . . . . .                                   | 21        |
| <b>2</b> | <b>Exact Diagonalization of the Heisenberg Spin Chain</b>    | <b>23</b> |
| 2.1      | From the Hubbard dimer to a quantum magnet . . . . .         | 23        |
| 2.1.1    | The classical Ising dimer . . . . .                          | 23        |
| 2.1.2    | The quantum Heisenberg dimer . . . . .                       | 24        |
| 2.2      | Exact diagonalization of a spin chain . . . . .              | 24        |
| 2.2.1    | The product-state basis . . . . .                            | 24        |
| 2.2.2    | A sparse matrix . . . . .                                    | 24        |
| 2.2.3    | The dimer solved in two ways . . . . .                       | 25        |
| 2.3      | The many-body spectrum and the many-body gap . . . . .       | 26        |
| 2.3.1    | Counting the eigenvalues . . . . .                           | 26        |
| 2.3.2    | The many-body gap and its scaling . . . . .                  | 26        |
| 2.4      | The XXZ model from classical order to entanglement . . . . . | 27        |
| 2.4.1    | The two ends of the XXZ chain . . . . .                      | 27        |
| 2.4.2    | The transition in the finite-size spectrum . . . . .         | 28        |
| 2.5      | Good quantum numbers of the Heisenberg chain . . . . .       | 28        |
| 2.5.1    | Conservation of the total spin . . . . .                     | 29        |
| 2.5.2    | The Zeeman field does not mix states . . . . .               | 29        |
| 2.5.3    | Block-diagonalizing a long chain . . . . .                   | 29        |
| 2.6      | Level crossings and magnetization curves . . . . .           | 30        |
| 2.6.1    | The level crossing of the dimer . . . . .                    | 30        |
| 2.6.2    | The magnetization staircase of longer chains . . . . .       | 31        |
| 2.6.3    | Excited states in a small field . . . . .                    | 31        |

|          |                                                                                  |           |
|----------|----------------------------------------------------------------------------------|-----------|
| 2.7      | The gapped dimerized chain . . . . .                                             | 32        |
| 2.7.1    | A chain with alternating bonds . . . . .                                         | 32        |
| 2.7.2    | Finite-size convergence of the gap . . . . .                                     | 32        |
| 2.8      | Diagnosing the gap with impurities and correlators . . . . .                     | 33        |
| 2.8.1    | A magnetic impurity . . . . .                                                    | 33        |
| 2.8.2    | Non-local static correlators . . . . .                                           | 33        |
| 2.9      | Dynamical correlators, and a first look at spin-1 . . . . .                      | 34        |
| 2.9.1    | The Lehmann representation . . . . .                                             | 34        |
| 2.9.2    | Discrete peaks of the uniform chain . . . . .                                    | 34        |
| 2.9.3    | A first look at spin-1 . . . . .                                                 | 34        |
| 2.10     | Spinon mean-field theory with Abrikosov fermions . . . . .                       | 35        |
| 2.10.1   | A single-particle picture of the excitations . . . . .                           | 35        |
| 2.10.2   | The Abrikosov auxiliary fermion representation . . . . .                         | 35        |
| 2.10.3   | Mean-field decoupling of the exchange . . . . .                                  | 36        |
| 2.10.4   | Spinon bands of the uniform and dimerized chains . . . . .                       | 36        |
| <b>3</b> | <b>Exact Diagonalization in the Fermionic Basis</b>                              | <b>38</b> |
| 3.1      | The many-body Fock space of fermions . . . . .                                   | 38        |
| 3.1.1    | Counting the many-body states . . . . .                                          | 38        |
| 3.1.2    | Spinful fermions and the cost of the calculation . . . . .                       | 39        |
| 3.1.3    | Exact diagonalization in the Fock basis . . . . .                                | 40        |
| 3.2      | The exact charge-density-wave transition of spinless fermions . . . . .          | 40        |
| 3.2.1    | The spinless chain with nearest-neighbor interaction . . . . .                   | 40        |
| 3.2.2    | Two solvable limits . . . . .                                                    | 40        |
| 3.2.3    | The exact many-body spectrum . . . . .                                           | 41        |
| 3.2.4    | Comparison with mean-field theory . . . . .                                      | 41        |
| 3.3      | Chemical potential, conserved quantum numbers, and the charging energy . . . . . | 42        |
| 3.3.1    | Conservation of the particle number . . . . .                                    | 42        |
| 3.3.2    | The charging energy . . . . .                                                    | 42        |
| 3.4      | The exact magnetization of the Hubbard chain . . . . .                           | 43        |
| 3.4.1    | The magnetization of the exact ground state . . . . .                            | 43        |
| 3.4.2    | Lieb's theorem . . . . .                                                         | 44        |

|          |                                                                                |           |
|----------|--------------------------------------------------------------------------------|-----------|
| 3.4.3    | Turning on an explicit symmetry-breaking field . . . . .                       | 44        |
| 3.4.4    | Comparison of the charge-density wave and the Hubbard magnetism . . . .        | 45        |
| 3.5      | The Heisenberg model from the exact Hubbard dimer . . . . .                    | 45        |
| 3.5.1    | The singlet-triplet gap of the Hubbard dimer . . . . .                         | 45        |
| 3.5.2    | Excitations as magnons . . . . .                                               | 46        |
| 3.6      | Spin-charge separation . . . . .                                               | 47        |
| 3.6.1    | The many-body gap is not one thing . . . . .                                   | 47        |
| 3.6.2    | Nonlocal correlators of a metal and an insulator . . . . .                     | 47        |
| 3.6.3    | Dynamical correlators and the two energy scales . . . . .                      | 48        |
| <b>4</b> | <b>Matrix Product States for Spin Chains</b>                                   | <b>51</b> |
| 4.1      | From an exponential wavefunction to a matrix product state . . . . .           | 51        |
| 4.1.1    | Tensor networks as data compression . . . . .                                  | 51        |
| 4.1.2    | The formal matrix product state ansatz . . . . .                               | 52        |
| 4.1.3    | The cost of exact diagonalization and of matrix product states . . . . .       | 53        |
| 4.2      | Convergence diagnostics for the variational state . . . . .                    | 53        |
| 4.2.1    | A variational ansatz . . . . .                                                 | 53        |
| 4.2.2    | Energy fluctuations . . . . .                                                  | 54        |
| 4.2.3    | Bond dimension and excited states . . . . .                                    | 54        |
| 4.3      | Low-energy excitations and level crossings . . . . .                           | 54        |
| 4.3.1    | The lowest spin excitation in the bulk . . . . .                               | 55        |
| 4.3.2    | Level crossings in a magnetic field . . . . .                                  | 55        |
| 4.4      | Entanglement entropy and why matrix product states work in one dimension . . . | 55        |
| 4.4.1    | Separable versus entangled states . . . . .                                    | 55        |
| 4.4.2    | The reduced density matrix and the von Neumann entropy . . . . .               | 56        |
| 4.4.3    | The Schmidt decomposition and the bound on the entanglement . . . . .          | 56        |
| 4.4.4    | The area law, and why one dimension is cheap . . . . .                         | 57        |
| 4.4.5    | Why two dimensions is expensive . . . . .                                      | 58        |
| 4.4.6    | Where matrix product states struggle even in 1D . . . . .                      | 58        |
| 4.5      | Boundary conditions . . . . .                                                  | 59        |
| 4.5.1    | Open boundaries and a single cut . . . . .                                     | 59        |
| 4.5.2    | Periodic boundaries and the cost of two cuts . . . . .                         | 59        |

|          |                                                                                     |           |
|----------|-------------------------------------------------------------------------------------|-----------|
| 4.6      | Entanglement entropy as a diagnostic for quantum phase transitions . . . . .        | 60        |
| 4.6.1    | The transverse-field Ising model . . . . .                                          | 60        |
| 4.6.2    | The entanglement peak and the order parameter . . . . .                             | 60        |
| 4.7      | The Heisenberg chain at thermodynamic-limit scale . . . . .                         | 61        |
| 4.7.1    | Magnetization at zero field and around a magnetic impurity . . . . .                | 61        |
| 4.7.2    | The correlation length of a dimerized chain from an impurity response . . .         | 61        |
| 4.7.3    | Excited-state magnetization profiles and the many-body gap . . . . .                | 62        |
| 4.8      | Fractionalization in spin- $\frac{1}{2}$ and spin-1 chains at large scale . . . . . | 62        |
| 4.8.1    | Non-local static correlators . . . . .                                              | 62        |
| 4.8.2    | Fractionalization in the spin-1 chain . . . . .                                     | 63        |
| <b>5</b> | <b>Matrix Product States for Fermionic Models</b>                                   | <b>66</b> |
| 5.1      | The Jordan-Wigner mapping from spins to fermions . . . . .                          | 66        |
| 5.1.1    | Spin models and fermionic models . . . . .                                          | 66        |
| 5.1.2    | Matching the local Hilbert spaces . . . . .                                         | 67        |
| 5.1.3    | The string operator . . . . .                                                       | 67        |
| 5.1.4    | Why nearest-neighbor hopping barely notices the string . . . . .                    | 68        |
| 5.1.5    | The practical recipe . . . . .                                                      | 69        |
| 5.2      | The spinless interacting chain at large scale . . . . .                             | 69        |
| 5.2.1    | The model and its two limits . . . . .                                              | 70        |
| 5.2.2    | The equivalence with the XXZ chain . . . . .                                        | 70        |
| 5.2.3    | Charge order from a pinning field . . . . .                                         | 70        |
| 5.2.4    | The phase transition at $V_c$ . . . . .                                             | 71        |
| 5.3      | Correlators as a diagnostic of the phases . . . . .                                 | 72        |
| 5.3.1    | The nonlocal particle-particle correlator . . . . .                                 | 72        |
| 5.3.2    | Pairing correlators and the Cooper-pair susceptibility . . . . .                    | 72        |
| 5.4      | Spin-charge separation in the Hubbard model at large scale . . . . .                | 73        |
| 5.4.1    | The Hubbard chain and its two kinds of excitations . . . . .                        | 73        |
| 5.4.2    | Charge gap from the particle-particle correlator . . . . .                          | 73        |
| 5.4.3    | Gapless spin excitations from the spin-spin correlator . . . . .                    | 74        |
| 5.4.4    | Pairing correlators in the Hubbard model . . . . .                                  | 74        |
| 5.5      | The correlation entropy and the validity of mean-field theory . . . . .             | 74        |

|       |                                                                              |    |
|-------|------------------------------------------------------------------------------|----|
| 5.5.1 | The need for a many-body description . . . . .                               | 75 |
| 5.5.2 | Definition via the correlation matrix . . . . .                              | 75 |
| 5.5.3 | Applied to the spinless chain . . . . .                                      | 76 |
| 5.5.4 | Driving a quantum magnet toward its mean-field solution . . . . .            | 76 |
| 5.6   | The general tensor-network algorithm . . . . .                               | 77 |
| 5.6.1 | Diagrammatic notation . . . . .                                              | 77 |
| 5.6.2 | Matrix product operators . . . . .                                           | 78 |
| 5.6.3 | Contraction and compression when applying $\mathcal{H}$ to a state . . . . . | 78 |
| 5.6.4 | The DMRG sweep as a variational search . . . . .                             | 79 |
| 5.6.5 | PEPS and MERA beyond matrix product states . . . . .                         | 80 |

# PHYS-E0510 – Advanced Computational Methods in Physics D

## Session 1

### Classical Magnetism and Mean-Field Theory

**Companion notebook:** `classical_magnetism.ipynb`    **Prerequisites:** none (second quantization is introduced from scratch)

## Contents and goals

In this session we build the minimal tools that we need to describe interacting electrons, which is second quantization, and we use them to answer a concrete question. The question is when repulsive electron–electron interactions spontaneously break a symmetry of the Hamiltonian. We will look at two symmetry-broken phases, classical magnetism and charge density waves, and we will treat both of them at the mean-field level. At the end of the session we will see a case where we can show that mean-field theory gives the wrong ground state, which is the Hubbard dimer, and this failure is the reason why we develop exact-diagonalization and tensor-network methods in the rest of the course.

## Learning outcomes

By the end of this session, you should be able to do the following.

- Write single-particle and many-body Hamiltonians in second-quantized form, and explain why the interaction term makes the many-body problem exponentially hard.
- Set up and run a mean-field self-consistency loop for the Hubbard and CDW models, and interpret the resulting exchange splitting, gap and order parameter.
- Derive the superexchange coupling  $J \sim t^2/U$  from degenerate perturbation theory and use it to predict collinear versus frustrated classical spin order.
- Identify when mean-field theory fails qualitatively, and explain why, using the entangled singlet ground state of the Hubbard dimer as the counterexample.

## 1.1 Single-particle versus many-body Hamiltonians

### 1.1.1 Single-particle Hamiltonians

Let us start by separating electronic Hamiltonians into two broad classes. The first class contains the Hamiltonians that are bilinear in the field operators, which we call single-particle Hamiltonians,

$$\mathcal{H}_0 = \sum_{ij} t_{ij} c_i^\dagger c_j, \quad (1)$$

where  $t_{ij}$  is a hopping amplitude, and we can think of it as the probability amplitude for an electron in orbital  $j$  to jump to orbital  $i$ . Since  $\mathcal{H}_0$  is only a matrix acting on a single-particle Hilbert space, every electron here moves essentially independently of the others, and to find the spectrum we only need to diagonalize an  $L \times L$  matrix for  $L$  orbitals. This is already enough to describe many materials, such as insulators, semiconductors and ordinary metals.

### 1.1.2 The quartic interaction term

The case we care about most is the many-body case. Here we again have the bilinear term, but we also add a term that is quartic in the fermionic operators,

$$\mathcal{H} = \mathcal{H}_0 + \sum_{ijkl} V_{ijkl} c_i^\dagger c_j^\dagger c_k c_l, \quad (2)$$

and  $V_{ijkl}$  gives the strength of this interaction. This term is responsible for essentially all of the exotic phenomena we are interested in for quantum materials, such as magnetism, charge density waves, superconductivity and every strongly correlated phase we will see later in the course. Second quantization is useful because it allows us to write both the single-particle and the many-body part of Eq. (2) in the same language.

### 1.1.3 The size of the many-body problem

The price of the quartic term is the size of the space where it acts. One electron on  $L$  orbitals has  $L$  states, so  $\mathcal{H}_0$  is an  $L \times L$  matrix. In contrast, any number of electrons on the same  $L$  orbitals has  $2^L$  occupation configurations, since each orbital is either empty or occupied, and the interacting  $\mathcal{H}$  is a  $2^L \times 2^L$  matrix. Figure 1 counts both, first for a chain of four sites and then as  $L$  grows.

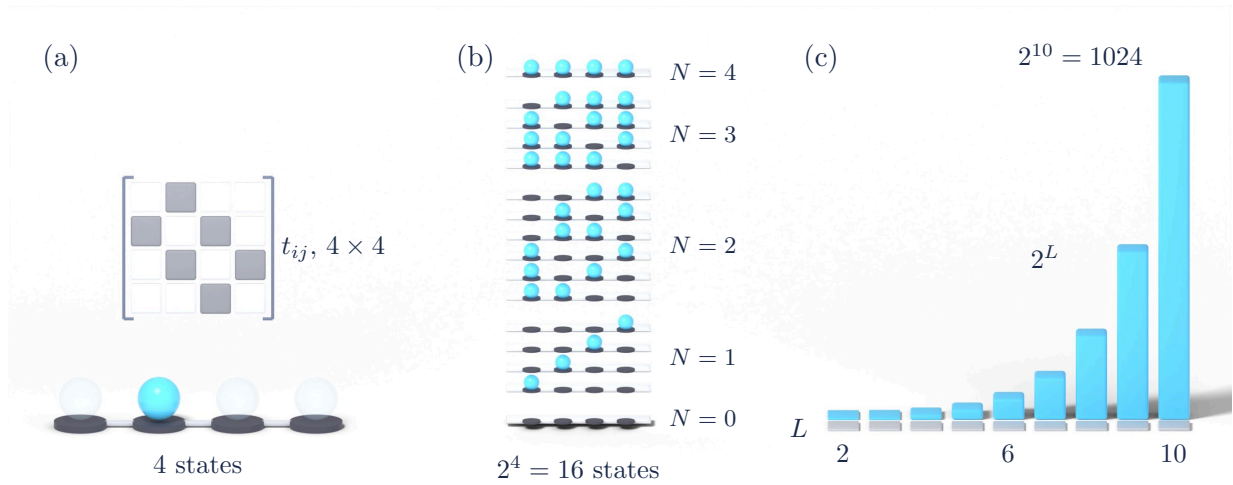


**Figure 1:** The dimension of the single-particle and of the many-body problem. (a) One electron on a chain of four sites can sit on any of the four sites, which we draw as one electron and three ghosts, so the hopping  $t_{ij}$  is a  $4 \times 4$  matrix with entries only between neighbors. (b) The same four sites with any number of electrons, from none to four. Each slab is one occupation configuration and a filled ball is an occupied site, and the  $2^4 = 16$  slabs come in groups of 1, 4, 6, 4 and 1 by electron number  $N$ . (c) The two dimensions as a function of  $L$  on the same linear scale, with  $L$  in front and  $2^L$  behind, meaning that the single-particle problem stays flat while the many-body one already reaches 1024 at  $L = 10$ .

## 1.2 Second quantization

### 1.2.1 Creation and annihilation operators

So let us set up this language. We define the fermionic annihilation and creation operators  $c_i, c_i^\dagger$  for orbital  $i$ , and a vacuum state  $|\Omega\rangle$  that has no electrons, so that  $c_i |\Omega\rangle = 0$  for every  $i$ . We can think of the vacuum as a vector and of the operators as matrices that map one vector to another. A single-particle basis state is then  $c_i^\dagger |\Omega\rangle$ , and the matrix elements of  $\mathcal{H}_0$  in this basis are the hopping amplitudes  $t_{ij}$  we started with.

### 1.2.2 Anticommutation and local degrees of freedom

How do we enforce mathematically that no site can hold more than one electron of a given species? We impose the canonical anticommutation relations,

$$\{c_i, c_j^\dagger\} = \delta_{ij}, \quad \{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0. \quad (3)$$

This algebraic statement does two things at the same time. First, swapping two fermions gives a minus sign, which is the antisymmetry of the wavefunction. Second, acting with  $c_i^\dagger$  twice on any state gives zero, which is the Pauli exclusion principle. In this course we will see three types of local degree of freedom that are built in this way.

- **Spinful fermions.** Each site has four possible states,  $|0\rangle, |\uparrow\rangle, |\downarrow\rangle$  and  $|\uparrow\downarrow\rangle$ . This is the realistic case, the one that we would use for a hydrogen atom.
- **Spinless fermions.** Each site has only two states,  $|0\rangle$  and  $|1\rangle$ . Formally, a spinful fermion is the same as two decoupled spinless fermions, one per spin flavor.
- **Spin- $\frac{1}{2}$  operators.** Again there are two states,  $|\uparrow\rangle$  and  $|\downarrow\rangle$ , but now the operators are *bosonic*, meaning that they commute on different sites instead of anticommuting. As we will see in Section 1.6, a local spin emerges from a spinful fermion once we project out double occupancy and the empty state. This is the origin of what is called spin-charge separation.

#### ✖ Computational companion

Open `classical_magnetism.ipynb`, section “Bandstructure of a tight binding chain” and “Finite size chains.” Diagonalize  $\mathcal{H}_0$  for a chain of  $L$  sites and check that the number of eigenvalues grows linearly in  $L$ , while their spacing gets smaller. This is the discrete precursor of a continuous band. Then, in “Density of states of a finite system as a function of the system size,” plot the density of states,  $\rho(\omega) = -\frac{1}{\pi} \text{Im Tr} [\omega - \mathcal{H}_0 + i0^+]^{-1}$ , and think about how it is related to what a tunneling-spectroscopy or ARPES experiment measures.

## 1.3 The tight-binding dimer as a worked example

### 1.3.1 Bonding and antibonding orbitals

Before we add any interactions, let us solve the smallest possible chain by hand, since we will come back to it many times. Let us take  $L = 2$  sites with hopping  $t$ , and let us include spin from the start, so each site can hold a spin-up and a spin-down electron independently, and the Hamiltonian reads

$$\mathcal{H}_0 = -t \sum_{\sigma} \left( c_{0\sigma}^\dagger c_{1\sigma} + c_{1\sigma}^\dagger c_{0\sigma} \right). \quad (4)$$

Spin never enters the hopping, so  $\mathcal{H}_0$  splits into two identical  $2 \times 2$  spinless problems, one per spin flavor, and each of them reads

$$\mathcal{H}_0^{(\sigma)} = -t \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \implies \varepsilon_{\pm} = \mp t, \quad |\pm\rangle = \frac{1}{\sqrt{2}} (|0\rangle \pm |1\rangle). \quad (5)$$

The state  $|+\rangle$ , at energy  $-t$ , is called the **bonding** orbital, and  $|-\rangle$ , at energy  $+t$ , is called the **antibonding** orbital. Now let us restore spin. Each of these two orbital levels can hold a spin-up and a spin-down electron, so we have  $2 \times 2 = 4$  single-particle eigenstates in total, even though there are only *two* different energies,  $\pm t$ , each of them doubly degenerate. This answers a question that you may have already asked yourself while looking at the notebook, which is why there are four eigenstates for two sites and why some of them are degenerate. The degeneracy counts spin, not orbital content, and it comes from the fact that  $\mathcal{H}_0$  commutes with the total spin, since nothing in  $\mathcal{H}_0$  distinguishes  $\uparrow$  from  $\downarrow$ .

### 1.3.2 The two-electron many-body basis

If we fill in electrons one at a time starting from  $|\Omega\rangle$ , we generate the full many-body basis for two spinful sites, as we set up in the previous section. At half filling with two electrons, for instance, there are  $\binom{4}{2} = 6$  states in total. Four of them are singly occupied, with one electron per site ( $\uparrow\downarrow, \downarrow\uparrow, \uparrow\uparrow, \downarrow\downarrow$ ), and two of them are doubly occupied, with both electrons on the same site. We should keep this counting in mind, since it is what we will use in Section 1.6 to build the effective spin model at strong coupling.

#### ✕ Computational companion

Section “The spectra of a dimer.” Diagonalize the two-site, spinful tight-binding Hamiltonian and check that you recover the bonding and antibonding energies  $\pm t$  and their spin degeneracy directly from the numerical spectrum.

## 1.4 Two microscopic interactions, two broken symmetries

Equation (2) is completely general, so in practice we have to choose a concrete form for  $V_{ijkl}$  and ask which symmetry-broken state it favors in the thermodynamic limit,  $L \rightarrow \infty$ . We will focus on two of the simplest choices, which are also well motivated physically.

### 1.4.1 The Hubbard model of spinful fermions

Let us keep only the interaction between opposite spins on the *same* site, which gives

$$\mathcal{H}_{\text{Hub}} = - \sum_{ij,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad n_{i\sigma} \equiv c_{i\sigma}^\dagger c_{i\sigma}. \quad (6)$$

Physically, this local repulsion is what the onsite electrostatic Coulomb interaction becomes once screening is included, and it is the minimal Hamiltonian we need for **magnetism**. Magnetic order breaks time-reversal and spin-rotational symmetry. The exact Hamiltonian is invariant under any spin rotation but its ground state is not, and if we apply time reversal to the ground state we get a different state with the opposite magnetization.

### 1.4.2 The spinless nearest-neighbor model

Now let us remove the spin degree of freedom and keep instead a density–density repulsion between neighboring sites,

$$\mathcal{H}_{\text{CDW}} = -t \sum_i \left( c_i^\dagger c_{i+1} + \text{h.c.} \right) + V \sum_i n_i n_{i+1}, \quad n_i \equiv c_i^\dagger c_i, \quad (7)$$

which is what we would get from a longer-range electrostatic repulsion once we truncate it to nearest neighbors. This is the minimal Hamiltonian for a **charge density wave (CDW)**. Here the broken symmetry is the *translational* symmetry of the lattice, and charge piles up on one sublattice while it is depleted on the other.

Note that the two models live on the same chain and differ only in what the interaction penalizes, which is two electrons on one site in the first case and two electrons on neighboring sites in the second. As a result, they differ in what orders, which is the spin in the first case and the charge in the second. Figure 2 shows the two side by side.

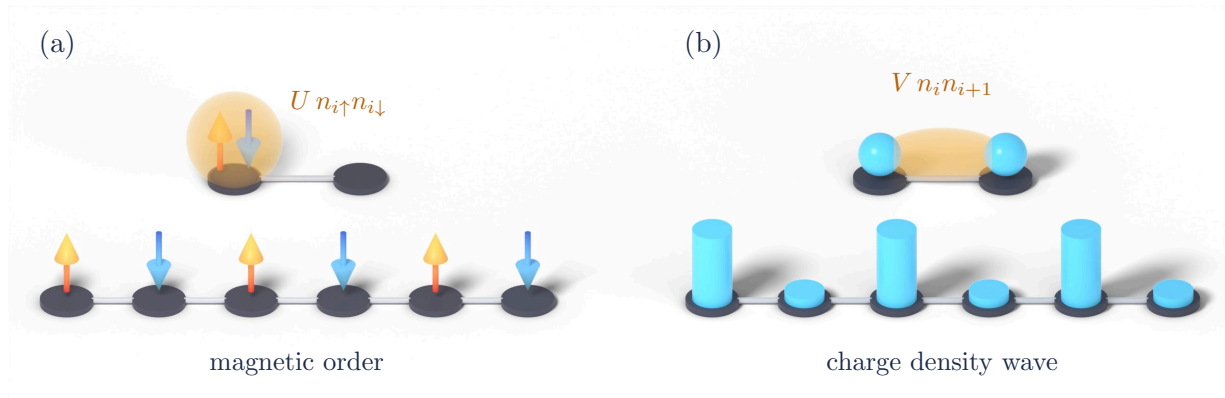


**Figure 2:** The two interactions of this section and the order that each one favors. (a) In the Hubbard model of Eq. (6), an up and a down electron on the same site cost  $U$ , so at half filling the electrons spread out with one per site and their spins align antiparallel from site to site, which is the antiferromagnet. (b) In the spinless model of Eq. (7), two electrons on neighboring sites cost  $V$ , so the charge piles up on every other site, which we draw as the height of a column, and the sites in between are left nearly empty, which is the charge density wave.

### 1.4.3 Where do $U$ and $V$ come from physically?

We will treat  $U$  and  $V$  as given parameters for the rest of the course, but let us stop for a moment on where they come from, because this also explains why both repulsive and attractive effective interactions are physically reasonable.

- **Direct electrostatics.** The screened Coulomb repulsion between electrons is always present, and it is always repulsive. Its onsite part gives us  $U$ , and its longer-range part, truncated to nearest neighbors, gives us  $V$ .
- **Quasiparticle-mediated interactions.** Let us take some other bosonic degree of freedom that couples to the electron density or spin, such as lattice vibrations, which are phonons, collective spin fluctuations, which are magnons, or collective charge fluctuations, which are plasmons and excitons. If we integrate it out, we generate an *effective* quartic interaction

of exactly the same form as Eq. (2), even though there was no bare electron–electron term at the start.

The interaction that we see in the end is the sum of all these contributions, and depending on which mechanism wins it can be repulsive or *attractive* in total. In this course we work with repulsive  $U, V > 0$ , which is the regime relevant for magnetism and CDW order. Attractive interactions instead favor Cooper pairing and superconductivity, a case that we will not study here, although it uses the same formal tools.

## 1.5 Mean-field theory

### 1.5.1 A single-particle approximation

Solving Eq. (6) exactly means working in a Hilbert space of dimension  $4^L$ , or  $2^L$  per spin species, which is exponential in the system size. So the question we want to ask is not how to solve it exactly, but how to solve it approximately. Is there some single-particle Hamiltonian  $\mathcal{H}_{\text{MF}}$  whose ground state is close to the true ground state of  $\mathcal{H}$ ? Finding this Hamiltonian is the main task of mean-field theory.

### 1.5.2 Decoupling the interaction

The simplest way to do this is to write each quartic term as a product of two bilinears and to replace one of the bilinears by its expectation value. We drop the fluctuation term that is left. This is exact only at  $U = 0$ , but we will see that it can still be a very good approximation away from this limit. The decoupling then reads

$$n_{i\uparrow}n_{i\downarrow} \longrightarrow \langle n_{i\uparrow} \rangle n_{i\downarrow} + n_{i\uparrow} \langle n_{i\downarrow} \rangle - \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle. \quad (8)$$

If we define the local magnetization as  $m_i \equiv \langle n_{i\uparrow} \rangle - \langle n_{i\downarrow} \rangle$ , the Hubbard interaction becomes an effective, spin-dependent onsite potential,

$$\mathcal{H}_{\text{MF}} = - \sum_{ij,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} - \frac{U}{2} \sum_i m_i \sigma_z + \text{const}. \quad (9)$$

where  $\sigma_z = \pm 1$  for  $\sigma = \uparrow, \downarrow$ , so the onsite term reads  $-\frac{U}{2}m_i\sigma$  site by site. As a result, spin-up electrons now see a shifted onsite energy  $-Um_i/2$ , and spin-down electrons see  $+Um_i/2$ . This splitting is generated entirely by the interaction, and it is what is called the **exchange splitting**. More generally, if we also keep expectation values such as  $\langle c_{i\uparrow}^\dagger c_{i\downarrow} \rangle$ ,  $\mathcal{H}_{\text{MF}}$  can describe non-collinear magnetization, with components  $m_i^x \equiv 2 \text{Re} \langle c_{i\uparrow}^\dagger c_{i\downarrow} \rangle$ ,  $m_i^y \equiv 2 \text{Im} \langle c_{i\uparrow}^\dagger c_{i\downarrow} \rangle$ , and  $m_i^z \equiv m_i$ , so in principle mean-field theory can capture ferromagnets, antiferromagnets, spin spirals and even skyrmion textures.

### 1.5.3 The self-consistency loop in practice

Concretely, the procedure that we follow has four steps.

1. Guess an initial value for the local order parameters, for example  $m_i^{(0)}$  for magnetism or  $\langle n_i \rangle^{(0)}$  for a CDW.

2. Build  $\mathcal{H}_{\text{MF}}$  from Eq. (9) using this guess, and diagonalize it.
3. Fill the lowest single-particle orbitals up to the target electron number, and recompute  $m_i$ , or  $\langle n_i \rangle$ , from the newly occupied orbitals.
4. Compare the new order parameters to the previous ones. If they have not changed within some tolerance, we are done, and this is the self-consistent solution. Otherwise, mix the old and new guesses and go back to step 2.

Figure 3 draws these four steps as a loop, each one on a chain of four sites. Since this is a nonlinear fixed-point problem, it can converge to different fixed points depending on where we start it, and this is the dependence on the initial guess that we come back to below.

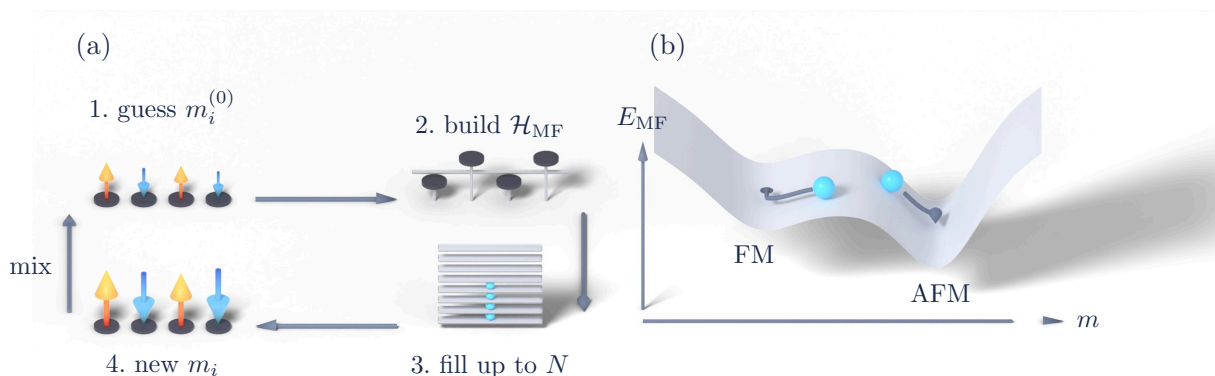


**Figure 3:** The self-consistency loop, which is what every mean-field calculation in this session runs. (a) The four steps as four stations, each drawn on a chain of four sites. Steps 2 and 3 are the two halves that alternate. An order parameter fixes a single-particle Hamiltonian through Eq. (9), which is drawn as the onsite energy of the spin-up electrons lowered where  $m_i > 0$  and raised where  $m_i < 0$ . Diagonalizing that Hamiltonian and filling its lowest orbitals up to the target electron number fixes a new order parameter, and at half filling these are the lowest four of the eight single-particle levels of four spinful sites. Convergence means that the two agree within a tolerance, and until they do we mix the old and new guesses and go around again. (b) The mean-field energy as a function of the order parameter, with a ferromagnetic valley and a lower antiferromagnetic valley. Two starting guesses on the two sides of the ridge roll into different valleys, meaning that the loop converges to a different self-consistent solution depending on where we start it.

#### 1.5.4 Mean-field theory as a variational method

There is an equivalent way to think about all of this, and in some sense a more useful one. Let us restrict the many-body ground state to be a single Slater determinant,  $|\Psi\rangle = c_{a_1}^\dagger c_{a_2}^\dagger \cdots |\Omega\rangle$ , and minimize  $\langle \mathcal{H} \rangle$  over the choice of single-particle orbitals  $\{a_n\}$ . Since  $\mathcal{H}_{\text{MF}}$  depends on  $\langle n_{i\sigma} \rangle$ , and  $\langle n_{i\sigma} \rangle$  itself depends on the ground state of  $\mathcal{H}_{\text{MF}}$ , minimizing the energy in this way is the same as the self-consistency loop we just described. We guess  $\{m_i\}$ , diagonalize  $\mathcal{H}_{\text{MF}}$ , recompute  $\{m_i\}$  from the filled orbitals, and repeat until it converges. So mean-field theory is the best approximation we can build out of *product states*, and this restriction to product states is what will give us problems in Section 1.9.

**x Computational companion**

Section “Magnetic order driven by interactions in a chain.” Run the self-consistency loop for a chain at fixed filling and look at the converged spin-up and spin-down bands. You should see one cosine band per spin, split by the exchange field, with only the spin-down band occupied at the filling used in the notebook.

**1.5.5 Gap opening at half filling**

Let us now force half filling and double the unit cell, so we have two sites with alternating majority spin. At  $U = 0$  this only folds the metallic cosine band onto itself. Once  $U > 0$ , the self-consistent solution opens a gap between the occupied and empty bands, and this gap grows with  $U$  and becomes linear,  $\Delta \sim U$ , once  $U \gg t$ . If we look at the single-particle spectral function instead of the eigenvalues, we see the same behavior, since the continuous metallic density of states at  $U = 0$  develops a clean gap that becomes wider with  $U$ , and this is what a spectroscopy experiment would measure.

**1.5.6 Multiple self-consistent solutions and their energetics**

Since the self-consistency loop is a *nonlinear* fixed-point problem, the solution it converges to depends on where we start it. A ferromagnetic initial guess converges to a metallic, ferromagnetic solution, while an antiferromagnetic initial guess converges to an insulating, antiferromagnetic solution. Both of them are legitimate stationary points of the mean-field energy, but only one of them is the true mean-field ground state with the lowest energy. If we take a half-filled chain with only nearest-neighbor hopping, the antiferromagnetic solution is always lower in energy, and the gap between the two scales as

$$E_{\text{FM}} - E_{\text{AFM}} \sim \frac{1}{U} \xrightarrow{U \rightarrow \infty} 0. \quad (10)$$

So the two solutions only become degenerate in the strict atomic limit  $U \rightarrow \infty$ , and at any finite  $U$  they are physically different states, one metallic and one insulating. Panel (b) of Figure 3 draws this as an energy landscape with two valleys, and a run that starts on the ferromagnetic side stays in the higher one.

**x Computational companion**

Section “The interacting Hubbard dimer.” Compare a self-consistent run seeded as a ferromagnet and one seeded as an antiferromagnet on the dimer of Section 1.3, now with  $U > 0$  switched on, and check numerically which solution has the lower variational energy and how the gap between them scales with  $U$ . Then go back to “Gap opening in the Hubbard model” with a ferromagnetic initialization, to see this dependence on the initial guess directly in the spectrum.

**1.6 From electrons to spins at strong coupling****1.6.1 Saturation of the local moment**

As  $U/t \rightarrow \infty$ , the local moment  $\langle n_{i\uparrow} \rangle - \langle n_{i\downarrow} \rangle$  saturates in magnitude to 1 on every site. Double occupancy and empty sites become forbidden in energy, and every site ends up with exactly one localized electron. In this regime the physics is better described by *spins* than by itinerant fermions, and let us now see in detail why.

### 1.6.2 The Hubbard dimer and its low-energy manifold

Let us take our two-site dimer again, with hopping  $t$ , interaction  $U$  and two electrons in total, so we are at half filling. We already counted a six-dimensional many-body basis for this problem in Section 1.3. For  $U \gg t$ , this basis splits into two groups.

- A four-dimensional **ground-state manifold** of singly occupied configurations, which are  $\uparrow\downarrow$ ,  $\downarrow\uparrow$ ,  $\uparrow\uparrow$  and  $\downarrow\downarrow$  across the two sites, at energy  $\sim 0$ .
- A **virtual manifold** of doubly occupied configurations, at high energy,  $\sim U$ .

Let us look closely at the ground-state manifold. It is the Hilbert space of two spin- $\frac{1}{2}$  degrees of freedom. In other words, our strongly interacting electronic problem has become a spin problem. Panel (c) of Figure 4 draws the six states with their energies.

### 1.6.3 Superexchange and the coupling $J = 4t^2/U$

The only term that connects the two manifolds is the hopping  $t$ . Since nothing in  $\mathcal{H}_{\text{Hub}}$  breaks spin rotation, symmetry alone already tells us that the effective low-energy Hamiltonian has to be proportional to  $\mathbf{S}_1 \cdot \mathbf{S}_2$  at leading order in spin operators. To find the coefficient, we take  $\mathcal{H}_U = U \sum_i n_{i\uparrow} n_{i\downarrow}$  as the unperturbed Hamiltonian, with the singly and doubly occupied configurations of Section 1.3 as its eigenstates, and the hopping  $V = -t \sum_{\sigma} (c_{0\sigma}^\dagger c_{1\sigma} + \text{h.c.})$  as the perturbation. The parallel configurations  $|\uparrow\uparrow\rangle$  and  $|\downarrow\downarrow\rangle$  have no doubly occupied virtual state to hop into, since Pauli exclusion blocks it, so they are already exact eigenstates and are not shifted at any order. This is our triplet, at  $E_{\text{triplet}} = 0$ . Panel (a) of Figure 4 draws this blocked hop, and panel (b) the hop that is allowed when the spins are antiparallel.

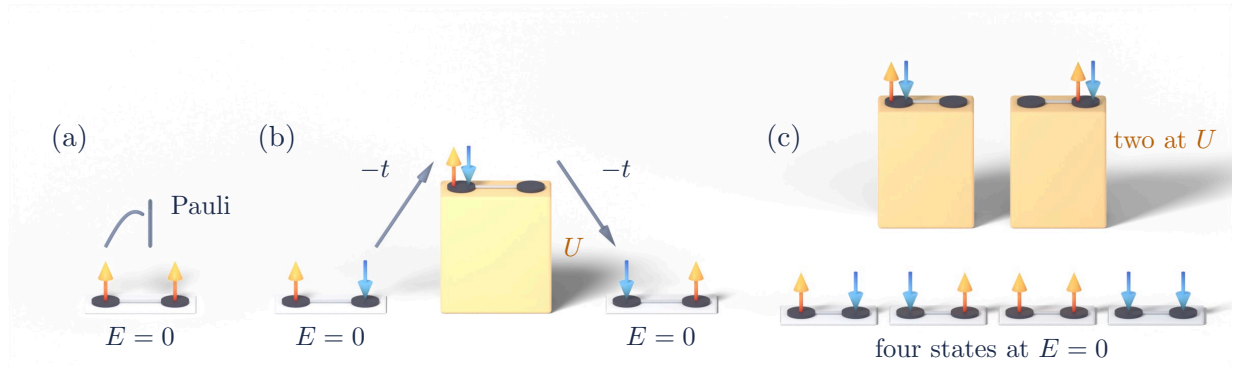


**Figure 4:** The two spin channels of the half-filled Hubbard dimer at strong coupling, which is where the  $J = 4t^2/U$  of Eq. (13) comes from. (a) With parallel spins there is no doubly occupied state to hop into, since Pauli exclusion blocks the process completely, and the triplet stays exactly at  $E_{\text{triplet}} = 0$  at every order. (b) With antiparallel spins either electron can hop onto its neighbor, passing through a virtual doubly occupied configuration at energy  $U$  and ending in the exchanged configuration. Each hop has a matrix element  $-t$  and the virtual state gives an energy denominator  $-U$ , so second-order perturbation theory lowers the antiparallel channel by an amount of order  $t^2/U$  and leaves the parallel one unchanged. (c) All six two-electron states of the dimer as levels. The four with one electron per site are at  $E = 0$  and form the ground-state manifold, which is the Hilbert space of two spins, and the two doubly occupied states are raised by  $U$ , and the hops of (b) visit them only virtually.

The antiparallel configurations are more subtle, since *either* electron can hop. Each one of  $|\uparrow\downarrow\rangle = c_{0\uparrow}^\dagger c_{1\downarrow}^\dagger |\Omega\rangle$  and  $|\downarrow\uparrow\rangle = c_{0\downarrow}^\dagger c_{1\uparrow}^\dagger |\Omega\rangle$  connects through  $V$  to *both* virtual doubly occupied states,

$|2, 0\rangle = c_{0\uparrow}^\dagger c_{0\downarrow}^\dagger |\Omega\rangle$  and  $|0, 2\rangle = c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger |\Omega\rangle$ , which are at energy  $U$  above the low-energy manifold. The matrix elements are  $\langle 2, 0 | V | \uparrow\downarrow \rangle = -t$  and  $\langle 0, 2 | V | \uparrow\downarrow \rangle = -t$ , and by the site-exchange symmetry of the problem we also have  $\langle 2, 0 | V | \downarrow\uparrow \rangle = +t$  and  $\langle 0, 2 | V | \downarrow\uparrow \rangle = +t$ , where the sign flips because of fermionic anticommutation once the two electrons are reordered onto the same site. Only the total spin is conserved here, not the sublattice, so the clean way to organize the calculation is to work directly in the singlet and triplet basis rather than in  $\{|\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle\}$ . Only the singlet combination  $|s\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$  has any overlap with the doubly occupied states, because the matrix elements of the triplet combination to  $|2, 0\rangle$  and  $|0, 2\rangle$  cancel by the sign flip above. By the same site-exchange symmetry, only the symmetric combination  $|d\rangle = \frac{1}{\sqrt{2}}(|2, 0\rangle + |0, 2\rangle)$  couples back to it, since the antisymmetric combination  $\frac{1}{\sqrt{2}}(|2, 0\rangle - |0, 2\rangle)$  is odd under the mirror and  $|s\rangle$  is even under it. Explicitly, we have

$$\langle d | V | s \rangle = \frac{1}{\sqrt{2}} [\langle 2, 0 | V | \uparrow\downarrow \rangle - \langle 2, 0 | V | \downarrow\uparrow \rangle + \langle 0, 2 | V | \uparrow\downarrow \rangle - \langle 0, 2 | V | \downarrow\uparrow \rangle] \frac{1}{\sqrt{2}} = \frac{1}{2} [-t - t - t - t] = -2t, \quad (11)$$

so the singlet sector reduces to an exact  $2 \times 2$  problem, with  $|s\rangle$  at energy 0 coupled to  $|d\rangle$  at energy  $U$  by the matrix element  $-2t$ . The orthogonal antisymmetric doubly occupied combination is decoupled and remains an exact eigenstate at energy  $U$ . Standard non-degenerate second-order perturbation theory on this  $2 \times 2$  block, in the form of Schrieffer–Wolff or equivalently Löwdin, gives

$$E_{\text{singlet}} \approx 0 + \frac{|\langle d | V | s \rangle|^2}{0 - U} = -\frac{4t^2}{U}, \quad (12)$$

which one can check is exactly the  $U \gg t$  expansion of the closed-form eigenvalue of the full  $2 \times 2$  matrix,  $E_- = \frac{U}{2} - \sqrt{(U/2)^2 + 4t^2} \rightarrow -4t^2/U$ . A full numerical exact diagonalization of the two-site, two-electron Hubbard model confirms both this asymptotic value and the exact triplet energy  $E_{\text{triplet}} = 0$  at every  $U/t$ , not only at strong coupling. Let us compare this to the exact spectrum of  $J \mathbf{S}_1 \cdot \mathbf{S}_2$  itself. Writing  $\mathbf{S}_{\text{tot}} = \mathbf{S}_1 + \mathbf{S}_2$  gives  $\mathbf{S}_1 \cdot \mathbf{S}_2 = \frac{1}{2} [S_{\text{tot}}(S_{\text{tot}} + 1) - \frac{3}{4} - \frac{3}{4}]$ , which is  $-\frac{3}{4}$  for the singlet ( $S_{\text{tot}} = 0$ ) and  $+\frac{1}{4}$  for the triplet ( $S_{\text{tot}} = 1$ ), meaning that  $E_{\text{singlet}} = -\frac{3}{4}J$  and  $E_{\text{triplet}} = \frac{1}{4}J$ , with a gap of exactly  $J$  between them. Matching this gap to the one we just computed fixes

$$J = E_{\text{triplet}} - E_{\text{singlet}} = \frac{4t^2}{U} \implies \mathcal{H}_{\text{eff}} = J \mathbf{S}_1 \cdot \mathbf{S}_2, \quad (13)$$

which is the **antiferromagnetic superexchange** coupling. Intuitively, virtual hopping into the doubly occupied states, which is blocked by Pauli exclusion for parallel spins, lowers the energy of the singlet combination of antiparallel configurations. This is why the effective low-energy interaction favors antialignment, even though the Hubbard repulsion itself has no explicit spin dependence. The same argument holds without change on any lattice with hoppings  $t_{ij}$ , so the half-filled, strongly interacting Hubbard model on *any* lattice maps onto a spin- $\frac{1}{2}$  **Heisenberg model**,

$$\mathcal{H}_{\text{Heis}} = \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j, \quad J_{ij} \sim \frac{t_{ij}^2}{U}. \quad (14)$$

with the same numerical prefactor as Eq. (13),  $J_{ij} = 4t_{ij}^2/U$ , for each bond treated in isolation in this way. If instead we have more than one electron per site, as in multi-orbital atoms, we map onto Heisenberg models with higher spin, which are spin-1 for two electrons per site, spin- $\frac{3}{2}$  for three, and so on. Additional weakly interacting orbitals can even flip the *sign* of  $J_{ij}$  and give

ferromagnetic rather than antiferromagnetic coupling, which is why real materials are not always antiferromagnets.

#### ✕ Computational companion

Section “The strongly interacting limit of the Hubbard model.” Compute  $E_{\text{FM}} - E_{\text{AFM}}$  as a function of  $U$  and check that it follows the  $1/U$  scaling we derived above. Then go to smaller  $U$  and see where the perturbative assumption  $t \ll U$  behind Eq. (13) starts to break down.

## 1.7 Classical magnetic order and frustration

If we now treat the spins in  $\mathcal{H}_{\text{Heis}}$  as classical vectors, which is an approximation very close in spirit to mean-field theory, finding the ground state becomes a direct energy minimization.

### 1.7.1 Bipartite lattices

On the square and honeycomb lattices, we can always split the sites into two sublattices  $A, B$  such that every bond connects  $A$  to  $B$ . For antiferromagnetic  $J > 0$ , the classical ground state is then  $\mathbf{S}_A = -\mathbf{S}_B$ , which is collinear Néel order.

### 1.7.2 Frustration

The situation is more interesting on lattices that are *not* bipartite, such as the triangular and kagome lattices, which are built from triangles that share corners or edges. On these lattices, no choice of two sublattices can satisfy every antiferromagnetic bond at the same time. The classical ground state becomes instead **non-collinear**, and neighboring spins rotate by  $120^\circ$  as we go around each triangle, which gives a spiral magnetic order with a magnetic unit cell of several sites. Figure 5 draws the Néel state, a single frustrated triangle and the  $120^\circ$  order side by side.

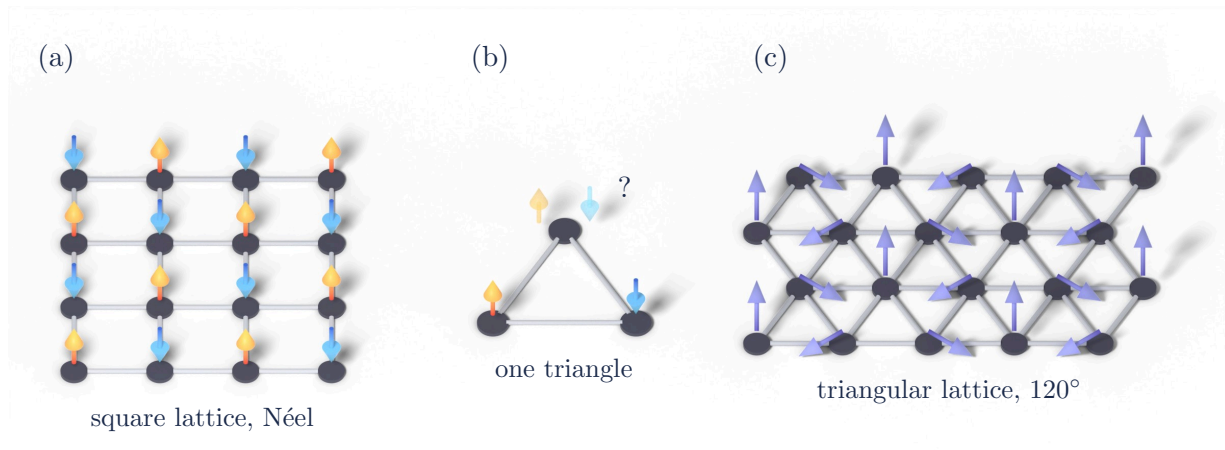


**Figure 5:** Classical ground states of the Heisenberg model of Eq. (14) with antiferromagnetic  $J > 0$ , obtained by treating every spin as a classical vector. (a) On a bipartite lattice every bond connects the two sublattices, so  $\mathbf{S}_A = -\mathbf{S}_B$  satisfies all of them at the same time and the order is collinear Néel. (b) A single triangle is where this fails. Once two spins are antiparallel and satisfy their bond, the third spin cannot be antiparallel to both, which we draw as two ghost arrows, so one bond is left unsatisfied regardless of its choice. (c) On the triangular lattice the bonds sit on edge-sharing triangles and no two-sublattice assignment can satisfy all of them, so the configuration with minimum energy is instead the non-collinear  $120^\circ$  spiral, with a magnetic unit cell of three sites. We draw it in one color since none of the three sublattices is up or down.

#### ✕ Computational companion

Section “Non-collinear magnetism in the Hubbard model from competing interactions” and “Non-collinear magnetic order from geometric frustration.” Add a second-neighbor hopping to the mean-field chain and see that it can also stabilize non-collinear order, since competing exchange paths play the same frustrating role as the triangular geometry. Then move to the triangular and kagome supercells and read off the  $120^\circ$  spiral directly from the self-consistent magnetization pattern.

### 1.7.3 Anisotropic exchange

Real materials often break the  $SU(2)$  spin-rotation symmetry of  $\mathcal{H}_{\text{Heis}}$  through spin-orbit coupling, which adds terms bilinear in spin that are *not* symmetric under a common rotation of all spins. Three of them appear often enough to have their own names.

- **Antisymmetric exchange**, also called **Dzyaloshinskii–Moriya exchange**,  $\mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j)$ , which appears when mirror symmetry is broken. It favors spins at  $90^\circ$  to each other, meaning non-collinear order even without any geometric frustration.
- **Ising anisotropy**, coupling only  $S_i^z S_j^z$ , which comes from strong spin-orbit coupling and single-ion anisotropy and pushes the spins toward classical behavior, restricted to a single axis or plane.
- **Kitaev exchange**, a *bond-dependent* Ising-like coupling where  $x$ -bonds couple  $S^x S^x$ ,  $y$ -bonds couple  $S^y S^y$  and  $z$ -bonds couple  $S^z S^z$ . On the honeycomb lattice, for example, no single spin configuration can satisfy the three bond types at the same time, which is why this term is intrinsically frustrating and a key ingredient of quantum spin liquid models.

We will not compute with any of these three terms in this course, but they are what we use as soon as spin-orbit coupling is strong, and they are behind most of the exotic magnets and

quantum spin liquid candidates that are studied today.

## 1.8 Charge density waves as a mean-field problem

### 1.8.1 Mean-field decoupling of the spinless model

The same tools apply to  $\mathcal{H}_{\text{CDW}}$  from Eq. (7). We decouple the density–density term as  $\langle n_i \rangle n_{i+1} + n_i \langle n_{i+1} \rangle - \langle n_i \rangle \langle n_{i+1} \rangle$  and iterate to self-consistency, as before. At  $V = 0$  the chain is a featureless, half-filled metal with  $n_i = \frac{1}{2}$  on every site. As we turn on  $V$ , we get the same qualitative evolution of the spectrum as in the Hubbard case, where a gap opens and grows as  $\sim V$  at large  $V$ .

### 1.8.2 The charge imbalance as order parameter

What changes is the order parameter, which is now the **charge imbalance**,

$$\delta n \equiv n_{\text{even}} - n_{\text{odd}}, \quad (15)$$

and it grows from 0 at  $V = 0$  toward  $\delta n \rightarrow 1$  at large  $V$ , meaning that the sites end up alternating between fully filled and fully empty. The broken symmetry here is translational rather than time-reversal, but note how closely the mechanism, and even the shape of the evolution of the spectrum, follows the magnetic case.

#### ✕ Computational companion

Sections “Gap opening in a spinless interacting model” and “Symmetry breaking in the spinless fermionic chain.” Track the gap and the charge imbalance  $\delta n$  as a function of  $V$ . Then seed the self-consistency loop with an explicit external CDW field and see how it selects which sublattice orders.

## 1.9 Where mean-field theory breaks down

So far mean-field theory has worked well every time, and the reason is that it is a very good technique when the true ground state *does* spontaneously break a symmetry. But nothing guarantees this in advance, and the Hubbard dimer at half filling gives us a clean counterexample.

### 1.9.1 The mean-field solution of the dimer

The exact Hamiltonian  $\mathcal{H}_{\text{Hub}}$  for two sites is fully symmetric under spin rotation and time reversal. Its mean-field decoupling, however, is only self-consistent with a *symmetry-breaking* ansatz once  $U$  passes a threshold. Below the threshold,  $\mathcal{H}_{\text{MF}}$  stays non-magnetic, and above it, the converged solution has finite local moments of opposite sign on the two sites, which eventually saturate, as in the regime we studied in Section 1.6. The mean-field gap follows this transition too, since it stays constant below the threshold and then grows linearly above it.

### 1.9.2 The exact singlet ground state

Let us now compare this to the *exact* many-body ground state, which looks quite different. In the strongly interacting limit, Section 1.6 already told us that the dimer maps onto  $\mathcal{H}_{\text{eff}} = J \mathbf{S}_1 \cdot \mathbf{S}_2$ ,

and we can diagonalize this by hand. Its exact ground state is the singlet

$$|\Psi_{\text{singlet}}\rangle = \frac{1}{\sqrt{2}} \left( |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right). \quad (16)$$

This state has  $\langle S_1^z \rangle = \langle S_2^z \rangle = 0$ . It does not break time-reversal symmetry, in direct contradiction with what the symmetry-broken mean-field solution told us to expect. The reason is structural and not a numerical accident. The state  $|\Psi_{\text{singlet}}\rangle$  is an entangled superposition, and it cannot be written as a single Slater determinant, for any choice of orbitals or spin quantization axis. Mean-field theory is built by construction from product states, as we saw in Section 1.5.4, so it can never reach this state.

### 1.9.3 Why this matters

The Hubbard dimer is the smallest Hamiltonian that shows this kind of failure, but the failure itself is completely generic. Whenever the true many-body ground state is entangled and not adiabatically connected to a product state, mean-field theory gets the physics qualitatively wrong, with the wrong symmetry, the wrong order, and sometimes a completely wrong phase. This defines the plan for the rest of the course. *Exact diagonalization*, in Sessions 2 and 3, solves small many-body Hamiltonians with no product-state restriction at all, and *tensor network* methods, in Sessions 4 and 5, allow us to recover the exact answer at system sizes where exact diagonalization is no longer possible.

|                        | Mean-field theory                                                                      | Exact diagonalization                                 | Tensor networks (MPS)                                  |
|------------------------|----------------------------------------------------------------------------------------|-------------------------------------------------------|--------------------------------------------------------|
| Ansatz                 | product state, a Slater determinant                                                    | unrestricted, full Hilbert space                      | bounded-entanglement state (MPS)                       |
| Cost vs. size $L$      | polynomial                                                                             | exponential, $\sim 2^L$                               | polynomial in $L$ and bond dimension                   |
| Captures entanglement? | no                                                                                     | yes, exactly                                          | yes, up to the bond dimension                          |
| Typical reach          | any $L$                                                                                | $L \lesssim 20$ spins, half that for spinful fermions | $L \sim 40$ to 100 and more in 1D                      |
| Fails when...          | the ground state is not adiabatically connected to a product state, as in this session | never in principle, only limited by $L$               | entanglement exceeds what the bond dimension can store |

**Table 1:** The three methods used in this course, side by side as a preview. For each method we show the ansatz, how the cost scales with system size  $L$ , whether it captures entanglement, the typical reach and when it fails.

We can think of Table 1 as a preview rather than a derivation, since we will develop and use each of these methods on its own starting from the next session.

### Closing summary

- Second quantization allows us to write single-particle and many-body ( $\mathcal{O}(4)$ -fermion) Hamiltonians in the same language, and the interaction term is what drives all correlated physics.

- Mean-field theory decouples the interaction into an effective single-particle problem that we solve self-consistently. Equivalently, it is a variational search over Slater determinants.
- The Hubbard model gives us magnetism, which breaks time-reversal and spin symmetry, and the spinless nearest-neighbor model gives us charge density waves, which break translational symmetry. Both come from essentially the same mean-field mechanism.
- In the strongly interacting limit, second-order perturbation theory maps the Hubbard model onto a Heisenberg spin model with  $J \sim t^2/U$ , which is the superexchange coupling. Classically this model shows collinear order on bipartite lattices and non-collinear, frustrated order on other lattices.
- Mean-field theory can fail qualitatively whenever the true ground state is entangled beyond any product state, as we saw for the singlet ground state of the Hubbard dimer. This failure is what motivates exact diagonalization and tensor networks, which we start in the next session.

# PHYS-E0510 – Advanced Computational Methods in Physics D

## Session 2

### Exact Diagonalization of the Heisenberg Spin Chain

**Companion notebook:** `quantum_magnetism.ipynb`    **Prerequisites:** Session 1 (second quantization and the superexchange derivation of the Heisenberg model)

## Contents and goals

In the last session we saw that mean-field theory has a limitation, since it only uses product states and the ground state of the Hubbard dimer is a singlet, which is an entangled state that does not break any symmetry. In this session we will not do any approximation. We will take the Heisenberg Hamiltonian that we obtained from superexchange, write it as a matrix in the full many-body Hilbert space, which has dimension  $2^L$ , and diagonalize it exactly. With this, we will learn how to read a many-body spectrum. First, we will use the many-body gap to see if a spin chain is gapped or gapless. Then we will see how a magnetic field or a change in the couplings gives rise to level crossings and phase transitions. We will also see how symmetries allow us to write the Hamiltonian in blocks, so that we can solve bigger systems, and how static and dynamical correlators tell us about the order and the excitations of the system. At the end we will ask if the excitations of a quantum magnet can be described as single-particle excitations, in terms of emergent fermions that are called spinons. All the results in this session are exact, and the price we pay is that the Hilbert space grows as  $2^L$ . This exponential growth is the reason why, starting in Session 4, we will use tensor-network methods.

## Learning outcomes

By the end of this session, you should be able to do the following.

- Build the Heisenberg Hamiltonian as an explicit matrix in the basis of many-body product states and diagonalize it exactly for a finite spin chain.
- Use the finite-size scaling of the many-body gap, which either follows a power law or saturates, to tell a gapless spin chain from a gapped one.
- Use conserved quantum numbers, which are the total spin and  $S_{\text{tot}}^z$ , to block-diagonalize the Hamiltonian, and explain level crossings and magnetization curves in a field.
- Compute static and dynamical spin correlators and connect them to a mean-field description of the excitations in terms of auxiliary fermions, which are called spinons.

## 2.1 From the Hubbard dimer to a quantum magnet

### 2.1.1 The classical Ising dimer

Let us start by recalling what a classical magnet with a broken symmetry looks like at the microscopic level, since it is the natural contrast to what comes next. Let us take the simplest magnetic Hamiltonian, which is an Ising coupling between two spins,

$$\mathcal{H}_{\text{Ising}} = J S_1^z S_2^z, \quad J > 0. \quad (17)$$

There is no  $S^x$  or  $S^y$  in it, so we can think of  $S_i^z = \pm \frac{1}{2}$  as a classical Ising variable. Minimizing the energy is simple, since we want  $S_1^z$  and  $S_2^z$  to have opposite sign, and there are exactly two ways to do that,  $|\uparrow\downarrow\rangle$  and  $|\downarrow\uparrow\rangle$ . Both are valid ground states and both break time-reversal symmetry, because flipping every spin takes one into the other. Each of them has a finite and well-defined local moment  $\langle S_i^z \rangle = \pm \frac{1}{2}$ . This is a small version of a classical magnet, which is a symmetry-broken state with a finite magnetization at every site.

### 2.1.2 The quantum Heisenberg dimer

Now let us keep the full quantum mechanics of the spin operators and couple all three components,

$$\mathcal{H}_{\text{Heis}} = J \mathbf{S}_1 \cdot \mathbf{S}_2 = J (S_1^x S_2^x + S_1^y S_2^y + S_1^z S_2^z). \quad (18)$$

This is the superexchange Hamiltonian that we derived in the last session from the strong-coupling limit of the Hubbard dimer, with  $J = 4t^2/U > 0$ . We already know from Session 1 that its exact ground state is the singlet  $|\Psi_{\text{singlet}}\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ , which is a single non-degenerate state with  $\langle S_i^z \rangle = 0$  on every site, and which cannot be written as a product state. From now on we will call this a **quantum magnet**. In contrast with the Ising ground states, this state does not break time-reversal symmetry, and it is entangled in an essential way. In this session we will compute this kind of ground state exactly, for chains longer than two sites, and we will see what we can learn from it and from the excited states above it.

## 2.2 Exact diagonalization of a spin chain

### 2.2.1 The product-state basis

Let us now generalize Eq. (18) to a chain of  $L$  spin- $\frac{1}{2}$ 's with nearest-neighbor exchange,

$$\mathcal{H}_{\text{Heis}} = J \sum_{i=1}^{L-1} \mathbf{S}_i \cdot \mathbf{S}_{i+1}, \quad J > 0 \text{ (antiferromagnetic)}. \quad (19)$$

Regardless of how complicated  $J_{ij}$  is on a given lattice, solving this Hamiltonian exactly always takes the same three steps. First we pick a basis of the many-body Hilbert space, then we write  $\mathcal{H}$  as a matrix in that basis, and finally we diagonalize it. The natural basis is the set of all product states  $|\sigma_1 \sigma_2 \cdots \sigma_L\rangle$  with  $\sigma_i \in \{\uparrow, \downarrow\}$ . There are two states for  $L = 1$ , four for  $L = 2$ , eight for  $L = 3$ , and in general  $2^L$  states for  $L$  sites. This is the same exponential growth of the many-body Hilbert space that we saw in Session 1 for the Hubbard model. It appears here again because a spin- $\frac{1}{2}$  chain is a projected part of that same fermionic Hilbert space, where every site is singly occupied.

### 2.2.2 A sparse matrix

To build the matrix we need the matrix elements of  $\mathbf{S}_i \cdot \mathbf{S}_j$ , and it is convenient to split it into a diagonal and an off-diagonal part using the raising and lowering operators  $S^\pm = S^x \pm iS^y$ ,

$$\mathbf{S}_i \cdot \mathbf{S}_j = S_i^z S_j^z + \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+). \quad (20)$$

The first term is diagonal in our product basis, since it multiplies each basis state by  $\pm \frac{1}{4}$  depending on whether  $\sigma_i, \sigma_j$  are parallel or antiparallel. The second term is the one that moves us inside

the basis. The operator  $S_i^+ S_j^-$  flips an antiparallel pair  $\downarrow_i \uparrow_j \rightarrow \uparrow_i \downarrow_j$  and gives zero on everything else, so it only connects basis states that differ by swapping one  $\uparrow\downarrow$  pair on two sites joined by a bond. This is why the Heisenberg matrix is *sparse*, even though it lives in a  $2^L$ -dimensional space, meaning that each row has at most  $L - 1$  off-diagonal entries, one per bond. Iterative solvers such as Lanczos use this structure to reach much bigger  $L$  than a dense diagonalization can. Figure 6 goes through the three steps for  $L = 4$ .

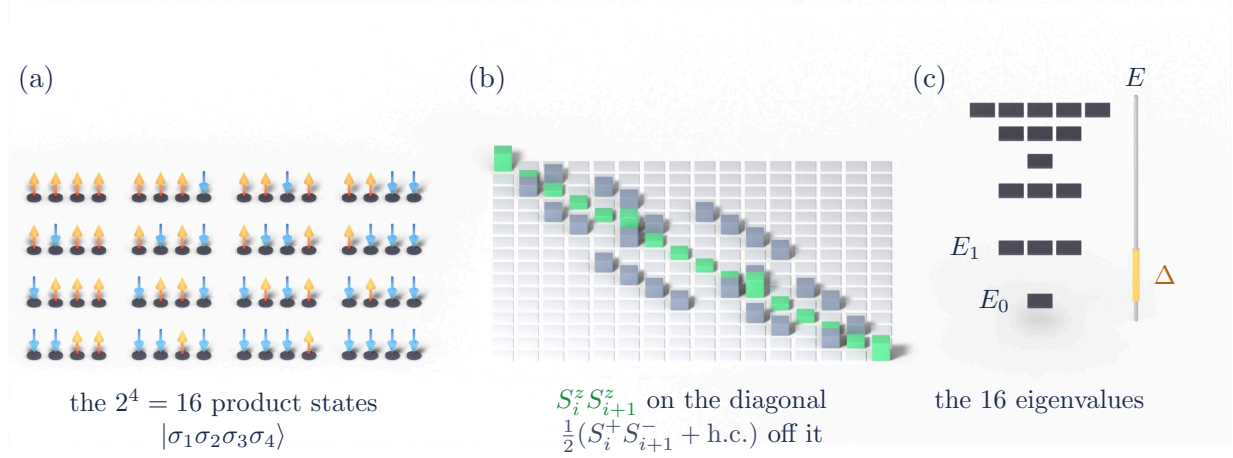


**Figure 6:** The three steps of exact diagonalization for the open Heisenberg chain of Eq. (19) with  $L = 4$ . (a) The basis, which is the  $2^4 = 16$  product states in the order a code would count them, with  $|\uparrow\uparrow\uparrow\uparrow\rangle$  at the back left and  $|\downarrow\downarrow\downarrow\downarrow\rangle$  at the front right. (b) The Hamiltonian in that basis, with one cell per matrix element in the same order and the height of a bar giving the size of the element. The  $S_i^z S_{i+1}^z$  term of Eq. (20) fills the diagonal and the flip-flop term puts at most  $L - 1 = 3$  bars in each row, so only 40 of the 256 cells are occupied, which is what we mean by a sparse matrix. (c) The result, which is the sixteen eigenvalues drawn as levels at their energy, with degenerate levels side by side. There is a singlet ground state at  $E_0 \approx -1.62J$ , a triplet at  $E_1 \approx -0.96J$ , and the many-body gap  $\Delta = E_1 - E_0$  of Eq. (23) in amber. At the top are the five members of the fully polarized  $S = 2$  multiplet at  $\frac{3}{4}J$ .

### 2.2.3 The dimer solved in two ways

Let us see this explicitly for  $L = 2$ . In the basis  $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$ , the stretched states  $|\uparrow\uparrow\rangle$  and  $|\downarrow\downarrow\rangle$  have no partner to flip into, so  $\mathcal{H}_{\text{Heis}} |\uparrow\uparrow\rangle = \frac{J}{4} |\uparrow\uparrow\rangle$ , and the same holds for  $|\downarrow\downarrow\rangle$ . On the remaining two-dimensional subspace  $\{|\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle\}$ , Eq. (20) gives the  $2 \times 2$  block

$$\mathcal{H}_{\text{Heis}} \Big|_{\{|\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle\}} = J \begin{pmatrix} -\frac{1}{4} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{4} \end{pmatrix} \implies E_{\pm} = J \left( -\frac{1}{4} \pm \frac{1}{2} \right), \quad |\pm\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle). \quad (21)$$

So  $E_- = -\frac{3}{4}J$  for the antisymmetric combination, which is the singlet we already knew, and  $E_+ = \frac{1}{4}J$  for the symmetric combination, which is degenerate with  $|\uparrow\uparrow\rangle$  and  $|\downarrow\downarrow\rangle$  at the same energy  $\frac{J}{4}$ . Together these three states form the **triplet**. Diagonalizing a  $4 \times 4$  matrix by hand already gives the full structure of the singlet and the triplet.

There is a second and faster way to get the same answer, and we will use it again because it generalizes. We define the total spin  $\mathbf{S}_{\text{tot}} = \mathbf{S}_1 + \mathbf{S}_2$ , so that  $\mathbf{S}_{\text{tot}}^2 = \mathbf{S}_1^2 + \mathbf{S}_2^2 + 2\mathbf{S}_1 \cdot \mathbf{S}_2$ , and hence

$$\mathcal{H}_{\text{Heis}} = J \mathbf{S}_1 \cdot \mathbf{S}_2 = \frac{J}{2} \left[ S_{\text{tot}}(S_{\text{tot}} + 1) - \frac{3}{4} - \frac{3}{4} \right], \quad (22)$$

where we used  $\mathbf{S}_i^2 = \frac{3}{4}$  for spin- $\frac{1}{2}$ . Since  $\mathbf{S}_{\text{tot}}^2$  has eigenvalues  $S_{\text{tot}}(S_{\text{tot}} + 1)$  with  $S_{\text{tot}} = 0$  or  $1$  for two spin- $\frac{1}{2}$ 's, Eq. (22) directly gives  $E(S_{\text{tot}} = 0) = -\frac{3}{4}J$  and  $E(S_{\text{tot}} = 1) = \frac{1}{4}J$ , in exact agreement with Eq. (21). Note also why the ground-state energy in the notebook is equal to the sum of the Ising and XY ground energies computed separately. On the two-dimensional subspace  $\{|\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle\}$ , the Ising part  $S_1^z S_2^z$  is proportional to the identity,  $-\frac{1}{4}\mathbb{I}$ , because *both* basis states have the same  $S_1^z S_2^z$  eigenvalue. Minimizing the sum of a constant and the XY block is the same as minimizing each one separately and adding them, and this is why the two energies add up here. This only happens for  $L = 2$ . For longer chains the Ising term is no longer a multiple of the identity on the subspace that the XY term mixes, and in general the two parts no longer have their minimum on the same state.

### ✕ Computational companion

Open `quantum_magnetism.ipynb` and work through the “Basics” block, which has the sections “Creating a spin\_chain object,” “Creating a Hamiltonian,” “Computing the ground state energy,” and “Computing expectation values.” Build the  $L = 2$  Heisenberg Hamiltonian directly from the spin operators, diagonalize it, and check numerically that you get  $E_{\text{singlet}} = -\frac{3}{4}J$  and  $E_{\text{triplet}} = \frac{1}{4}J$ . Then replace  $S^x$  by  $S^y$  in the expectation-value cell and think about why nothing changes.

## 2.3 The many-body spectrum and the many-body gap

### 2.3.1 Counting the eigenvalues

Now let us leave the case  $L = 2$ , which we can do by hand, and let the computer diagonalize Eq. (19) for increasing  $L$ . The number of eigenvalues we obtain is the dimension of the matrix,  $2^L$ , which is four for  $L = 2$ , sixteen for  $L = 4$ , sixty-four for  $L = 6$ , and so on, so it grows exponentially with system size in the same way as the basis. In practice, however, we almost never need the whole spectrum. A real experiment at low temperature only probes the states closest to the ground state, so from now on we will focus on the bottom of the many-body spectrum, which is the ground state  $E_0$  and the few low-lying excited states above it.

### 2.3.2 The many-body gap and its scaling

The most useful number that we can read from this part of the spectrum is the **many-body gap**,

$$\Delta(L) \equiv E_1(L) - E_0(L), \quad (23)$$

which is the energy cost of the lowest excitation above the ground state, and it is marked for  $L = 4$  in panel (c) of Figure 6. For the uniform Heisenberg chain,  $\Delta(L)$  decreases steadily as  $L$  grows, and it follows a power law instead of saturating to a finite value. This is the signature of a **gapless** system, meaning that its excitations cost arbitrarily little energy in the thermodynamic limit. Where does this power law come from? Qualitatively, it comes from the same free-fermion argument that we will use in Section 2.10. If we replace each spin operator by an auxiliary fermion  $f_{i\sigma}$ , which is called an Abrikosov fermion, and decouple the exchange term at the mean-field level,  $\mathcal{H}_{\text{Heis}}$  becomes a free-fermion **spinon** Hamiltonian with a gapless band and Fermi points at  $k_F = \pm\pi/2$ . The lowest excitations are then particle-hole pairs created at those Fermi points, which disperse *linearly* in momentum. A linearly dispersing excitation on a ring of  $L$  sites

is a one-dimensional particle-in-a-box problem, so its levels are spaced by

$$\Delta(L) \sim \frac{\pi v_s}{L}, \quad (24)$$

with  $v_s$  the velocity of the low-energy excitations, meaning that the gap follows a  $1/L$  power law and does not stay finite. Numerically, the finite-size data is well described by  $\Delta(L) \approx \pi^2 J/(2L)$ . To obtain  $v_s$  with this precision we need the exact Bethe-ansatz solution, since mean-field theory gives the right qualitative power law but not the precise coefficient. We will keep this picture of a particle in a box in mind, because we will see it again in a more literal form when we look at dynamical correlators in Section 2.9, and again when we build the explicit spinon band structure behind this argument in Section 2.10.

#### ✕ Computational companion

Section “Many-body energies of the Heisenberg model.” Diagonalize the uniform chain for  $L = 2, 4, 6, 8$  and plot the full spectrum each time, and check that the number of eigenvalues is  $2^L$ . Then plot only  $E_1(L) - E_0(L)$  and see how the gap shrinks with  $L$ . Think also about the biggest  $L$  for which you could still store the full spectrum on your own machine.

## 2.4 The XXZ model from classical order to entanglement

### 2.4.1 The two ends of the XXZ chain

Section 2.1 presented the Ising model and the Heisenberg model as two separate Hamiltonians, but it is more useful to see them as the two ends of a single family. Let us take

$$\mathcal{H}_{\text{XXZ}} = \sum_i \left[ J_{xy} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) + J_z S_i^z S_{i+1}^z \right], \quad J_z \equiv 1 \text{ fixed}, \quad (25)$$

and change  $J_{xy}$  from 0 to 1. At  $J_{xy} = 0$  we are back at the classical Ising model of Eq. (17), generalized to  $L$  sites. In the thermodynamic limit its ground state is doubly degenerate, with the Néel-ordered state  $|\uparrow\downarrow\uparrow\downarrow\cdots\rangle$  and its time-reversed partner, and each of them has a finite staggered moment that breaks the symmetry. At  $J_{xy} = 1$  we recover the isotropic Heisenberg model of Eq. (19), whose ground state, as we already know from the dimer, is unique and has no local moment, so it is a purely quantum magnet. This means that  $J_{xy}$  interpolates between a classical magnet with a broken symmetry and an entangled quantum magnet, and the natural question is how the ground state goes from one description to the other as we change  $J_{xy}$ .

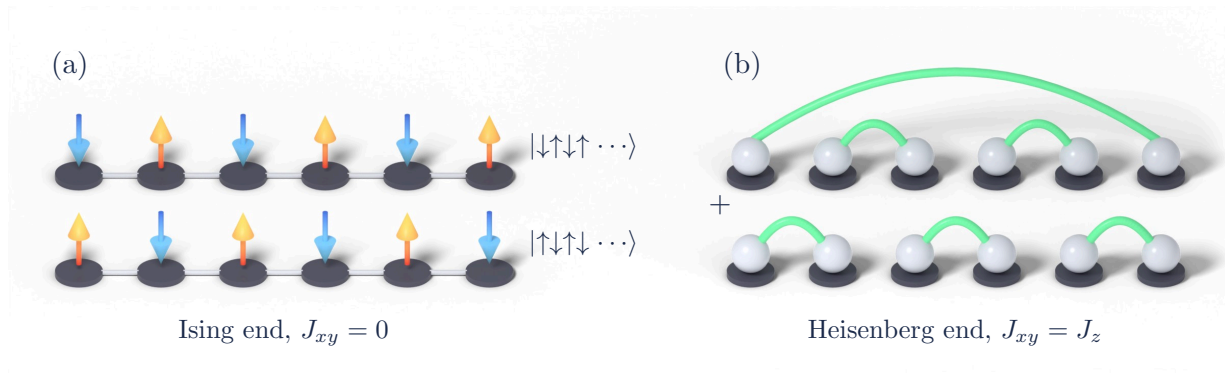


**Figure 7:** The two ends of Eq. (25). (a) The two classical ground states at the Ising end  $J_{xy} = 0$ , with  $|\uparrow\downarrow\uparrow\downarrow\cdots\rangle$  in front and  $|\downarrow\uparrow\downarrow\uparrow\cdots\rangle$  behind it. Each is a product state with a definite  $S^z$  on every site, each has a finite staggered moment, and the two are exchanged by time reversal. In the thermodynamic limit they are exactly degenerate and the system picks one of them, which is what symmetry breaking means here. On a finite chain, once  $J_{xy}$  is switched on, they are instead split by a tiny amount, and the growth of this splitting as  $J_{xy} \rightarrow 1$  is how the crossover to the unique, entangled Heisenberg ground state appears in the spectrum. (b) At the Heisenberg end  $J_{xy} = J_z$  there is no moment on any site, so the spins are drawn as spheres without arrows. You can think of the ground state as neighbors paired into singlets, drawn as the green bonds, which resonate between the two ways of pairing them. The two pairings are drawn in front and behind, and the second one pairs the two ends as on a ring. This is a cartoon of the entanglement and not the exact state, which also contains singlets between distant sites.

### 2.4.2 The transition in the finite-size spectrum

The finite-size spectrum answers this question directly. At small  $J_{xy}$  the two classical Néel states are not exactly degenerate on a finite chain, since only an infinite chain can spontaneously break a symmetry. However, they are very close in energy, and we can see the tiny splitting between them directly on the screen, which is what remains of the classical double degeneracy at finite size. As we increase  $J_{xy}$  toward 1, this splitting grows continuously, and for any finite  $L$  it becomes a finite gap between two clearly non-degenerate states once  $J_{xy}$  is close enough to 1. What changes as we make  $L$  bigger is how close to  $J_{xy} = 1$  this crossover is. For longer chains, the two low-lying states stay nearly degenerate over a longer range of  $J_{xy}$ , and the crossover becomes sharper and approaches the exact transition of the XXZ chain in the thermodynamic limit, which the Bethe-ansatz solution places exactly at the isotropic,  $SU(2)$ -symmetric point  $J_{xy} = J_z$ . In other words, just by following how two eigenvalues of a finite-size spectrum move and split as we change a coupling constant, we can already detect a quantum phase transition, before we reach the thermodynamic limit. We will use this technique many times in the rest of the course.

#### ✕ Computational companion

Section “From classical to quantum magnetism.” Plot the low-lying spectrum of  $\mathcal{H}_{\text{XXZ}}$  as a function of  $J_{xy}$  at fixed  $L$ . Identify the near-degenerate pair at small  $J_{xy}$  and follow how it splits as  $J_{xy} \rightarrow 1$ . Then increase  $L$  and see how the crossover of the splitting becomes sharper and moves, following the exact transition of the thermodynamic limit at the isotropic point.

## 2.5 Good quantum numbers of the Heisenberg chain

### 2.5.1 Conservation of the total spin

Section 2.2 used the identity  $\mathbf{S}_1 \cdot \mathbf{S}_2 = \frac{1}{2}[\mathbf{S}_{\text{tot}}^2 - \mathbf{S}_1^2 - \mathbf{S}_2^2]$  as a shortcut for the dimer, and it is useful to ask why it worked. The reason is that  $\mathbf{S}_{\text{tot}}^2$  and  $S_{\text{tot}}^z$  commute with  $\mathcal{H}_{\text{Heis}}$ , and this is not special to two sites. Because Eq. (19) is built only from dot products  $\mathbf{S}_i \cdot \mathbf{S}_j$ , it is invariant under any global spin rotation. Noether's theorem in its operator form then tells us that the total spin  $\mathbf{S}_{\text{tot}} = \sum_i \mathbf{S}_i$  is conserved for *any*  $L$  and any choice of exchange couplings  $J_{ij}$ , which we write as

$$[\mathcal{H}_{\text{Heis}}, \mathbf{S}_{\text{tot}}^2] = 0, \quad [\mathcal{H}_{\text{Heis}}, S_{\text{tot}}^z] = 0. \quad (26)$$

So every eigenstate of  $\mathcal{H}_{\text{Heis}}$  can be labeled by a definite total spin  $S$  and a definite projection  $m$ . These are the singlet ( $S = 0$ ) and triplet ( $S = 1$ ) labels that we used for the dimer, which now become good quantum numbers for a chain of any length.

### 2.5.2 The Zeeman field does not mix states

Let us now add a uniform magnetic field,

$$\mathcal{H}(B) = \mathcal{H}_{\text{Heis}} - B S_{\text{tot}}^z. \quad (27)$$

This term singles out the  $z$ -axis, so it breaks the full  $\text{SU}(2)$  spin-rotation symmetry down to rotations about  $z$  only. However, let us look at what it does to our two conserved quantities. It commutes with  $S_{\text{tot}}^z$ , since it is built only from this operator. And because  $[\mathbf{S}_{\text{tot}}^2, S_{\text{tot}}^z] = 0$  is a general identity of the algebra of angular momentum,  $\mathcal{H}(B)$  *also* commutes with  $\mathbf{S}_{\text{tot}}^2$ . So both quantum numbers survive in the presence of the field, meaning that adding  $B$  cannot mix eigenstates of  $\mathcal{H}_{\text{Heis}}$  with each other, and it can only shift the energy of each one by  $-Bm$ . This is why the spectrum as a function of the field that you see in the notebook is a set of straight lines and not of curves. Each state with a definite  $m$  shifts linearly,  $E(B) = E(0) - Bm$ , and states only bend or avoid each other once we add a term that does not commute with  $S_{\text{tot}}^z$ , such as a transverse field.

Let us apply this to the dimer. The singlet has  $m = 0$  and stays flat,  $E_{\text{singlet}}(B) = -\frac{3}{4}J$ . The three members of the triplet split according to their own  $m = -1, 0, +1$ . The  $m = 0$  member is also flat, at  $E = \frac{1}{4}J$ , while the  $m = \pm 1$  members disperse as  $E = \frac{1}{4}J \mp B$ . These are the two flat lines that you can see in the zero-field spectrum of the notebook. They are at different energies, separated by exactly the many-body gap  $\Delta = J$  of Eq. (23), and what distinguishes them is not  $m$ , which is 0 for both, but the total spin  $S$ , which is 0 for one and 1 for the other.

### 2.5.3 Block-diagonalizing a long chain

The main use of Eq. (26) is computational. Since  $S_{\text{tot}}^z = \sum_i S_i^z$  is conserved, the full  $2^L \times 2^L$  Hamiltonian never mixes basis states with different numbers of up spins. If  $n_{\uparrow}$  counts the up spins, then  $m = n_{\uparrow} - L/2$  is fixed within each block, and  $\mathcal{H}_{\text{Heis}}$  is block-diagonal with blocks of dimension

$$\dim(m) = \binom{L}{L/2 + m}. \quad (28)$$

The largest block is at  $m = 0$  (for even  $L$ ), with  $\dim(0) = \binom{L}{L/2} \sim 2^L / \sqrt{\pi L/2}$  from Stirling's approximation. This is still exponential in  $L$ , but it is a factor  $\sim \sqrt{L}$  smaller than the full Hilbert

space, and what matters most is that it can be diagonalized independently of every other block. If the chain is also periodic, translational invariance gives us a second conserved quantity, which is the total momentum  $k$ , and combining  $S_{\text{tot}}^z$  sectors with momentum sectors makes the largest block smaller by roughly another factor of  $L$ . Using every available conserved quantity together with the sparse-matrix Lanczos techniques of Section 2.2 is how exact-diagonalization codes reach the  $L \sim 20$  spins that are the limit of this session. Without it,  $2^{20} \approx 10^6$  would already be a heavy dense-matrix computation, and  $L = 30$  would be out of reach.

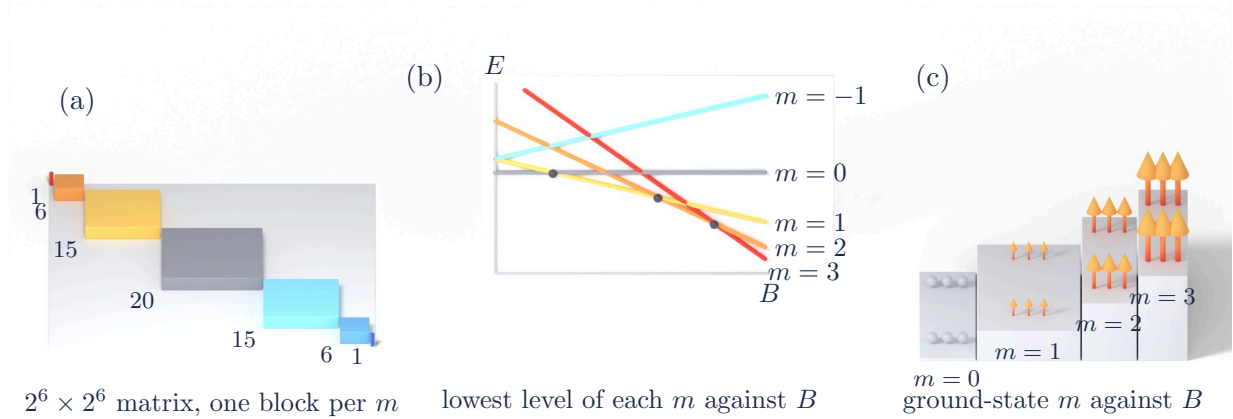


**Figure 8:** What the conservation of  $S_{\text{tot}}^z$  gives us, for the open chain of  $L = 6$ . (a) Block structure of  $\mathcal{H}_{\text{Heis}}$  in the  $S_{\text{tot}}^z$  basis, with the blocks to scale and  $m = +3$  at the back. Because  $S_{\text{tot}}^z$  is conserved, the Hamiltonian never connects basis states with different numbers of up spins, so the  $2^L \times 2^L$  matrix splits into one block per magnetization sector, of dimension  $\binom{L}{L/2+m}$  as in Eq. (28), and every element outside the blocks is zero. Each block is diagonalized independently of the others, and even the largest one, at  $m = 0$ , is already smaller than the full space by a factor  $\sim \sqrt{L}$ . (b) The lowest level of each block, in the color of its block, as a function of the field of Eq. (27). We leave out  $m = -2$  and  $m = -3$ , which rise out of the frame immediately. Every line is straight,  $E_m(B) = E_m(0) - Bm$ , and the dark beads mark where a different block takes over the bottom of the fan, at  $B \approx 0.49J$ ,  $1.39J$  and  $1.87J$ . (c) The ground-state magnetization obtained from (b), which is the staircase of Section 2.6, with the chain standing on each plateau. On the singlet plateau the spins are spheres with no moment, and on the next plateaus they are arrows whose length is the average moment  $m/L$  per site. The moment is saturated from  $B = J[1 + \cos(\pi/L)] \approx 1.87J$  on, which is the one-magnon edge of the open chain and tends to the  $2J$  of the infinite chain as  $L$  grows.

### ✕ Computational companion

Sections “Energies of a Heisenberg model as a function of the external magnetic field” and “Quantum numbers in the Heisenberg model.” Plot the dimer spectrum as a function of  $B$  and check the linear evolution without mixing that Eq. (27) predicts. Identify which line is the singlet and which is the  $m = 0$  member of the triplet, and check that they are exactly  $\Delta = J$  apart at  $B = 0$ . Then think about which field-dependent term would bend the lines instead of keeping them straight.

## 2.6 Level crossings and magnetization curves

### 2.6.1 The level crossing of the dimer

Equation (27) does more than split levels. Since different  $m$ -sectors disperse with different slopes, they can cross, and a crossing at the bottom of the spectrum is a **level crossing of the ground**

**state.** For the dimer we can find it exactly. The ground state is the singlet, at  $-\frac{3}{4}J$ , until the  $m = +1$  triplet branch  $E = \frac{1}{4}J - B$  goes below it, which happens when

$$\frac{1}{4}J - B = -\frac{3}{4}J \implies B = J. \quad (29)$$

Below  $B = J$  the ground state is the singlet, with zero magnetization, and above  $B = J$  it is the fully polarized member of the triplet  $|\uparrow\uparrow\rangle$ , with saturated magnetization  $\langle S_{\text{tot}}^z \rangle = 1$ . This is the simplest example of a quantum phase transition driven by a field, which here is a single sharp level crossing between a sector with  $S = 0$  and a sector with  $S = 1$ .

### 2.6.2 The magnetization staircase of longer chains

Longer chains show the same phenomenon, repeated many times. As  $B$  grows from zero, the ground state moves step by step through sectors of increasing total spin,  $S = 0 \rightarrow 1 \rightarrow 2 \rightarrow 3 \rightarrow \dots$ , and each step appears as a sudden jump in the ground-state magnetization  $\langle S_{\text{tot}}^z \rangle$ , which gives a magnetization staircase. Panels (b) and (c) of Figure 8 show both for  $L = 6$ , the crossings at the bottom of the fan and the staircase that they give. Because bigger chains have their low-lying  $S$ -sectors closer together in energy, these crossings happen at smaller and smaller fields as  $L$  grows, and in the thermodynamic limit the staircase becomes the continuous magnetization curve of an infinite antiferromagnetic chain. Once  $B$  is larger than roughly the bandwidth of the low-energy spectrum, which is  $B \gtrsim zJ$  with  $z$  the coordination number, the ground state saturates completely and every spin points along the field. For a chain,  $z = 2$  and the saturation field is exactly  $B_{\text{sat}} = 2J$ . This fully polarized state is in fact an *exact* eigenstate of  $\mathcal{H}_{\text{Heis}}$  itself, and it is a rare case where the many-body ground state is a simple product state, since the exchange term has nothing left to do once every spin is maximally aligned. Changing  $B \rightarrow -B$  gives the same staircase with the opposite sign of magnetization, which is the time-reversal partner of the  $B > 0$  curve.

### 2.6.3 Excited states in a small field

Let us also look at the excited states in a small field, before any level crossing has happened. The ground state stays a total- $S = 0$  singlet with zero magnetization on every site. The first excited states, which are the  $S = 1$  members of the triplet, do have a finite total magnetization, but this magnetization is not localized anywhere. Instead, it is spread over the whole chain, which is one more sign that these are delocalized many-body excitations and not a single flipped spin at one site. Higher excited states repeat this pattern with different sign structures, and several of them are related to each other by time reversal. This whole family of spread-out excitations, which look roughly like the states of a particle in a box, is what the dynamical correlator of Section 2.9 will allow us to resolve in detail.

#### ✕ Computational companion

Sections “Level crossings in the Heisenberg model,” “Many-body wavefunctions in a magnetic field,” “Level crossings as a function of the magnetic field,” and “Magnetization of moderately large Heisenberg model.” Check the crossing of the dimer at  $B = J$  from Eq. (29). Then move to chains with  $L = 6$  and  $L = 10$  and follow the full magnetization staircase, its saturation field, and its mirror symmetry under  $B \rightarrow -B$ .

## 2.7 The gapped dimerized chain

### 2.7.1 A chain with alternating bonds

Section 2.3 told us that the uniform Heisenberg chain is gapless, with  $\Delta(L) \rightarrow 0$  as a power law. Let us now build a chain that is gapped, by alternating the exchange coupling from bond to bond,

$$\mathcal{H}_{\text{dimer}} = \sum_i J_i \mathbf{S}_i \cdot \mathbf{S}_{i+1}, \quad J_i = J [1 + (-1)^i \delta], \quad (30)$$

so odd and even bonds alternate between  $J(1 + \delta)$  and  $J(1 - \delta)$ . At  $\delta = 0$  we recover the uniform, gapless chain. At the opposite limit  $\delta \rightarrow 1$ , the weak bonds vanish and the chain splits into  $L/2$  decoupled dimers, each one exactly the  $L = 2$  problem of Section 2.2. The exact ground state is then a product of singlets, one per strong bond, and the lowest excitation is a single dimer going from its singlet into its triplet, which costs exactly  $\Delta_\infty = J(1 + \delta)$ , the same singlet-triplet gap that we computed in Eq. (21). Turning the weak bond back on changes this picture, since the singlets now couple to each other and the triplet excitation gets some dispersion, but it does not close the gap. For any finite  $\delta$ , no matter how small, the dimerized chain stays gapped, with a finite  $\Delta_\infty$  that goes smoothly to zero only as  $\delta \rightarrow 0$ . Figure 9 shows the two chains side by side.

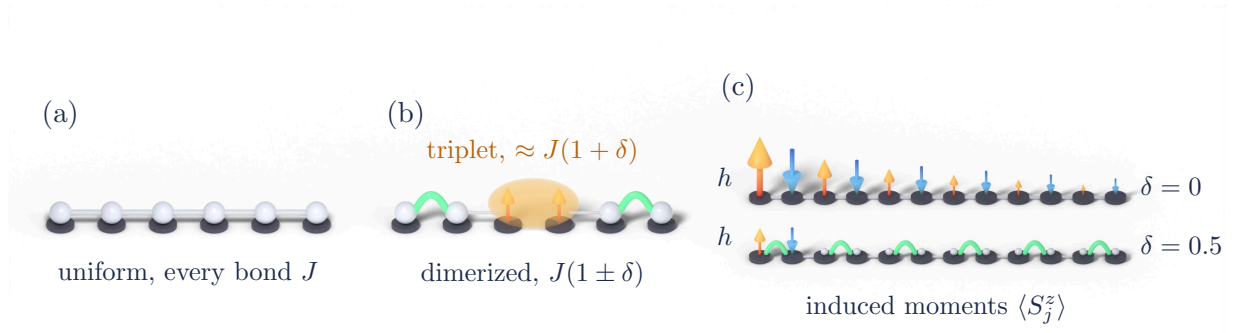


**Figure 9:** The uniform and the dimerized chain of Eq. (30). (a) At  $\delta = 0$  every bond is the same and no pair of sites is singled out. (b) At finite  $\delta$  the strong bonds, drawn as green singlets, alternate with weak ones, drawn thin. The lowest excitation is one strong bond lifted from its singlet into a triplet, here its  $m = +1$  member with both spins up, which costs about  $J(1 + \delta)$  and is what keeps the chain gapped. (c) A field  $h$  pins the first spin of a chain of  $L = 12$ , and the arrows are the induced moments  $\langle S_j^z \rangle$  of the exact ground state, to scale, for  $h = 0.2J$ . Along the uniform chain at the back they alternate in sign and decay slowly, which is the algebraic decay of Section 2.8, and since on the open chain they add up to zero, the far end compensates. Along the dimerized chain in front, with  $\delta = 0.5$  and its strong bonds drawn as singlets, the first singlet takes almost all of the response and the moment is gone by the third dimer, which is the exponential decay set by  $\xi$ . Moments below 0.02 are drawn as small spheres.

### 2.7.2 Finite-size convergence of the gap

This qualitative difference appears very clearly in how  $\Delta(L)$  approaches its value in the thermodynamic limit. For the gapless uniform chain, we already saw the slow power-law approach of Eq. (24), and even  $L \sim 20$  is not enough to be sure that the gap goes to zero. For the dimerized chain, a finite gap defines its own length scale, which is the correlation length  $\xi \sim v_s/\Delta_\infty$ , and the finite-size corrections to the gap are suppressed exponentially,  $\Delta(L) - \Delta_\infty \sim e^{-L/\xi}$ , and not as a power law. This is why, numerically, the gap of a dimerized chain already looks converged at  $L \sim 12$  to 14, while the gap of the uniform chain still changes visibly at the same size. The

presence or absence of a length scale  $\xi$  is what separates fast, exponential finite-size convergence from slow, power-law convergence.

### ✕ Computational companion

Section “Gap of a many-body spin chain.” Compute  $\Delta(L)$  for the uniform chain ( $\delta = 0$ ) and for a dimerized chain ( $\delta > 0$ ), and compare how fast each one saturates as you increase  $L$ . Check that the dimerized gap has converged well before the uniform one.

## 2.8 Diagnosing the gap with impurities and correlators

Comparing gaps at different  $L$  works, but it needs several system sizes. Is there a way to tell gapped from gapless behavior with a *single* calculation? There is, and the way we do this is by looking at how the system responds in space, instead of how its energy changes with size.

### 2.8.1 A magnetic impurity

Let us put a small local field on one site,  $\mathcal{H} \rightarrow \mathcal{H}_{\text{Heis}} - h S_{i_0}^z$ , and measure the induced magnetization profile  $\langle S_j^z \rangle$  as a function of the distance  $r = |j - i_0|$  from the impurity. For the gapless uniform chain, this response decays *algebraically*,  $\langle S_j^z \rangle \sim r^{-1}$ , which is the usual signature of critical, scale-free correlations in a one-dimensional gapless system. For the gapped dimerized chain, the same measurement decays *exponentially*,  $\langle S_j^z \rangle \sim e^{-r/\xi}$ , with the same correlation length  $\xi$  that controlled the finite-size convergence of the gap in Section 2.7. Panel (c) of Figure 9 shows both profiles for a chain of twelve sites. So the way the response to a local perturbation dies out as we move away from it already tells us, from a single system size, if the chain is gapped or gapless.

### 2.8.2 Non-local static correlators

We can get the same information without any impurity, by computing the connected two-point correlator

$$C(i, j) = \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle - \langle \mathbf{S}_i \rangle \cdot \langle \mathbf{S}_j \rangle. \quad (31)$$

In a quantum magnet  $\langle \mathbf{S}_i \rangle = 0$  everywhere, so this reduces to the bare correlator  $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ . For a classical magnet described by a product state, on the other hand,  $C(i, j)$  is exactly zero, since in a product state the expectation value factorizes. So a nonzero  $C(i, j)$  is a direct signature of entanglement beyond any mean-field description, which is the same failure of mean-field theory that we found for the Hubbard dimer in Session 1. Formally, this static correlator is related to the impurity response of the previous paragraph by linear response, through a Kubo-formula argument, meaning that the magnetization induced at  $j$  by a small field at  $i$  is, to leading order, proportional to  $C(i, j)$  itself. As a result,  $C(i, j)$  shows the same two behaviors, with power-law decay for the gapless chain and exponential decay, with a rate set by  $\delta$ , for the dimerized one. The bigger the dimerization, the bigger the gap and the faster  $C(i, j)$  decays, which gives a diagnostic from a single calculation for how gapped a quantum magnet is.

### ✕ Computational companion

Sections “Magnetization of a Heisenberg model with a magnetic impurity,” “Magnetization of a dimerized Heisenberg model with a magnetic impurity,” and “Non-local static correlators.” Compare the decay of the induced magnetization for the uniform and the dimerized chains. Then compute Eq. (31) directly for several values of the dimerization and check that a faster decay goes together with a bigger gap.

## 2.9 Dynamical correlators, and a first look at spin-1

### 2.9.1 The Lehmann representation

So far we have only used static, equal-time expectation values. A **dynamical spin correlator** contains more information, because it resolves excitations by their energy as well as by their position. We define

$$S(i, \omega) = \langle 0 | S_i^z \delta(\omega - (\mathcal{H} - E_0)) S_i^z | 0 \rangle. \quad (32)$$

This looks abstract, but it becomes clearer once we insert a resolution of the identity in the exact eigenbasis of  $\mathcal{H}$ ,  $\mathbb{1} = \sum_n |n\rangle \langle n|$ , which turns Eq. (32) into the Lehmann representation

$$S(i, \omega) = \sum_n |\langle n | S_i^z | 0 \rangle|^2 \delta(\omega - (E_n - E_0)). \quad (33)$$

We can read this as a spectroscopy experiment. If we inject a spin flip at site  $i$  with energy  $\omega$ , we get a nonzero response exactly when there is an eigenstate  $|n\rangle$  at energy  $E_n = E_0 + \omega$  that is connected to the ground state by a local spin flip, and the weight is given by the size of the overlap  $\langle n | S_i^z | 0 \rangle$ .

### 2.9.2 Discrete peaks of the uniform chain

For the spin- $\frac{1}{2}$  uniform chain,  $S(i, \omega)$  shows a sequence of discrete peaks, spread over the whole chain and separated by gaps, which is the particle-in-a-box quantization that we anticipated in Eq. (24). As  $L$  grows, these peaks move to lower  $\omega$ , following the shrinking many-body gap of Section 2.3, and more of them appear as the low-energy spectrum becomes denser.

### 2.9.3 A first look at spin-1

If we do the same calculation for a spin-1 Heisenberg chain instead of spin- $\frac{1}{2}$ , the profile of  $S(i, \omega)$  looks qualitatively different. The reason for this is that the two cases are in different phases. The spin- $\frac{1}{2}$  chain is gapless in the thermodynamic limit, as we have seen in this session, while the spin-1 chain is what is called a **topological quantum magnet**, which has a full gap in the bulk but gapless, fractionalized spin- $\frac{1}{2}$  excitations pinned to the two ends of an open chain. Half-integer and integer spin chains behave so differently because of the Lieb–Schultz–Mattis theorem, which says that a translationally invariant,  $SU(2)$ -symmetric chain with half-integer spin per site cannot have a unique, gapped ground state, while it puts no such restriction on integer spin. In our small finite-size dynamical correlators we can already see hints of this, in the form of a low-energy excitation that lives mostly at the two edges and becomes softer as  $L$  grows, well below a much larger bulk gap that roughly does not depend on the size. To resolve this fractionalization clearly, however, we need system sizes well beyond what exact diagonalization can reach, and this is the job that tensor networks will do for us in Session 4.

**x Computational companion**

Section “Dynamical correlators.” Compute  $S(i, \omega)$  for the spin- $\frac{1}{2}$  Heisenberg chain, make the system smaller and follow how the discrete peaks move. Then add a magnetic field to see how the Zeeman shifts of Section 2.5 appear directly in the peak positions of the correlator.

**2.10 Spinon mean-field theory with Abrikosov fermions****2.10.1 A single-particle picture of the excitations**

Everything we have computed so far treats the ground state and its excitations as many-body objects, without any single-particle description. However, we can ask the same question that we asked in Session 1 about the Hubbard model, which is whether there is an auxiliary single-particle Hamiltonian whose spectrum reproduces, at least qualitatively, the low-energy excitations of  $\mathcal{H}_{\text{Heis}}$ . The answer is yes, and it comes from writing the quantum spin operators themselves in terms of auxiliary fermions.

**2.10.2 The Abrikosov auxiliary fermion representation**

We introduce one fermion  $f_{i\sigma}$  per site and per spin flavor and write

$$S_i^\alpha = \frac{1}{2} \sum_{\sigma\sigma'} f_{i\sigma}^\dagger \tau_{\sigma\sigma'}^\alpha f_{i\sigma'}, \quad \alpha = x, y, z, \quad (34)$$

with  $\tau^\alpha$  the Pauli matrices, together with the local constraint  $\sum_\sigma f_{i\sigma}^\dagger f_{i\sigma} = 1$  on every site, meaning that there is exactly one auxiliary fermion per site, no more and no fewer. This constraint is an essential part of the construction, since it is what makes the representation exact and not approximate. A spinful fermion per site without the constraint has four states, which are the empty state, the singly occupied states ( $\uparrow$  or  $\downarrow$ ) and the doubly occupied state. The constraint removes the empty and the doubly occupied configurations and leaves exactly the two singly occupied states  $\{|\uparrow\rangle, |\downarrow\rangle\}$ , which is the spin- $\frac{1}{2}$  Hilbert space we started with. These auxiliary fermions are not electrons. They never hop in or out of the constrained subspace, and they only describe the same two-dimensional local Hilbert space in the language of fermions. Panel (a) of Figure 10 shows the four states of one site and the two that the constraint keeps.

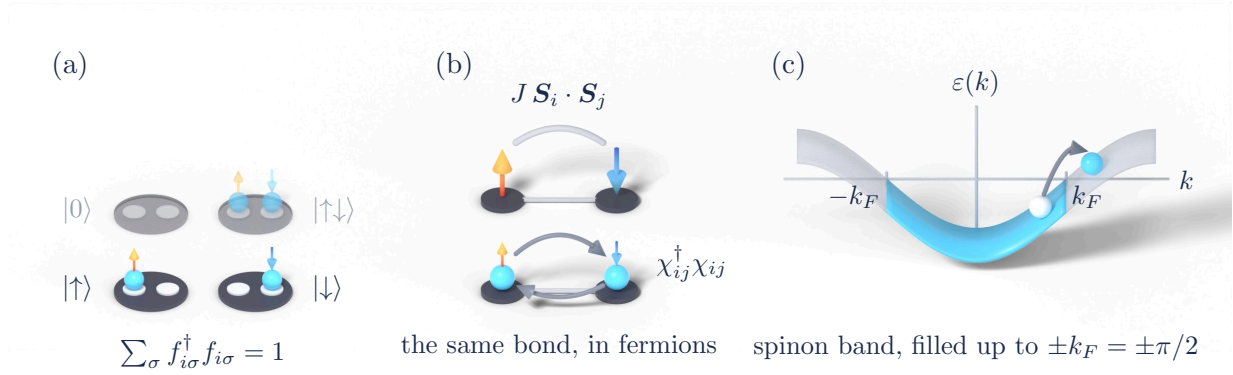


**Figure 10:** Spins as Abrikosov fermions, Eq. (34). (a) One site as two fermion slots,  $\uparrow$  on the left and  $\downarrow$  on the right, and its four states. The empty and the doubly occupied ones, drawn ghosted, are removed by the constraint, and the two that remain are exactly the spin- $\frac{1}{2}$ . (b) One bond drawn twice, with the spin exchange at the back and the same two sites in the language of fermions at the front. There Eq. (35) replaces the exchange by the bond operator, where the up fermion hops across the bond in one direction and the down fermion in the other direction, which leaves one fermion per site and the two spins flipped. (c) The spinon band  $\varepsilon(k) = -J\chi \cos k$  of the uniform chain, from Eq. (36), filled up to the Fermi points  $k_F = \pm\pi/2$ , with a particle-hole pair at the right Fermi point, made of a hole just below  $k_F$  and a spinon just above it. This is the excitation that costs arbitrarily little energy, and it gives the gapless spinons behind Eq. (24).

### 2.10.3 Mean-field decoupling of the exchange

Substituting Eq. (34) into  $\mathbf{S}_i \cdot \mathbf{S}_j$  and using the constraint on each site, one finds the identity

$$\mathbf{S}_i \cdot \mathbf{S}_j = -\frac{1}{2} \chi_{ij}^{\dagger} \chi_{ij} + \frac{1}{4} n_i n_j, \quad \chi_{ij} \equiv \sum_{\sigma} f_{i\sigma}^{\dagger} f_{j\sigma}, \quad (35)$$

where  $\chi_{ij}$  is the fermionic **bond operator**, shown in panel (b) of Figure 10. This turns the quartic spin exchange into a quartic fermion interaction, which is the kind of term that we learned to handle in Session 1, by decoupling it at the mean-field level. We introduce the self-consistent bond amplitude  $\chi_{ij} \equiv \langle \sum_{\sigma} f_{i\sigma}^{\dagger} f_{j\sigma} \rangle$  and Lagrange multipliers  $\lambda_i$  that enforce the occupancy constraint on average, and Eq. (35) becomes an effective free-fermion Hamiltonian, which is called the **spinon** Hamiltonian,

$$\mathcal{H}_{\text{MF}} = - \sum_{ij} \frac{J_{ij} \chi_{ij}}{2} \sum_{\sigma} f_{i\sigma}^{\dagger} f_{j\sigma} + \text{h.c.} + \sum_i \lambda_i (n_i - 1). \quad (36)$$

This is the same kind of self-consistency loop as in the Hubbard mean-field theory of Session 1. We guess  $\chi_{ij}$ , diagonalize the resulting single-particle Hamiltonian, compute  $\chi_{ij}$  again from the filled spinon orbitals, and repeat until convergence.

### 2.10.4 Spinon bands of the uniform and dimerized chains

The advantage is that Eq. (36) is a tight-binding model, and we already know how to read its spectrum. For the uniform chain, the self-consistent  $\chi_{ij} \equiv \chi$  is the same on every bond, which gives a simple cosine spinon band  $\varepsilon(k) = -J\chi \cos k$  with gapless Fermi points, and therefore gapless spin excitations, as shown in panel (c) of Figure 10. This agrees with everything we

found directly from exact diagonalization in Section 2.3. For the dimerized chain of Eq. (30), the bond amplitude follows the alternation of  $J_i$ , which gives a dimerized tight-binding chain for the spinons, similar to the Su-Schrieffer-Heeger model. Its spectrum opens a gap set by the difference between the hopping amplitudes of the strong and the weak bonds, in the same way as the many-body gap of Section 2.7. The same construction can be generalized to two dimensions, where a similar mean-field ansatz on, for example, the honeycomb lattice gives gapless **Dirac spinons**, which is the auxiliary-fermion language behind many candidate quantum spin liquids. We will not compute spinon bands in the notebook, but this picture is useful to keep, since it is the language in which most proposals for quantum spin liquids are written.

## Closing summary

- Exact diagonalization means writing the Heisenberg Hamiltonian as a matrix in the full  $2^L$  product-state basis and diagonalizing it directly, without any restriction to product states. The exact singlet ( $-\frac{3}{4}J$ ) and triplet ( $\frac{1}{4}J$ ) energies of the dimer are the smallest worked example of this.
- The many-body gap  $\Delta(L) = E_1 - E_0$  shrinks with system size. A power-law decay signals a gapless chain, such as the uniform Heisenberg chain with  $\Delta \sim \pi^2 J/2L$ , while saturation to a finite value, with exponentially fast finite-size convergence, signals a gapped chain, such as the dimerized chain.
- The XXZ model interpolates continuously between the classical, symmetry-broken Ising limit and the quantum, entangled Heisenberg limit. The finite-size splitting of the two lowest states already shows where the exact phase transition of the thermodynamic limit is.
- The total spin  $\mathbf{S}_{\text{tot}}^2$  and  $S_{\text{tot}}^z$  are exactly conserved quantities of the Heisenberg Hamiltonian, for any  $L$ . They block-diagonalize the exponentially large Hilbert space into much smaller sectors, they guarantee that a uniform field only splits levels linearly and does not mix them, and they are what allows exact diagonalization to reach  $L \lesssim 20$  spins.
- A sequence of level crossings driven by the field, between successive total-spin sectors, gives the magnetization staircase of a finite chain. Impurity responses and non-local static correlators decay algebraically when the chain is gapless and exponentially when it is gapped, so they diagnose from a single calculation the same physics as the gap scaling.
- Dynamical correlators resolve excitations in both space and energy through the Lehmann representation. Comparing spin- $\frac{1}{2}$  and spin-1 chains gives our first hint of the fractionalized, topological physics of the spin-1 chain, which we will study properly with tensor networks in Session 4.
- Writing spins as constrained Abrikosov fermions and decoupling the exchange term at the mean-field level gives an effective free-fermion description of the excitations in terms of spinons. The spinons are gapless for the uniform chain and gapped for the dimerized chain, and the self-consistency loop is the same as in the Hubbard mean-field theory of Session 1.
- All of this is numerically exact, but the cost is still exponential in  $L$ . Even with every symmetry that we can use, exact diagonalization stops around  $L \sim 20$  spins, and this limit is the reason why we will use the matrix-product-state methods of Session 4.

# PHYS-E0510 – Advanced Computational Methods in Physics D

## Session 3

### Exact Diagonalization in the Fermionic Basis

**Companion notebook:** `quantum_interacting_fermions.ipynb` **Prerequisites:** Session 1 (second quantization, the Hubbard model, mean-field theory) and Session 2 (exact diagonalization, though we rebuild everything we need directly in the fermionic language here)

## Contents and goals

In Session 1 we built the Hubbard model from second quantization and solved it at the mean-field level, and at the end we saw that mean-field theory can fail badly, even for the smallest example, which is the Hubbard dimer at half filling. In Session 2 we started from this failure and solved the resulting Heisenberg spin model exactly, with no restriction to product states, by diagonalizing it directly in the spin basis. In this session we go back one more step and diagonalize the *original* fermionic Hamiltonian exactly, in the fermionic Fock space, without first mapping it to spins. This is more than a change of language, because it allows us to see things that a spin model cannot describe. These are the charge physics, a real chemical potential, a real difference between an insulator and a metal, and an exact numerical test of the mean-field prediction for the magnetization in Session 1. We will find that mean-field theory gives a magnetization of the Hubbard chain that is wrong qualitatively, and not only quantitatively, and this kind of failure is the reason why we want to solve problems exactly when the cost allows it. At the end we will see how spin and charge decouple from each other as the interaction grows, which is a many-body effect called spin-charge separation. In Session 5 we will take this exact fermionic approach again and use tensor networks to reach much larger system sizes.

## Learning outcomes

By the end of this session, you should be able to do the following.

- Diagonalize interacting fermionic Hamiltonians directly in Fock space and explain how the Hilbert-space dimension scales with system size and spin.
- Use the ground-state degeneracy, a sweep of the chemical potential and the charging energy to identify a charge-density-wave transition and to control the particle number of the ground state.
- Test the mean-field prediction for the magnetization of Session 1 against the exact Hubbard result and explain the disagreement with Lieb's theorem.
- Identify spin-charge separation from static and dynamical correlators, and connect the strong-coupling limit to the Heisenberg model of Session 2.

## 3.1 The many-body Fock space of fermions

### 3.1.1 Counting the many-body states

Let us start by building again the many-body tools that we used for spins in Session 2, but now directly with fermionic creation and annihilation operators. Remember from Session 1 that a

single-particle Hamiltonian on  $L$  orbitals is an  $L \times L$  matrix, and diagonalizing it has a polynomial cost. As soon as we add any quartic term, which is an interaction term, this is no longer true. We then have to diagonalize  $\mathcal{H}$  in the full many-body Fock space, which is spanned by all the ways to distribute the electrons among the  $L$  orbitals, and this space grows exponentially with  $L$ .

Let us count this explicitly, starting from the smallest case. We take two spinless sites, labeled 0 and 1. The many-body basis has exactly four states,

$$|\Omega\rangle, \quad c_0^\dagger |\Omega\rangle, \quad c_1^\dagger |\Omega\rangle, \quad c_0^\dagger c_1^\dagger |\Omega\rangle, \quad (37)$$

which are the empty state, the two singly-occupied states and the doubly-occupied state, so  $\mathcal{H}$  is a  $4 \times 4$  matrix in this basis. If we add a third site, the counting becomes  $1 + 3 + 3 + 1 = 8$  states, with one empty configuration, three with one electron, three with two electrons and one fully filled, which is  $2^3$ . In general, for  $L$  spinless orbitals the Fock space has dimension  $2^L$ . Every orbital is either empty or filled, independently of the others, so we have one binary choice per orbital. Let us compare this with the single-particle sector alone, which is spanned by  $c_i^\dagger |\Omega\rangle$  for  $i = 1, \dots, L$  and only has dimension  $L$ . Restricting to one electron is what gives single-particle physics a polynomial cost, and removing this restriction is what gives many-body physics an exponential cost. Panel (b) of Figure 11 shows the eight states of three orbitals.

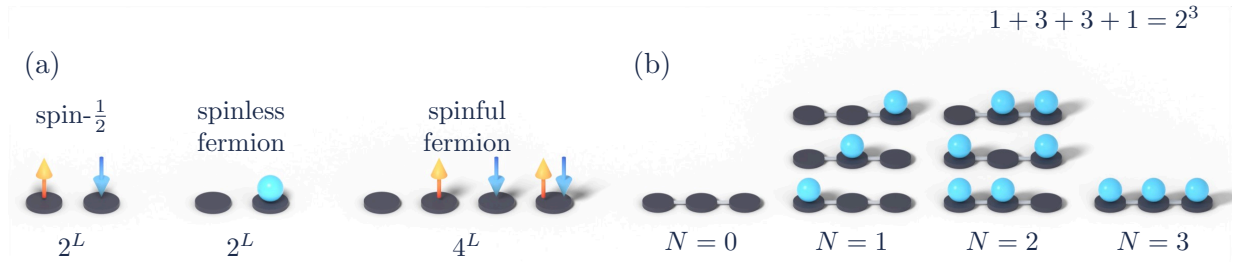


**Figure 11:** The local Hilbert spaces and the many-body basis built from them. (a) The states of a single site. There are two for a spin- $\frac{1}{2}$ , up and down, two for a spinless fermion, empty and occupied, and four for a spinful fermion, empty, up, down and doubly occupied, so a chain of  $L$  sites has  $2^L$ ,  $2^L$  and  $4^L$  many-body states. (b) The complete many-body basis of three spinless orbitals, with a ball on every occupied orbital and the states grouped by their particle number  $N$ . Across the panel there is one empty configuration, three with a single electron, three with two electrons and one completely filled state, so in total there are  $1 + 3 + 3 + 1 = 8 = 2^3$  basis states. Every additional orbital doubles this number, because each orbital is either empty or filled independently of the others, and this doubling is the exponential growth that separates many-body from single-particle physics.

### 3.1.2 Spinful fermions and the cost of the calculation

If the fermions have spin, each site has *four* local states,  $|0\rangle$ ,  $|\uparrow\rangle$ ,  $|\downarrow\rangle$  and  $|\uparrow\downarrow\rangle$ , as in Session 1. We can also think of a spinful chain as  $2L$  spinless orbitals, where the spin is just one more orbital index, so the Fock space has dimension  $2^{2L} = 4^L$ . The exponent is twice the one of the spinless case, since every site now has two binary choices instead of one, and panel (a) of Figure 11 shows this next to the spin and the spinless fermion. Note that this is the same counting as for the spin chains of Session 2, since a spin- $\frac{1}{2}$  chain with  $L$  sites also has a Hilbert space of dimension  $2^L$ , the same as for spinless fermions. The reason for this is that there is an exact mapping between spinless fermions and spin- $\frac{1}{2}$  degrees of freedom, site by site, which is called the Jordan-Wigner

transformation, and we will see it in detail in Session 5. In practice, this means two things for the cost of our calculations.

- Solving an interacting **spinless** fermionic chain costs the same as solving a quantum **spin** chain of the same length,  $\sim 2^L$ .
- Solving an interacting **spinful** fermionic chain, such as the Hubbard model, costs the square of that,  $\sim 4^L$ , so with the same computer we can only reach about half the system size.

### 3.1.3 Exact diagonalization in the Fock basis

As in Session 2, once we have  $\mathcal{H}$  written as an explicit  $2^L \times 2^L$  matrix in this Fock basis, or as a  $4^L \times 4^L$  matrix, the ground state is its lowest eigenvector. This is a set of  $2^L$  complex coefficients, or  $4^L$  of them, one for each basis configuration. Any expectation value we want, such as  $\langle n_i \rangle$ ,  $\langle S_i^z \rangle$ , correlators or spectra, is then obtained with ordinary linear algebra on this eigenvector. There is no approximation and no restriction to product states, which is what exact diagonalization gives us, and now we do it directly in the fermionic language.

#### ✕ Computational companion

Sections “Creating a fermion\_chain object,” “Creating a Hamiltonian,” “Computing the ground state energy,” and “Computing expectation values.” Build a small fermionic chain object, write a many-body Hamiltonian directly with the fermionic operators, and compute its ground state energy and a few expectation values. This is the fermionic version of what you did with spin operators in Session 2, so compare the two interfaces side by side.

## 3.2 The exact charge-density-wave transition of spinless fermions

### 3.2.1 The spinless chain with nearest-neighbor interaction

Let us now use these tools for the simplest interacting model we have, which is the spinless nearest-neighbor chain from Session 1,

$$\mathcal{H}_{\text{CDW}} = -t \sum_i \left( c_i^\dagger c_{i+1} + \text{h.c.} \right) + V \sum_i \left( n_i - \frac{1}{2} \right) \left( n_{i+1} - \frac{1}{2} \right), \quad n_i \equiv c_i^\dagger c_i. \quad (38)$$

This is the  $\mathcal{H}_{\text{CDW}}$  of Session 1, with  $n_i \rightarrow n_i - \frac{1}{2}$  inside the interaction, which is only a shift for bookkeeping. If we expand it, it adds a constant and, automatically, a chemical potential of  $-V/2$  per site. This chemical potential is chosen so that the model is exactly at half filling, without the need to add and tune a separate  $\mu$  by hand.

### 3.2.2 Two solvable limits

Two limits of Eq. (38) are easy to solve directly. At  $V = 0$  we have the free tight-binding chain of Session 1, which has a single cosine band filled up to the Fermi points, so it is a metal with a unique, non-degenerate ground state. At  $V \rightarrow \infty$  we can neglect the hopping, and the interaction alone is minimized by the classical alternating pattern  $1, 0, 1, 0, \dots$ , with one electron on every other site. There are exactly *two* such states, related by a shift of the pattern by one site, and they are degenerate. This is the charge-density wave, and its defining property is that the ground state is twofold degenerate, in contrast with the unique metallic ground state at  $V = 0$ . Figure 12 shows the two limits next to each other.

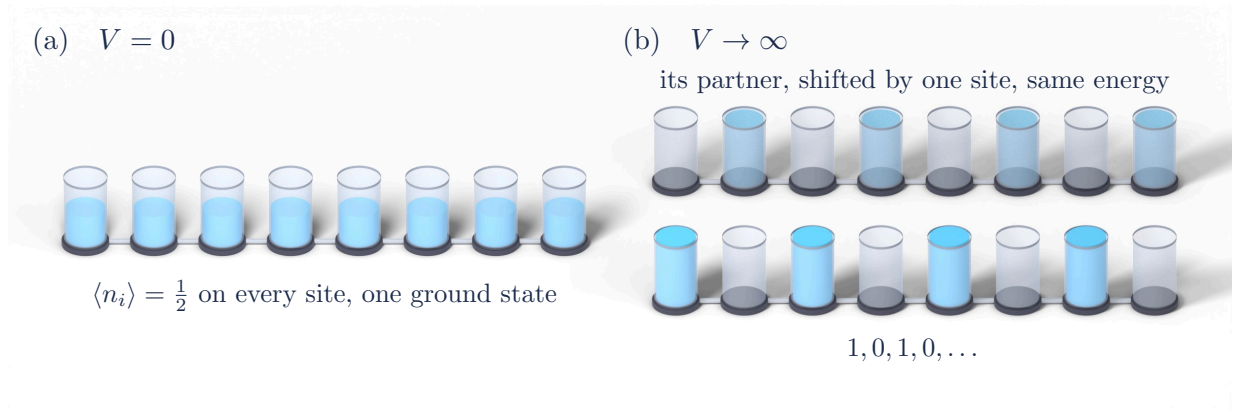


**Figure 12:** The two solvable limits of Eq. (38), where the occupation of every site is drawn as the filling of a cup. (a) At  $V = 0$  the chain is a free tight-binding metal at half filling, with the same average density  $\frac{1}{2}$  on every site and a unique ground state. (b) As  $V \rightarrow \infty$  the hopping becomes irrelevant and the interaction alone selects the alternating  $1, 0, 1, 0, \dots$  pattern, drawn in front. If we shift this pattern by one site we obtain a second state with the same energy, drawn behind it as a ghost, and this twofold degeneracy is the defining property of the charge-density wave.

### 3.2.3 The exact many-body spectrum

Exact diagonalization allows us to see this on a finite chain. We diagonalize Eq. (38) at fixed  $L$  and plot the low-lying eigenvalues, measured from the ground state, as a function of  $V$ . At small  $V$  we see a unique ground state and then a small gap to a dense set of excited states. This gap is a finite-size effect, roughly the level spacing  $\sim t/L$  of the free-fermion band, and it becomes smaller as we go from  $L = 12$  to  $L = 14$ , as we expect if it closes in the thermodynamic limit and leaves a continuum. As  $V$  grows, one excited state separates from this continuum and goes down toward the ground state, until it becomes exactly degenerate with it as  $V \rightarrow \infty$ . This is the CDW partner state. Unlike the metallic gap, this near-degeneracy does *not* close by adding more excited states below it. Instead, a large gap opens above the ground state, which is now twofold degenerate, and this gap grows asymptotically as  $\Delta \sim V$ . This linear growth has a simple interpretation. At large  $V$ , the cheapest way to excite the system is to introduce a single domain wall into the alternating pattern, which is a local defect where the two patterns of the charge order meet. Each domain wall costs an energy of order  $V$  independently of the size of the system, and this is the finite gap, independent of the size of the system, that we see in the numerics.

### 3.2.4 Comparison with mean-field theory

Let us compare this with the mean-field treatment of the same model in Session 1. There, the self-consistent gap also opened continuously as  $V$  increased and also grew linearly at large  $V$ , and here exact diagonalization confirms both features quantitatively. The reason for this is that the CDW breaks a *discrete* symmetry, which is the translation by one site, a  $\mathbb{Z}_2$  symmetry, and the breaking of a discrete symmetry of this kind is allowed even in a one-dimensional quantum system at zero temperature. We should keep this in mind, because in Section 3.4 we will see a case where mean-field theory tries to break a *continuous* symmetry, and there the result is completely different.

### ✕ Computational companion

Sections “Many-body energies of an interacting fermionic model” and “Towards interaction-induced symmetry breaking.” Plot the low-lying many-body spectrum of the spinless chain as a function of  $V$  for two system sizes, and identify by eye where the first excited state becomes degenerate with the ground state, which is the CDW transition. Then look at how the large- $V$  gap scales with  $V$  and check the linear behavior we derived above.

## 3.3 Chemical potential, conserved quantum numbers, and the charging energy

### 3.3.1 Conservation of the particle number

So far we have kept the electron number fixed at half filling. Let us now add a chemical potential explicitly,

$$\mathcal{H}(\mu) = \mathcal{H}_{\text{CDW}} - \mu \sum_i n_i \equiv \mathcal{H}_{\text{CDW}} - \mu N, \quad (39)$$

where  $N = \sum_i n_i$  is the operator of the total particle number. The important structural property here is that  $[\mathcal{H}_{\text{CDW}}, N] = 0$ . The hopping moves an electron from one site to another without changing the total number, and the interaction only counts electrons, so it also commutes with  $N$ . Since  $\mathcal{H}_{\text{CDW}}$  and  $N$  commute, they have a common eigenbasis, which means that adding the  $-\mu N$  term does not change any eigenvector of  $\mathcal{H}_{\text{CDW}}$ . It only shifts each eigenenergy by  $-\mu N$ , where  $N$  is the fixed particle number of that eigenstate. As a result, every eigenvalue of  $\mathcal{H}(\mu)$  is a straight line as a function of  $\mu$ , with slope  $-N$  given only by the particle number of that state relative to the one of the ground state.

This has a direct and useful consequence. Different excited states have different particle numbers, so they have different slopes, and as we sweep  $\mu$  these lines cross. At a crossing, the *ground state* itself changes, meaning that below the crossing the lowest-energy state has  $N$  electrons and above it the lowest-energy state has  $N \pm 1$ . In other words,  $\mu$  is a parameter that directly controls the electron number of the ground state, in the same way as a gate voltage does in a real quantum dot or nanostructure.

### 3.3.2 The charging energy

Let us make this quantitative. We define  $E(N)$  as the lowest eigenvalue of  $\mathcal{H}_{\text{CDW}}$  restricted to the  $N$ -particle sector. The state with  $N$  particles is the ground state of  $\mathcal{H}(\mu)$  when  $E(N) - \mu N$  is lower than  $E(N \pm 1) - \mu(N \pm 1)$ , and this condition can be written as a window,

$$E(N) - E(N - 1) < \mu < E(N + 1) - E(N). \quad (40)$$

The width of this stability window is the **charging energy**,

$$U_c(N) \equiv [E(N + 1) - E(N)] - [E(N) - E(N - 1)], \quad (41)$$

which is the discrete second derivative of the ground-state energy with respect to the particle number. It measures how much harder it is to add one more electron than it was to add the previous one, and it is the quantity that gives the flat plateaus that you see when you plot the ground-state occupation  $\langle N \rangle$  against  $\mu$ . On a plateau,  $\mu$  can change without changing  $N$ , because

it has not yet reached the addition energy in Eq. (40). As  $V$  grows, the interaction makes it more expensive to put more charge on sites that are already crowded, so  $U_c$  grows and the plateaus in the  $\langle N \rangle$ -versus- $\mu$  curve become wider, which is what the notebook shows when you compare a weakly and a strongly interacting chain. Figure 13 shows the staircase for a ring of eight sites.

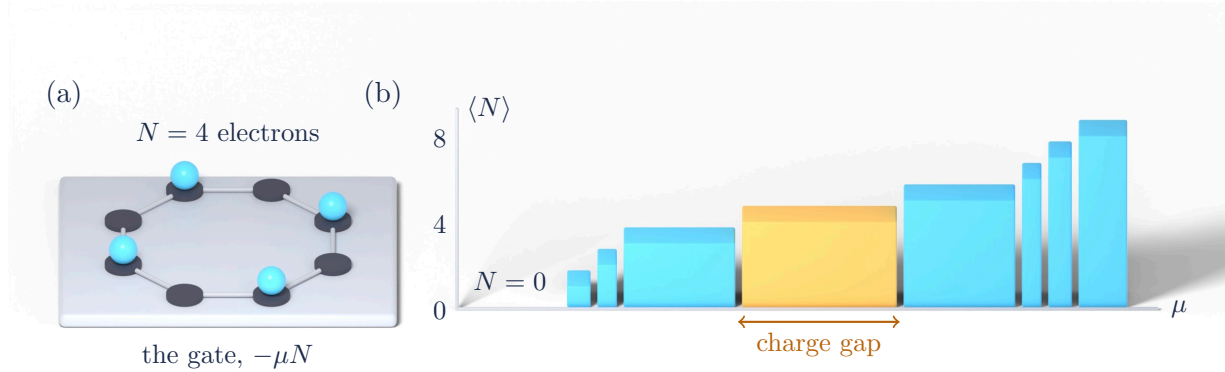


**Figure 13:** The chemical potential as a gate on the electron number. (a) A ring of eight sites on a gate, which is the term  $-\mu N$  of Eq. (39), here with  $N = 4$  electrons, which is half filling. (b) The particle number of the ground state against  $\mu$  for the ring at  $V = 4t$ , computed exactly from Eq. (38). We use a ring because the ends of an open chain blur the plateaus. Every block except the last one, which continues to arbitrarily large  $\mu$ , is a plateau, meaning the window of Eq. (40) in which  $N$  does not change, and its width is the charging energy of Eq. (41). The widest plateau is at half filling, with about  $3.8t$  against less than  $3t$  for its neighbors, and this width is the charge gap of the charge-density wave.

#### ✕ Computational companion

Sections “Energies of an interacting fermionic model as a function of the chemical potential,” “Quantum numbers in the interacting fermionic model,” “Level crossings in the interacting fermionic model,” and “Electronic density as a function of the chemical potential.” Track the particle number of each many-body eigenstate as  $\mu$  is swept, see how the ground state changes its particle number at the level crossings, and confirm that the width of each occupation plateau grows with the interaction strength, as the charging energy of Eq. (41) says.

### 3.4 The exact magnetization of the Hubbard chain

#### 3.4.1 The magnetization of the exact ground state

Now let us include spin again and repeat this exercise for the Hubbard chain,

$$\mathcal{H}_{\text{Hub}} = -t \sum_{i,\sigma} \left( c_{i\sigma}^\dagger c_{i+1\sigma} + \text{h.c.} \right) + U \sum_i \left( n_{i\uparrow} - \frac{1}{2} \right) \left( n_{i\downarrow} - \frac{1}{2} \right), \quad (42)$$

which, as in Eq. (38), differs from the Hubbard Hamiltonian of Session 1 only by the same shift for bookkeeping, which is an automatic chemical potential that keeps us at half filling.

We now meet a problem. If we diagonalize  $\mathcal{H}_{\text{Hub}}$  exactly and compute the local magnetization  $m_i \equiv \langle n_{i\uparrow} \rangle - \langle n_{i\downarrow} \rangle$  site by site, we find  $m_i = 0$  *identically*, on every site and for every  $U$ , independently of how strong the interaction is. This is in direct contradiction with the mean-field theory of Session 1. There, for any  $U > 0$  on a bipartite half-filled chain, the self-consistency

loop converges to a finite staggered moment,  $m_i = (-1)^i m$ , with  $m$  growing toward saturation as  $U \rightarrow \infty$ . Exact diagonalization and mean-field theory do not only differ quantitatively here, since they disagree about whether the ground state is magnetic at all. Figure 14 shows the two answers next to each other, and it also shows where the antiferromagnetism is in the exact answer, which is in the correlations.

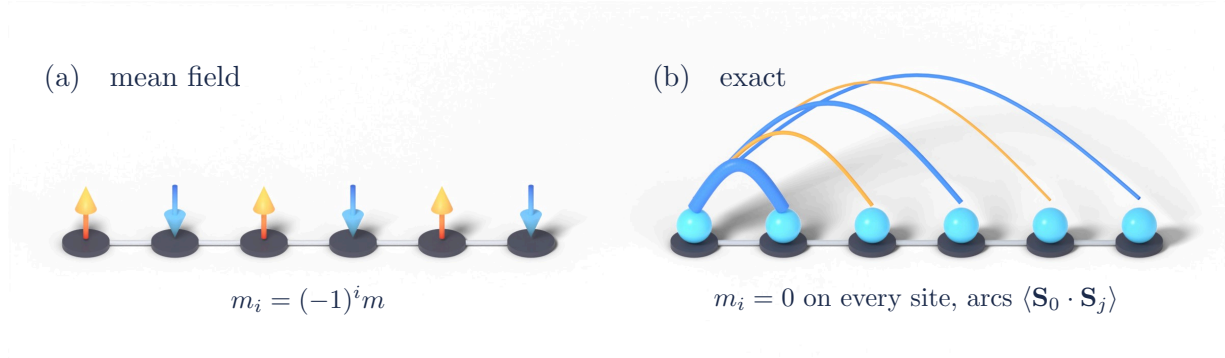


**Figure 14:** Two answers for the half-filled Hubbard chain of Eq. (42). (a) Mean-field theory finds a finite staggered moment  $m_i = (-1)^i m$ , with an arrow on every site. (b) The exact ground state of a chain of six sites at  $U = 4t$  has no moment on any site, so every electron is drawn without an arrow. The antiferromagnetism is instead in the correlation  $\langle \mathbf{S}_0 \cdot \mathbf{S}_j \rangle$  between the first site and site  $j$ , drawn as an arc whose thickness is its size, blue where it is negative and orange where it is positive, so every arc has the color of the arrow that panel (a) puts on site  $j$ . The sign alternates with distance,  $-0.54$  for the neighbor and  $+0.12, -0.17, +0.06, -0.11$  further away, which is the staggered pattern of panel (a), now carried by correlations rather than by moments.

### 3.4.2 Lieb's theorem

The reason for this is an exact symmetry argument. The Hamiltonian Eq. (42) is invariant under any global spin rotation, so it commutes with the total spin operators,  $[\mathcal{H}_{\text{Hub}}, \mathbf{S}^2] = [\mathcal{H}_{\text{Hub}}, S_z^{\text{tot}}] = 0$ , and its eigenstates can be labeled by a definite total spin  $S$ . For the repulsive Hubbard model on any bipartite lattice at half filling there is an exact result that fixes this completely, which is called **Lieb's theorem**. It says that the ground state is unique and has total spin  $S = \frac{1}{2}|N_A - N_B|$ , where  $N_A, N_B$  are the sizes of the two sublattices. On our chain the two sublattices have the same size, so  $S = 0$  exactly, which is a spin singlet, for every  $U$  and every chain length. A unique state with total spin zero that is invariant under rotations cannot have a nonzero expectation value of  $S_i^z$  on any single site. The reason is that a spin rotation would map it to another valid ground state with the opposite sign of  $m_i$ , and the uniqueness of the ground state does not allow two different ground states. Mean-field theory, by construction, only searches among single Slater determinants, and a Slater determinant with staggered spin breaks spin-rotation symmetry *explicitly* from the first guess. So it can never describe a rotationally invariant, entangled singlet, which is the same structural failure that we saw for the Hubbard dimer in Session 1.

### 3.4.3 Turning on an explicit symmetry-breaking field

We can see this failure directly if we interpolate between the exact model and the mean-field ansatz. We add an explicit staggered field,

$$\mathcal{H}(h) = \mathcal{H}_{\text{Hub}} + h \sum_i (-1)^i (n_{i\uparrow} - n_{i\downarrow}), \quad (43)$$

which is the single-particle term that mean-field theory would have generated if it had found a self-consistent staggered solution, as in the  $\mathcal{H}_{\text{MF}}$  of Session 1. At  $h = 0$  we recover the exact result,  $m = 0$ . As  $h$  increases from zero,  $m(h)$  grows *continuously* and does not jump to a finite value. The quantum fluctuations, which are contained in the entangled singlet ground state, act against the ordering field, and only when  $h$  is large enough to overcome these fluctuations does  $m(h)$  approach the mean-field saturation value. This is the standard test for spontaneous symmetry breaking. The true order parameter is defined as  $m \equiv \lim_{h \rightarrow 0^+} \lim_{L \rightarrow \infty} m(h, L)$ , and the order of the two limits is very important. At any finite  $L$ , symmetry forces  $m(h=0, L) = 0$  exactly, so we must take  $L \rightarrow \infty$  *first*. Even after doing that, this limit still gives zero for the one-dimensional Heisenberg antiferromagnet, which is the model that this one reduces to at large  $U$ , as we will see in Section 3.5. One-dimensional quantum antiferromagnets do not have true long-range magnetic order, only quasi-long-range order with power-law spin correlations, and this is the same gapless behavior that we will see again in Section 3.6. This is the reason why mean-field theory fails so badly here. It does not only miss quantitative corrections, because it predicts an ordered phase that does not exist in one dimension.

#### 3.4.4 Comparison of the charge-density wave and the Hubbard magnetism

|                       | CDW (Section 3.2)                                                | Hubbard magnetism (this section)                                                   |
|-----------------------|------------------------------------------------------------------|------------------------------------------------------------------------------------|
| Symmetry broken       | discrete, $\mathbb{Z}_2$ , translation by one site               | continuous, $\text{SU}(2)$ , spin rotation                                         |
| Mean-field prediction | finite $\delta n$ , growing continuously with $V$                | finite staggered $m$ , growing continuously with $U$                               |
| Exact 1D result       | agrees qualitatively, with the onset of order and a gap $\sim V$ | disagrees, since $m = 0$ identically and the ground state is a unique spin singlet |

**Table 2:** The two symmetry-breaking scenarios we have seen so far. For each one we list which symmetry is broken, what mean-field theory predicts, and whether the exact one-dimensional result agrees.

Table 2 compares the two symmetry-breaking scenarios that we have seen so far. Mean-field theory gives the right qualitative result for the discrete CDW transition, but a very wrong result for the continuous Hubbard magnetization.

#### ✕ Computational companion

Sections “Magnetization of an interacting Hubbard model” and “Magnetization of a Hubbard model with staggered magnetization.” First confirm  $m_i = 0$  at every site of the exact Hubbard ground state, however large  $U$  is. Then switch on the staggered field of Eq. (43), see how  $m$  grows smoothly from zero, and check how the field strength needed to saturate  $m$  changes as you increase  $U$ .

### 3.5 The Heisenberg model from the exact Hubbard dimer

#### 3.5.1 The singlet-triplet gap of the Hubbard dimer

Let us now verify with exact diagonalization the superexchange result  $J \sim t^2/U$  that we derived in Session 1 with degenerate perturbation theory. We take the Hubbard dimer,  $L = 2$ , at half

filling, and work in the sector with zero total  $S_z$ , which is spanned by the four states

$$|1\rangle = c_{0\uparrow}^\dagger c_{1\downarrow}^\dagger |\Omega\rangle, \quad |2\rangle = c_{0\downarrow}^\dagger c_{1\uparrow}^\dagger |\Omega\rangle, \quad |3\rangle = c_{0\uparrow}^\dagger c_{0\downarrow}^\dagger |\Omega\rangle, \quad |4\rangle = c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger |\Omega\rangle, \quad (44)$$

which are the same singly- and doubly-occupied configurations as in Session 1. The hopping connects a singly occupied state to a doubly occupied one, but never  $|1\rangle$  directly to  $|2\rangle$  or  $|3\rangle$  directly to  $|4\rangle$ . With the shift in Eq. (42), the singly-occupied states are at  $-U/2$  and the doubly-occupied ones at  $+U/2$ . So if we add the constant  $U/2$  to all of them, in this basis  $\mathcal{H}_{\text{Hub}}$  becomes

$$\mathcal{H}_{\text{Hub}} \longrightarrow \begin{pmatrix} 0 & 0 & -t & t \\ 0 & 0 & t & -t \\ -t & t & U & 0 \\ t & -t & 0 & U \end{pmatrix} \quad \text{in the basis } \{|1\rangle, |2\rangle, |3\rangle, |4\rangle\}. \quad (45)$$

This block can be diagonalized easily if we use symmetric and antisymmetric combinations, which are  $|a\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle)$ , the  $S_z = 0$  member of the triplet,  $|b\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle)$ , the singlet, and in the same way  $|c\rangle = \frac{1}{\sqrt{2}}(|3\rangle + |4\rangle)$  and  $|d\rangle = \frac{1}{\sqrt{2}}(|3\rangle - |4\rangle)$  for the doubly-occupied states. A short calculation shows that  $|a\rangle$  and  $|c\rangle$  are already exact eigenstates,

$$\mathcal{H}_{\text{Hub}} |a\rangle = 0 \cdot |a\rangle, \quad \mathcal{H}_{\text{Hub}} |c\rangle = U |c\rangle, \quad (46)$$

while  $|b\rangle$  and  $|d\rangle$  mix into a  $2 \times 2$  block,

$$\mathcal{H}_{\text{Hub}}|_{\{b,d\}} = \begin{pmatrix} 0 & -2t \\ -2t & U \end{pmatrix} \implies E_{\pm} = \frac{U \pm \sqrt{U^2 + 16t^2}}{2}. \quad (47)$$

The lower eigenvalue,  $E_-$ , is the exact ground state. We compare it with the  $S_z = \pm 1$  states  $|\uparrow\uparrow\rangle$  and  $|\downarrow\downarrow\rangle$ , which are exactly degenerate and both have energy 0, like  $|a\rangle$ , because Pauli exclusion blocks all hopping for parallel spins. We then see that the full ground state is the total spin singlet ( $S = 0$ ), strictly below the  $S = 1$  triplet at energy 0, as Lieb's theorem guaranteed in Section 3.4. The exact singlet-triplet gap is therefore

$$\Delta_{s-t} = 0 - E_- = \frac{\sqrt{U^2 + 16t^2} - U}{2} \xrightarrow{U \gg t} \frac{4t^2}{U}, \quad (48)$$

which reproduces, with a completely independent and exact calculation, not only the  $t^2/U$  scaling but also the same numerical prefactor that Session 1 obtained with perturbation theory for the effective coupling  $J = 4t^2/U$  of  $\mathcal{H}_{\text{eff}} = J \mathbf{S}_1 \cdot \mathbf{S}_2$ . If we expand Eq. (48) to leading order in  $t/U$  we obtain  $\Delta_{s-t} \rightarrow 4t^2/U$ , with exactly the same prefactor. This is a useful check, since two completely different techniques, one perturbative and with spins only, and one exact and fermionic, give the same physics and not only the same scaling.

### 3.5.2 Excitations as magnons

We can study the excited states further, as in Session 2, by adding a Zeeman field  $-\hbar S_z^{\text{tot}}$ . Since  $[\mathcal{H}_{\text{Hub}}, S_z^{\text{tot}}] = 0$ , this again leaves every eigenvector unchanged and only shifts the eigenenergies linearly in  $\hbar$ , by an amount given by the  $S_z^{\text{tot}}$  of each state. The three states that we called the triplet split linearly into  $S_z^{\text{tot}} = -1, 0, +1$  branches, while the singlet ground state, which has  $S_z^{\text{tot}} = 0$ , does not move at all. This is the same field dependence as for the Heisenberg dimer of Session 2, and the physical interpretation is also the same. The lowest excitations above a singlet

ground state are spin-1 objects, which are called magnons, and their Zeeman splitting is a direct and numerically exact signature of the spin physics inside the fermionic Hubbard model. The same mapping works, qualitatively, for longer chains, since the exact fermionic spectrum at large  $U/t$  reproduces the exact spin spectrum of a Heisenberg chain with  $J_{ij} \sim t_{ij}^2/U$ , and this is what it means to say that the two models are equivalent at strong coupling.

#### ✕ Computational companion

Section “Connection between the Hubbard and Heisenberg models.” Diagonalize the Hubbard model for increasing  $U/t$  and compare its low-energy many-body spectrum directly with the Heisenberg spectrum from the notebook of Session 2. Check that the states that map onto each other converge as  $U$  grows, and see how fast the mapping fails as you decrease  $U$  back toward  $t$ .

## 3.6 Spin-charge separation

We now have all the elements to understand one of the main features of the one-dimensional Hubbard model, which is that at strong coupling its charge and spin degrees of freedom behave in completely different ways.

### 3.6.1 The many-body gap is not one thing

Equation (48) already showed that the singlet-triplet gap of the dimer decreases like  $1/U$  at large  $U$ . If we follow the same gap as a function of the chain length  $L$ , this trend remains and becomes even stronger. At  $U = 0$  the gap is a purely single-particle level spacing that comes from the finite size, and it closes as a clean power law,  $\Delta \sim 1/L$ . Turning on  $U$  makes the gap *smaller* at fixed  $L$ , and increasing  $U$  further makes it even smaller. At first this looks wrong, since we expect the Hubbard model to become more insulating as  $U$  grows, not less gapped. The answer is that this gap is the **spin gap**, which is the energy needed to change the total spin from  $S = 0$  to  $S = 1$ , and in Section 3.5 we saw that it is given by  $J \sim t^2/U$ , which indeed decreases with  $U$ . In the thermodynamic limit this spin gap vanishes, because the Heisenberg chain that the Hubbard model maps to at strong coupling is itself gapless. All this does not tell us anything yet about the **charge gap**, the energy needed to add or remove an electron, which is a completely different quantity that we have to compute separately.

### 3.6.2 Nonlocal correlators of a metal and an insulator

A simple way to distinguish a metal from an insulator, using only the ground state, is to look at how a static correlator decays with distance. We define the nonlocal particle correlator and the nonlocal spin correlator,

$$C_c(i, j) \equiv \langle c_{i\sigma}^\dagger c_{j\sigma} \rangle, \quad C_s(i, j) \equiv \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle, \quad (49)$$

both computed in the many-body ground state. Physically,  $C_s(i, j)$  measures how strongly the spin at site  $i$  is correlated with the spin at site  $j$ . Even at strong coupling, where the model reduces to the gapless Heisenberg chain,  $C_s(r)$  decays as a power law and not exponentially, because the spin sector has no gap that suppresses the propagation over long distances. What grows with  $U$  is the *amplitude* of this correlator, not its decay rate. At  $U = 0$  the spin of each site is only weakly correlated with its neighbors, since itinerant electrons barely feel the spin of

the other electrons. At large  $U$  every site has a singly-occupied local moment that is better and better formed and strongly antiferromagnetically correlated with its neighbors, so the correlations approach the ones of the ideal Heisenberg chain.

$C_c(i, j)$ , on the other hand, measures the amplitude to add an electron at site  $i$  and later find it at site  $j$ . In a metal this decays only as a power law,  $C_c(r) \sim \sin(k_F r)/r$ , because the gapless charge excitations allow the particle to propagate arbitrarily far at almost no energy cost. In an insulator, instead, any propagation needs a virtual excitation with an energy of the order of the charge gap  $\Delta_c$ , and the correlator decays exponentially,  $C_c(r) \sim e^{-r/\xi_c}$ , with a correlation length  $\xi_c$  set by  $\Delta_c$ , roughly  $\xi_c \sim v/\Delta_c$  for some characteristic velocity  $v$ . This is the behavior we see in the Hubbard chain. At  $U = 0$ ,  $C_c(r)$  decays slowly, as a power law, while at large  $U$ , say  $U = 10t$ , it goes to zero within a few sites, which is a clear exponential decay. This shows that the charge sector is gapped and insulating, in agreement with the linearly growing charge scale that we will see again below. So the interactions act in opposite directions on the two channels. They strongly suppress the charge fluctuations while they make the spin correlations stronger, even though the energy scale  $J \sim t^2/U$  of these spin fluctuations becomes smaller.

#### ✕ Computational companion

Sections “Gap of an interacting Hubbard model,” “Non-local static correlators for the spin response,” and “Non-local static correlators for the particle-particle response.” Plot the singlet-triplet gap against  $L$  for a few values of  $U$  and confirm the  $1/U$  trend derived above. Then plot  $C_c(1, j)$  and  $C_s(1, j)$  against  $j$  for weak and strong  $U$ , and check which one changes from power-law to exponential decay as  $U$  grows. This is your direct numerical evidence for a charge gap together with a gapless spin sector.

### 3.6.3 Dynamical correlators and the two energy scales

Static correlators tell us about decay lengths, and dynamical correlators tell us about the excitation energies, which makes them the many-body generalization of the single-particle density of states of Session 1. We define the dynamical particle and spin correlators with their Lehmann representations, which are spectral representations,

$$S_c(\omega) = \sum_n \left| \langle n | c_{i\sigma}^\dagger | 0 \rangle \right|^2 \delta(\omega - (E_n - E_0)), \quad S_s(\omega) = \sum_n \left| \langle n | S_i^+ | 0 \rangle \right|^2 \delta(\omega - (E_n - E_0)), \quad (50)$$

where the sums run over all many-body eigenstates  $|n\rangle$  of  $\mathcal{H}_{\text{Hub}}$ .  $S_c(\omega)$  selects the excitation energies that we reach by adding a single electron, which is the charge sector, and  $S_s(\omega)$  selects the excitation energies that we reach by flipping a single spin, which is the spin sector. At a large but fixed interaction, say  $U = 60t$ , the two are very different.  $S_c$  has almost no weight up to a large threshold energy, and this threshold moves up as  $U$  increases.  $S_s$  has weight starting at a much lower energy, and its overall lineshape closely follows the spin structure factor of the Heisenberg chain from Session 2, as we expect from the mapping at strong coupling.

If we follow the peak position of each correlator as a function of  $U$ , the difference becomes completely explicit. The leading charge peak moves to higher energy *linearly* in  $U$ , since it costs  $\sim U/2$  to overcome the local repulsion when we add a second electron to a site that is already singly occupied. The leading spin peak instead moves to *lower* energy, decreasing  $\sim 1/U$ , as we derived in Section 3.5. Charge and spin excitations follow opposite trends with the same parameter  $U$ , and their energies move apart without bound as  $U$  increases. This is what we call **spin-charge separation**. In the strongly correlated one-dimensional Hubbard chain, charge

transport is exponentially suppressed, and essentially absent in the thermodynamic limit, while spin transport remains gapless and, in this precise sense, easy, even though both live on the same lattice of electrons. Figure 15 shows what the two excitations are and how far apart their energies are.

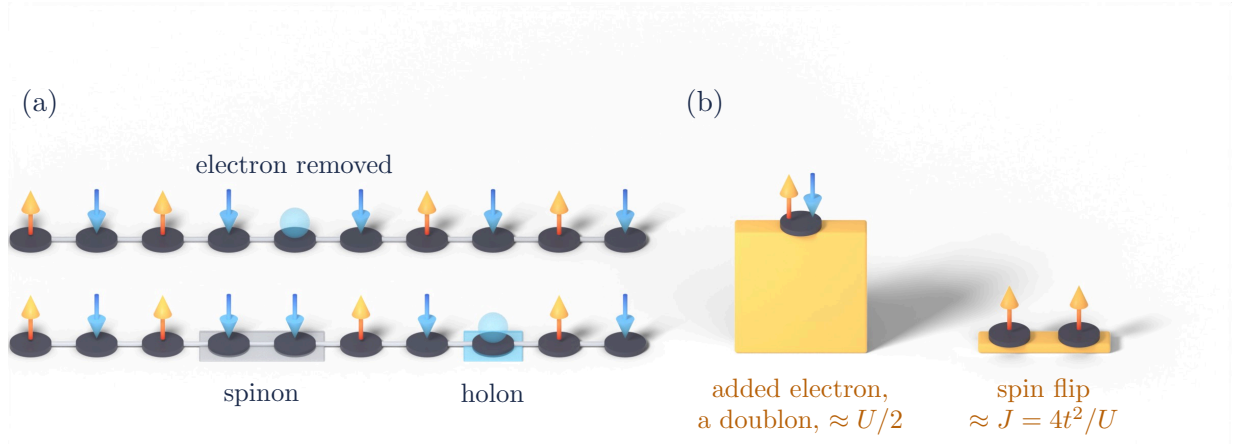


**Figure 15:** Spin-charge separation in the half-filled Hubbard chain of Eq. (42). (a) Behind, an electron is removed from the antiferromagnetic chain, and in front, the same chain is shown after the hole has hopped three sites to the right. The hole is now an empty site without spin, which is called the holon and carries the charge. Where it started, it has left two parallel neighbors, which are called the spinon and carry the spin, so one removed electron has become two objects that move apart. (b) The two energy scales at  $U = 10t$ , drawn to scale as two towers. Adding an electron on a singly occupied site makes a doubly occupied site, called a doublon, which is what  $S_c(\omega)$  of Eq. (50) reaches, and it costs about  $U/2$ . Flipping a spin against its neighbor, which is what  $S_s(\omega)$  reaches, costs about  $J = 4t^2/U = 0.4t$ .

#### ✕ Computational companion

Sections “Dynamical particle-particle correlators in the Hubbard model,” “Dynamical spin-spin correlators in the Hubbard model,” and “Interaction dependence of the dynamical excitations in the Hubbard model.” Compute both dynamical correlators at a large, fixed  $U$  and compare their line-shapes. Then follow how the leading peak of each one moves as you scan  $U$ , and confirm the contrast between linear growth and  $1/U$  decay that defines spin-charge separation.

### Closing summary

- Exact diagonalization directly in the fermionic Fock space has a Hilbert space dimension of  $2^L$  for spinless fermions or  $4^L$  for spinful fermions, which in the spinless case is the same as the  $2^L$  cost of the equivalent spin problem of Session 2, and it has no restriction to product states.
- The spinless nearest-neighbor chain shows an exact charge-density-wave transition, in which a unique metallic ground state at  $V = 0$  becomes a twofold-degenerate, gapped insulator as  $V \rightarrow \infty$ , with a large- $V$  gap that grows as  $\sim V$ . This is in good qualitative and quantitative agreement with the mean-field treatment of Session 1, since the broken symmetry here is only discrete.
- A conserved chemical potential term allows us to control the particle number of the ground state directly, and the width of the resulting occupation plateaus is the charging energy, which is the discrete second derivative of the ground-state energy with respect to  $N$ .

- The exact magnetization of the Hubbard model is *zero* at every site and for every  $U$ , in sharp and structural disagreement with the mean-field prediction of finite staggered order in Session 1. Lieb's theorem guarantees a unique, rotationally invariant spin singlet ground state at half filling, which no single Slater determinant can describe. This is the exact numerical confirmation of the failure of mean-field theory that we pointed out at the end of Session 1.
- An exact diagonalization of the Hubbard dimer reproduces the  $t^2/U$  superexchange scaling of Session 1 from first principles, and adding a Zeeman field shows that the low-energy excitations are magnons, as for the Heisenberg dimer of Session 2.
- At strong coupling the Hubbard chain shows spin-charge separation. The charge sector is gapped, with a gap that grows linearly in  $U$  and nonlocal correlators that decay exponentially, while the spin sector stays gapless, with a spin gap that decreases as  $1/U$  and power-law correlators, which is the physics of the Heisenberg chain it maps to.
- All of this was limited by the growth as  $2^L$  and  $4^L$ , to  $L \sim 20$  sites for spinless fermions and about half that for the Hubbard chain. In Session 5 we will come back to this same fermionic approach, with the Jordan-Wigner mapping and tensor-network methods, and reach system sizes where the thermodynamic limit becomes directly visible.

# PHYS-E0510 – Advanced Computational Methods in Physics D

## Session 4

### Matrix Product States for Spin Chains

**Companion notebook:** `mps_quantum_magnets.ipynb`    **Prerequisites:** exact diagonalization of the Heisenberg model (Session 2)

## Contents and goals

In the last two sessions we solved quantum many-body problems exactly. First we solved the Heisenberg chain in the spin basis, and then the spinless and Hubbard chains in the fermionic basis. This worked, and the gaps, the level crossings and the correlators all came out of the numerics with no approximation. However, both times we found the same limitation. The Hilbert space of  $L$  spin- $\frac{1}{2}$ 's has dimension  $2^L$ , and  $4^L$  for spinful fermions, and this number grows too fast for us to handle. At around  $L \sim 20$  spins even a very good computer runs out of memory, and we are still far from the thermodynamic limit, which is where the interesting physics appears, such as quantum phase transitions, fractionalization and the emergence of gaps. So the question for this session is concrete. Is there a way to represent the many-body wavefunction that does not have an exponential cost, at least for the states we are interested in? The answer is yes, and the method is called matrix product states (MPS), which is the simplest member of the larger family of tensor network methods. We will see why this representation is efficient, why it works so well in one dimension, and how to check numerically if we can trust it. In the second half of the session we will repeat the study of the Heisenberg model of Session 2, but now at 40 to 100 spins and more, which is large enough to see the physics of the thermodynamic limit that before we could only guess.

## Learning outcomes

By the end of this session, you should be able to do the following.

- Explain why the matrix product state ansatz compresses an exponentially large wavefunction into a cost that is linear in  $L$  and quadratic in the bond dimension  $\chi$ .
- Use entanglement entropy and the area law to explain why matrix product states work well in one dimension, and where we expect them to fail, which is in 2D and for volume-law states.
- Check the convergence of a variational MPS calculation with energy fluctuations, and use entanglement entropy as a diagnostic for a quantum phase transition.
- Run MPS calculations at 40 to 100 spins and more to distinguish the gapless spin- $\frac{1}{2}$  Heisenberg chain from the gapped and fractionalized spin-1 Haldane phase.

## 4.1 From an exponential wavefunction to a matrix product state

### 4.1.1 Tensor networks as data compression

Before we write any equations, let us start with an analogy. Let us take a photograph with a high resolution, and let us say that we want to store it with much less memory. We do not remove

information at random. Instead, we use the fact that real photographs have a lot of structure, since pixels that are close to each other are correlated, and a compressed format such as JPEG can give an image that looks the same as the original with only a small fraction of the original pixels. Tensor networks do the same thing, but for the wavefunctions of quantum many-body systems. The role of the pixels is played by the  $2^L$  complex coefficients of the wavefunction in the computational basis. The role of the compression algorithm is played by a specific way of writing these coefficients as a product of small pieces, and the parameter that controls how much we compress is what is called the **bond dimension**. In this section we will make this analogy precise.

#### 4.1.2 The formal matrix product state ansatz

For a chain of  $L$  spins, each with  $d$  local states where  $d = 2$  for spin- $\frac{1}{2}$ ,  $d = 3$  for spin-1 and so on, an arbitrary wavefunction is

$$|\Psi\rangle = \sum_{s_1, \dots, s_L} C(s_1, \dots, s_L) |s_1\rangle \otimes \dots \otimes |s_L\rangle, \quad (51)$$

and to specify  $|\Psi\rangle$  exactly we have to give all  $d^L$  numbers  $C(s_1, \dots, s_L)$  independently. The matrix product state ansatz makes a specific proposal for how to generate these coefficients without storing them one by one. For every site  $n$  and every local state  $s_n$ , we introduce a matrix  $M_n^{s_n}$ , and we write

$$C(s_1, \dots, s_L) = M_1^{s_1} M_2^{s_2} \dots M_L^{s_L}. \quad (52)$$

For open boundary conditions,  $M_1^{s_1}$  is a  $1 \times \chi_1$  row vector and  $M_L^{s_L}$  is a  $\chi_{L-1} \times 1$  column vector, so the product of matrices in Eq. (52) gives a single number, as it must for  $C$  to be a scalar coefficient. The internal matrices  $M_n^{s_n}$  are  $\chi_{n-1} \times \chi_n$ , and the integer  $\chi$  is the **bond dimension**, which we will mostly take uniform along the chain. The bond dimension is the one parameter that controls how much this ansatz can represent, and it will be the central quantity of this session. Figure 16 shows the two ways of storing the same state next to each other.

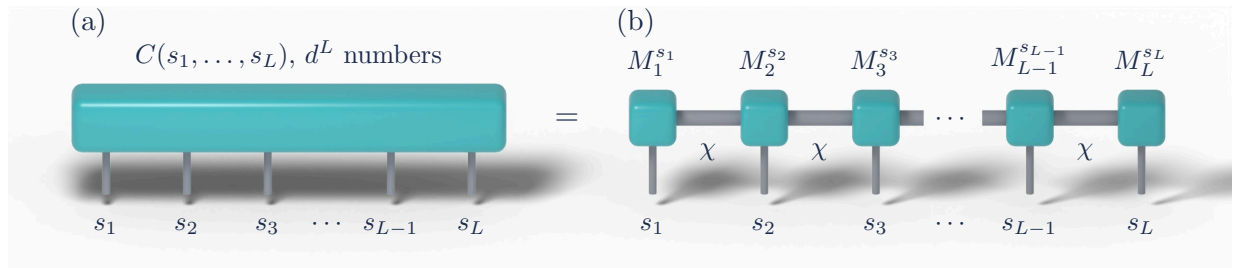


**Figure 16:** The state of Eq. (51) stored in two ways. (a) The coefficients  $C(s_1, \dots, s_L)$  as one tensor with  $L$  physical legs, one per site, which means  $d^L$  numbers to store. (b) The matrix product state of Eq. (52), where the same legs hang from a chain of small tensors. Each site has one tensor  $M_n^{s_n}$ , with a vertical *physical* leg that runs over the  $d$  local states of that site and horizontal *bond* legs of dimension  $\chi$  that join it to its neighbors. Joining two legs means summing over the shared index, so contracting the horizontal legs from left to right is the matrix product of Eq. (52). The two end tensors have a single bond leg each, a row vector and a column vector, which is why the whole contraction gives one number. The only difference between the panels is where the numbers are stored, either in one block that grows as  $d^L$  or in  $L$  small tensors of  $d\chi^2$  numbers each, as in Eq. (53).

Let us count parameters, because this is the main point. Storing  $C(s_1, \dots, s_L)$  directly costs  $d^L$  numbers, which is exponential in  $L$ . Storing the matrices  $\{M_n^{s_n}\}$  instead costs

$$N_{\text{MPS}} \sim L d \chi^2, \quad (53)$$

which is *linear* in the system size  $L$  and only quadratic in the bond dimension  $\chi$ . So if we can represent the states we are interested in with a fixed and moderate  $\chi$ , we have turned an exponential problem into a polynomial one. This raises a natural question. Is it true that the states we are interested in, which are ground states and low-lying excited states of local Hamiltonians, can be described in this way with a  $\chi$  that stays moderate as  $L$  grows? We will answer this in detail once we introduce entanglement entropy in Section 4.4, but the short answer is yes, in one dimension, and this is the reason why this course has a Session 4.

### 4.1.3 The cost of exact diagonalization and of matrix product states

Before we justify this theoretically, let us first look at what it gives us in practice. If we solve the Heisenberg chain  $\mathcal{H}_{\text{Heis}} = J \sum_n \mathbf{S}_n \cdot \mathbf{S}_{n+1}$  by exact diagonalization, the time to find the ground state grows exponentially with  $L$ , because we work with vectors and matrices of size  $2^L$ . If instead we solve it variationally with the matrix product state ansatz of Eq. (52), at fixed bond dimension the cost grows close to linearly in  $L$ . The two curves cross at around  $L \sim 14$  to 16. Below this size exact diagonalization is faster, since there is no reason to use a variational method when the exact answer is cheap. Above it, matrix product states are faster, and the difference keeps growing with the system size. For example, systems of 50, 70 and even 80 spins can be solved on a laptop in seconds, while exact diagonalization would need more memory than the largest supercomputers have once we pass  $L \sim 40$  to 50. This difference in scaling, exponential versus polynomial, is the basis of the rest of the session.

#### ✕ Computational companion

Sections “Energy of the Heisenberg model as a function of the system size” and “Near linear scaling with system size with matrix product states.” Plot the ground-state energy per site against  $L$  and see how it converges to a value in the thermodynamic limit. As an independent convergence check, compare it with the exact Bethe-ansatz result  $e_0 = J(\frac{1}{4} - \ln 2) \approx -0.4431J$ . Then compare the time of exact diagonalization with the time of the matrix product state solver as you increase  $L$ , and find the system size beyond which the tensor network method is the only option.

## 4.2 Convergence diagnostics for the variational state

### 4.2.1 A variational ansatz

Matrix product states are a variational ansatz. We do not solve the Schrödinger equation exactly, and instead we search for the best approximation to the ground state, or to an excited state, within the family of states described by Eq. (52) at some fixed  $\chi$ . This gives a practical question that we did not have with exact diagonalization. How do we know if our variational state is good, without knowing the exact answer?

### 4.2.2 Energy fluctuations

Let us assume that our solver has converged to some normalized state  $|\Omega\rangle$ , with energy  $E_\Omega = \langle\Omega|\mathcal{H}|\Omega\rangle$ . If  $|\Omega\rangle$  was an exact eigenstate of  $\mathcal{H}$ , then  $\mathcal{H}|\Omega\rangle = E_\Omega|\Omega\rangle$  and the variance of the energy,

$$(\Delta E)^2 \equiv \langle\Omega|\mathcal{H}^2|\Omega\rangle - \langle\Omega|\mathcal{H}|\Omega\rangle^2, \quad (54)$$

would be exactly zero. So a natural diagnostic is to compute  $(\Delta E)^2$  using only the variational state, without any knowledge of the true ground state, and to check how close it is to zero. Let us make this quantitative. We write  $|\Omega\rangle$  as mostly the true ground state  $|0\rangle$  with a small admixture  $\varepsilon$  of the first excited state  $|1\rangle$ ,

$$|\Omega\rangle = \sqrt{1 - \varepsilon^2} |0\rangle + \varepsilon |1\rangle, \quad \varepsilon \ll 1. \quad (55)$$

If we expand  $\langle\Omega|\mathcal{H}|\Omega\rangle$  and  $\langle\Omega|\mathcal{H}^2|\Omega\rangle$  to  $\mathcal{O}(\varepsilon^2)$  using  $\mathcal{H}|0\rangle = E_0|0\rangle$  and  $\mathcal{H}|1\rangle = E_1|1\rangle$ , a short calculation gives

$$E_\Omega - E_0 = \varepsilon^2(E_1 - E_0), \quad (\Delta E)^2 = \varepsilon^2(E_1 - E_0)^2 + \mathcal{O}(\varepsilon^4). \quad (56)$$

Two results follow from this, and both make this diagnostic very useful. First,  $(\Delta E)^2 \rightarrow 0$  if and only if  $\varepsilon \rightarrow 0$ , meaning that  $|\Omega\rangle$  converges to a true eigenstate, so the fluctuation is a good measure of the unknown distance to the exact answer. Second, if we compare the two relations in Eq. (56), we find that  $(\Delta E)^2 \approx (E_\Omega - E_0)(E_1 - E_0)$ , so the energy fluctuation tells us at the same time how much our state is mixed with an excited state *and* roughly how large the gap to this excited state is. In practice we follow  $(\Delta E)^2$  as we increase the bond dimension  $\chi$ . It should decrease monotonically and finally become flat near machine precision once  $\chi$  is large enough for the physics of the problem.

### 4.2.3 Bond dimension and excited states

Everything we said for the ground state also applies to any targeted eigenstate. An excited-state solver also converges toward some  $|\Omega_k\rangle \rightarrow |k\rangle$  as  $\chi$  increases, and we can follow the same energy fluctuation, Eq. (54), evaluated on  $|\Omega_k\rangle$ . What changes is *how fast* this convergence happens. Higher excited states are in general more entangled than the ground state, since they explore a larger part of the Hilbert space. As we will see in Section 4.4, entanglement is what a finite bond dimension has difficulty to capture, so these states need a larger  $\chi$  before their energy fluctuation goes to zero. This is a generic feature of tensor network calculations. The ground state converges first and fastest, and each higher excited state needs a bit more bond dimension to reach the same convergence.

#### ✕ Computational companion

Sections “The role of the bond dimension” and “The role of bond dimension in excited states.” Plot the ground-state energy and its fluctuation, Eq. (54), against  $\chi$  for the Heisenberg chain, and see how the fluctuation goes to zero as  $\chi$  grows. Then repeat this for several excited states at the same time, and check that higher states need a larger  $\chi$  to converge to the same fluctuation tolerance.

## 4.3 Low-energy excitations and level crossings

Before we build the full formalism of entanglement entropy, let us see what matrix product states give us physically, using as a diagnostic the same first excited state that we just discussed.

### 4.3.1 The lowest spin excitation in the bulk

Let us take the Heisenberg chain and compute the matrix element  $\langle 0 | S_n^x | 1 \rangle$  between the ground state and the first excited state, as a function of the site  $n$  where we act with the spin operator. Physically, this is the amplitude for creating the lowest-energy spin excitation at site  $n$ . For the spin- $\frac{1}{2}$  chain, this profile looks like the ground-state wavefunction of a particle in a box, with maximal amplitude at the center of the chain and a smooth decay toward both edges. This is the particle-in-a-box picture that we already saw in the dynamical correlators of Session 2. The lowest spin excitation is a wave spread over the whole chain, and on an *open* chain the boundaries turn it into a standing wave that vanishes at both edges. This is the behavior of a delocalized spin excitation in the bulk, and it is our first hint that the low-energy physics of the spin- $\frac{1}{2}$  chain is in the bulk. Once we have systems large enough to make the comparison convincing, in Section 4.8, we will come back to this profile and compare it with the very different one of spin-1.

### 4.3.2 Level crossings in a magnetic field

The other natural quantity to follow is how the ground state changes as we turn on a magnetic field,  $\mathcal{H} = J \sum_n \mathbf{S}_n \cdot \mathbf{S}_{n+1} - B \sum_n S_n^z$ . Since  $\sum_n S_n^z$  commutes with the exchange term, the field  $B$  never mixes eigenstates of  $\mathcal{H}|_{B=0}$ . It only shifts their energies by  $-B \times (\text{total } S^z)$ , and sectors with different total  $S^z$  cross each other as  $B$  increases. For  $L = 2$  there is exactly one such crossing, from the  $S = 0$  singlet to the  $S = 1$  triplet. For  $L = 4$  there are two,  $S = 0 \rightarrow S = 1 \rightarrow S = 2$ , and as we increase  $L$ , more and more crossings appear, closer and closer together in  $B$ . This is a direct and numerically clean way to see that the spin- $\frac{1}{2}$  Heisenberg chain is gapless in the thermodynamic limit. The staircase of crossings becomes a smooth ramp as  $L \rightarrow \infty$ , meaning that there are excitations arbitrarily close in energy to the ground state at any nonzero  $B$ .

#### ✕ Computational companion

Sections “Low energy excitations of a Heisenberg model” and “Level crossings as a function of the magnetic field with matrix product states.” Reproduce the particle-in-a-box profile of the matrix element. Separately, follow the total spin of the ground state as a function of  $B$  for  $L = 2, 4, 10, 30$ , and see how the discrete staircase of Session 2 becomes what looks like a continuous ramp once  $L$  is large enough.

## 4.4 Entanglement entropy and why matrix product states work in one dimension

For two sections we have used the matrix product state ansatz without justifying it. Let us now do this properly, because the justification also tells us when this approach will fail.

### 4.4.1 Separable versus entangled states

Let us split our system into two regions,  $A$  and  $B$ , where we can take  $A$  as the left half of the chain and  $B$  as the right half. We say that a state  $|\Psi\rangle$  is **separable** if it can be written as a simple tensor product,

$$|\Psi\rangle = |\phi\rangle_A \otimes |\chi\rangle_B, \quad (57)$$

for some states  $|\phi\rangle_A$  and  $|\chi\rangle_B$  that live only on  $A$  and only on  $B$ . A basis state such as  $|\uparrow\downarrow\rangle$  is trivially of this form,  $|\uparrow\rangle_A \otimes |\downarrow\rangle_B$ . A state where every spin points along  $x$  is also of this form,

which is less obvious but follows directly, since  $|\rightarrow\rangle \otimes |\rightarrow\rangle = \frac{1}{2}(|\uparrow\rangle + |\downarrow\rangle) \otimes (|\uparrow\rangle + |\downarrow\rangle)$  is still a product. Every classical configuration, and in fact every state that we can write without any correlation between  $A$  and  $B$ , is separable in this sense. But now let us take the two-site singlet that we already saw in Session 1,

$$|\Psi_{\text{singlet}}\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle). \quad (58)$$

No choice of  $|\phi\rangle_A$  and  $|\chi\rangle_B$  gives this state. If we try to write it as a product, we find that we need two different terms with opposite relative sign, which a single product cannot give. We call such a state **entangled**. This is the distinction between classical and quantum states, and we need a way to quantify *how* entangled a state is, and not only whether it is entangled or not.

#### 4.4.2 The reduced density matrix and the von Neumann entropy

Given the full density matrix  $\rho = |\Psi\rangle\langle\Psi|$ , we define the **reduced density matrix** of subsystem  $A$  by tracing out everything in  $B$ ,

$$\rho_A \equiv \text{Tr}_B \rho. \quad (59)$$

The **entanglement entropy** across the cut is then the usual von Neumann entropy of  $\rho_A$ ,

$$S_A \equiv -\text{Tr} [\rho_A \ln \rho_A]. \quad (60)$$

If  $|\Psi\rangle$  is separable,  $\rho_A = |\phi\rangle\langle\phi|$  is a rank-one projector, its only nonzero eigenvalue is 1, and  $S_A = -1 \ln 1 = 0$ . If  $|\Psi\rangle$  is the singlet, a direct computation of  $\rho_A$ , where we trace out site  $B$ , gives  $\rho_A = \frac{1}{2}\mathbb{I}$ , with two equal eigenvalues  $\frac{1}{2}, \frac{1}{2}$ , so  $S_A = -2 \times \frac{1}{2} \ln \frac{1}{2} = \ln 2$ , which is the maximal possible entropy for a single spin- $\frac{1}{2}$ . So  $S_A$  goes smoothly from no entanglement to maximal entanglement, as we want.

#### 4.4.3 The Schmidt decomposition and the bound on the entanglement

Now let us connect this to the matrix product state ansatz. We cut the chain at bond  $n$ , between sites  $n$  and  $n+1$ . We can reshape the coefficient tensor of any state as a matrix between the left block  $(1, \dots, n)$  and the right block  $(n+1, \dots, L)$ , and with a singular value decomposition of this matrix we can write the state in the **Schmidt form**

$$|\Psi\rangle = \sum_{\alpha=1}^r \lambda_{\alpha} |\alpha\rangle_A \otimes |\alpha\rangle_B, \quad \sum_{\alpha} \lambda_{\alpha}^2 = 1, \quad (61)$$

with  $|\alpha\rangle_A$  and  $|\alpha\rangle_B$  orthonormal on each side and  $r$  the Schmidt rank. For a generic state,  $r$  can be as large as  $d^{\min(n, L-n)}$ , which is exponential in the block size. However, for a matrix product state built as in Eq. (52), the sum over the bond index at position  $n$  runs only over  $\chi_n$  values by construction. This means that the coefficient tensor factorizes through an index of dimension  $\chi_n$ , so the Schmidt rank at that cut is at most  $\chi_n$ . If we put the Schmidt form into Eq. (60), we get  $\rho_A = \sum_{\alpha} \lambda_{\alpha}^2 |\alpha\rangle\langle\alpha|$ , so

$$S_A = -\sum_{\alpha=1}^r \lambda_{\alpha}^2 \ln \lambda_{\alpha}^2 \leq \ln r \leq \ln \chi_n, \quad (62)$$

with equality in the last step exactly when all  $\chi_n$  Schmidt weights are equal,  $\lambda_{\alpha}^2 = 1/\chi_n$ . This is the most important equation of this session, and it says that *the bond dimension sets an*

upper limit to the entanglement entropy that the ansatz can represent. If the state we want has entanglement entropy  $S_A$  across some cut, we need at least  $\chi \gtrsim e^{S_A}$  there to describe it. So the question of whether matrix product states are a good choice for a given problem becomes the question of how  $S_A$  behaves as we increase the system size. Figure 17 shows what crosses a cut, for two spins, for a whole chain, for a square lattice and for a random state.

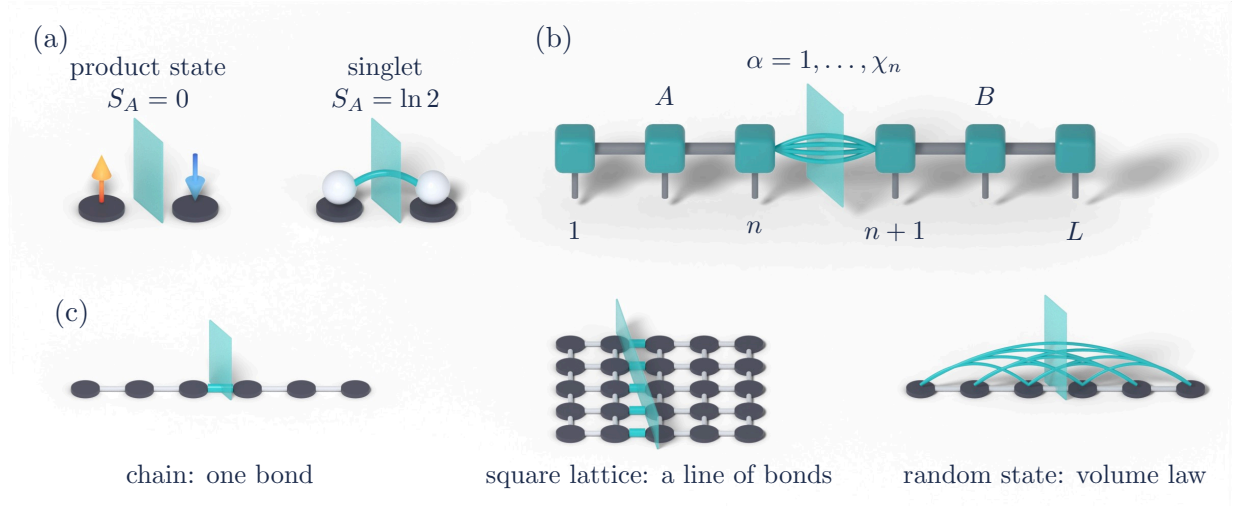


**Figure 17:** What crosses a cut. (a) The two cases of the section on separable and entangled states. Nothing crosses the cut of the product state  $|\uparrow\rangle_A \otimes |\downarrow\rangle_B$ , while the singlet, which is two spins with no moment of their own, is held together by one strand across the cut, and  $S_A = \ln 2$ . (b) The Schmidt decomposition of Eq. (61) read directly from a matrix product state. Cutting the chain at bond  $n$  separates it into blocks  $A$  and  $B$  and shows the single bond index  $\alpha$  that joined them, which is drawn opened into its  $\chi_n$  values. Since this index takes only  $\chi_n$  values by construction, the sum in Eq. (61) has at most  $\chi_n$  terms, the Schmidt rank obeys  $r \leq \chi_n$ , and the entropy across the cut obeys the bound of Eq. (62). All the information that the two halves of the chain share has to pass through this one index. (c) What a cut separates in a gapped ground state, which is one bond of a chain and a whole line of bonds of a square lattice, while for a random state there are strands everywhere, so that the entropy grows with the volume of the block, which is called the volume law.

#### 4.4.4 The area law, and why one dimension is cheap

The key physical fact is the following. For the ground state of a *gapped*, local, one-dimensional Hamiltonian, correlations decay exponentially beyond some correlation length  $\xi$ , and it turns out that  $S_A$  *saturates* to a constant that does not depend on  $L$  as soon as the block  $A$  is a few  $\xi$  away from both its boundary and the far end of the chain. This is what is called the area law, and it is proven for gapped one-dimensional systems. Only the physics within  $\sim \xi$  of the cut contributes to the entanglement, and everything deep inside  $A$  or  $B$  does not matter for it. For a *gapless* critical chain there is no finite  $\xi$ , and conformal field theory tells us that  $S_A$  grows instead, but only logarithmically, as  $S_A \sim \frac{c}{3} \ln n$  for a cut in the bulk of an infinite or periodic chain. With open boundaries, which we use in all this session for the reasons given in Section 4.5, this is roughly halved to  $S_A \sim \frac{c}{6} \ln n$ . In both cases this is much cheaper than the generic case. A uniformly random state in the Hilbert space has  $S_A$  growing linearly with the size of the smaller block, which is a *volume law* and is the content of Page's theorem. This would force  $\chi$  to grow exponentially with system size, and the ansatz would lose its purpose. Ground states of local 1D

Hamiltonians live in a very small and special part of the full Hilbert space, with low or at most logarithmically growing entanglement. It is because they live in this part that a bond dimension  $\chi$  that stays moderate, or grows only polynomially, as  $L \rightarrow \infty$  can describe them accurately. Panel (c) of Figure 17 shows the three cases next to each other.

A clean way to see the saturation directly is to solve an exactly dimerized chain, where sites are grouped into decoupled pairs,  $\mathcal{H} = J \sum_k \mathbf{S}_{2k-1} \cdot \mathbf{S}_{2k}$  with no coupling between pairs. The exact ground state is a product of singlets,  $|\Psi\rangle = \bigotimes_k |\Psi_{\text{singlet}}\rangle_{2k-1,2k}$ . Now let us cut this state anywhere. Every cut either falls *inside* a singlet, which contributes  $\ln 2$  as follows from Eq. (60) above, or falls *between* singlets, which contributes nothing, since the two halves factorize exactly there. However large we choose the block  $A$ , as long as its boundary is between dimers,  $S_A$  is either 0 or  $\ln 2$  per boundary point, independent of the size of  $A$ . This is the area law in its simplest form. Entanglement is a property of the *boundary* of the cut and not of its volume, and in one dimension a boundary is only a point, or two points for a block in the interior, so it costs  $\mathcal{O}(1)$  for any system size.

#### ✕ Computational companion

Sections “Entanglement entropy of the ground state,” “Size dependence of the entanglement entropy,” and “Bond dimension dependence of the entanglement entropy.” Compute  $S_A$  at every bond of a Heisenberg chain for a few values of  $\chi$ , and check that increasing  $\chi$  beyond some value does not change the profile anymore. This saturation is a direct numerical confirmation of the bound in Eq. (62). Then follow the entanglement entropy at the central bond as you increase  $L$ , and check that it grows only very slowly, as expected from the area-law scaling described above, which for the gapless Heisenberg chain is logarithmic.

#### 4.4.5 Why two dimensions is expensive

The same argument of counting bonds, done in two dimensions, gives the opposite conclusion. Let us divide a 2D lattice into decoupled clusters, for example plaquettes of four spins each that are fully coupled inside and disconnected from each other, and repeat the exercise. A rectangular block  $A$  now cuts a number of bonds between clusters that is proportional to the *perimeter* of  $A$ , and not a fixed number of points. Doubling the linear size of  $A$  roughly doubles the number of clusters at the boundary, and so it doubles  $S_A$ . A matrix product state has to turn the 2D lattice into an effective 1D chain that snakes through the rows, so the bond in the middle of this snake has to carry the entanglement of a whole row. As a result,  $\chi$  has to grow *exponentially* with the linear dimension of the system to keep the truncation error fixed. Matrix product states can still be used in two dimensions, and some of the best available numerics for the 2D Hubbard model and for frustrated triangular and kagome-lattice antiferromagnets are obtained in this way. However, this only works on narrow cylinders and with a much larger  $\chi$  than a comparable 1D calculation would need. We will not do two-dimensional calculations in this course, and the goal of the argument is to explain why everything else in this session is specific to one dimension.

#### 4.4.6 Where matrix product states struggle even in 1D

Bounded area-law entanglement is a property of *ground states* of *gapped or mildly critical, local* Hamiltonians. It fails, and matrix product states fail with it, in a few situations that we will not compute in this course but that we should keep in mind. First, entanglement grows *linearly* in time under quantum quench dynamics, so time evolution with matrix product states can only be

trusted up to some maximal time set by  $\chi$ . Second, highly excited states deep in the many-body spectrum typically violate the area law completely. Third, long-range interactions effectively bring back a higher-dimensional connectivity, even in a chain that is formally 1D.

## 4.5 Boundary conditions

### 4.5.1 Open boundaries and a single cut

Before we move to the physics, there is one more practical point. The choice between open and periodic boundary conditions matters a lot for tensor networks, even though it matters very little for exact diagonalization, where periodic boundary conditions only add one more coupling term to the Hamiltonian matrix. With open boundary conditions, a cut in the bulk separates exactly *one* bond of the chain, so the area-law argument above applies directly.

### 4.5.2 Periodic boundaries and the cost of two cuts

With periodic boundary conditions the chain is a ring, and any bipartition into two contiguous arcs cuts the ring at *two* points instead of one, since the two arcs are neighbors of each other at both ends. Both cuts contribute to the entanglement entropy across the partition, so periodic boundary conditions roughly *double*  $S_A$  compared with open boundary conditions on the same chain. By Eq. (62), doubling the entropy means that we need roughly the *square* of the bond dimension to reach the same accuracy. This is why almost every practical matrix product state calculation, including all the rest of this session, uses open boundary conditions, because periodic chains are much more expensive for the same physical answer. Figure 18 shows the two cases next to each other.

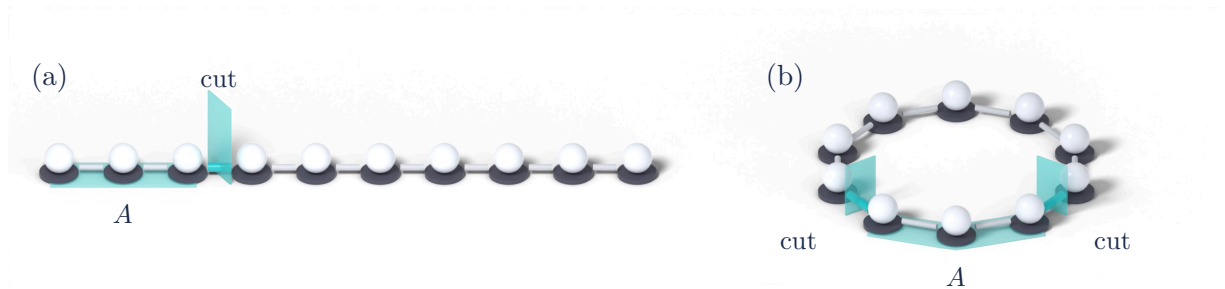


**Figure 18:** Why open boundaries are much cheaper. The teal tray marks the block  $A$  whose entanglement entropy we compute, and each pane shows a cut, with the bond that it separates drawn in teal. (a) On an open chain, a contiguous block touches the rest of the system at a single point, so one bond is cut. (b) On a ring the same block is next to the rest at both of its ends, so any bipartition cuts two bonds and each one contributes, which roughly doubles  $S_A$ . Through the bound of Eq. (62), a doubled entropy costs us the *square* of the bond dimension for the same accuracy.

#### ✕ Computational companion

Section “Open and closed boundary conditions.” Compute the entanglement entropy at the central bond of the Heisenberg chain with both open and periodic boundary conditions as a function of  $L$ , and check numerically that the periodic curve is roughly at twice the open one.

## 4.6 Entanglement entropy as a diagnostic for quantum phase transitions

### 4.6.1 The transverse-field Ising model

Entanglement entropy is not only a way to estimate the cost of a tensor network calculation. It is also a physical diagnostic, and the cleanest case where we can see this is a quantum phase transition. Let us take the transverse-field Ising chain,

$$\mathcal{H}_{\text{TFI}} = -J \sum_n S_n^z S_{n+1}^z - B_x \sum_n S_n^x. \quad (63)$$

This model has two exactly solvable limits. At  $B_x = 0$ , only the  $S^z S^z$  term survives, and even though  $S_n^z$  is a quantum operator, the Hamiltonian is diagonal in the  $S^z$  basis. The ground state is then the classical fully polarized ferromagnet  $|\uparrow\uparrow\cdots\uparrow\rangle$ , or its degenerate partner  $|\downarrow\downarrow\cdots\downarrow\rangle$ . At  $B_x \rightarrow \infty$ , we can instead neglect the exchange term completely, and the ground state is again classical, this time fully polarized along  $x$ ,  $|\rightarrow\rightarrow\cdots\rightarrow\rangle$ . Both limits are separable product states, so by Eq. (60) their entanglement entropy is exactly zero. Between these limits,  $\mathcal{H}_{\text{TFI}}$  must interpolate between two very different classical orders, and it does so through a quantum phase transition. The exact solution of this model comes from mapping the spins to free fermions with a Jordan-Wigner transformation, which we will see in detail in Session 5, and for the normalization used here it places the critical point at  $B_x = J/2$ . Figure 19 shows the chain at the two ends of the field and at the transition.

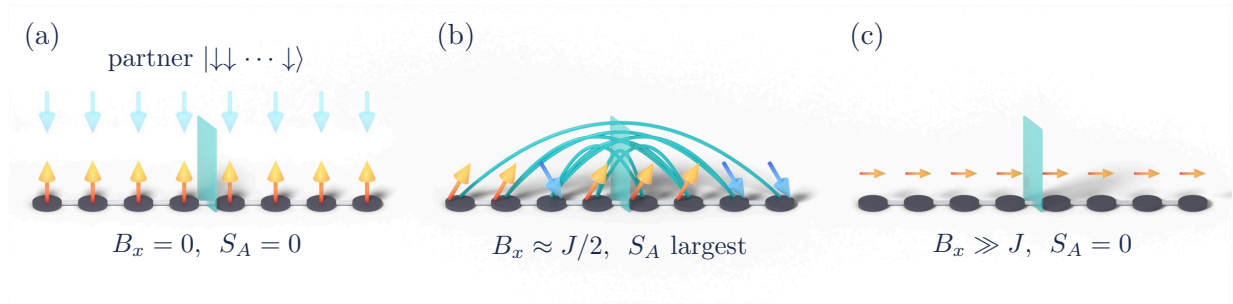


**Figure 19:** The transverse-field Ising chain of Eq. (63) at three fields, each cut at its central bond. (a) At  $B_x = 0$  every arrow points along  $z$ , and the all-down state drawn behind it is its degenerate partner. Both are product states, so nothing crosses the cut. (b) Near the critical field  $B_x = J/2$  the arrows tilt toward  $x$  and the chain breaks into domains of every size, and here the largest number of strands cross the cut, which is the peak of  $S_A$  found in the subsection on the entanglement peak and the order parameter. (c) For  $B_x \gg J$  every arrow points along  $x$ , which is again a product state with nothing across the cut. The point to look at is that both ends are classical and only the middle is not.

### 4.6.2 The entanglement peak and the order parameter

Both classical limits have zero entanglement entropy, while the state between them is quantum, meaning a superposition that cannot be reduced to a single classical spin configuration. So  $S_A$  has to rise from zero somewhere in the middle and go back down, and the natural guess is that it has its peak at the phase transition. This is what the numerics show. If we compute  $S_A$  at the central bond of a long chain as a function of  $B_x/J$ , we see that it vanishes at both  $B_x = 0$  and  $B_x \rightarrow \infty$ , with a clear maximum at the critical point. For a chain of  $\sim 100$  spins, which is close enough to the thermodynamic limit, this peak is at  $B_x/J = 0.5$ , the exact value given above.

We can compare this with a completely independent and more familiar diagnostic, which is the order parameter  $\langle S_n^z \rangle$ . For  $B_x < 0.5$ , the ground state keeps a finite  $\langle S_n^z \rangle$ , the ferromagnetic order parameter of the Ising phase. For  $B_x > 0.5$ , quantum fluctuations remove it completely and  $\langle S_n^z \rangle \rightarrow 0$ , and only  $\langle S_n^x \rangle \neq 0$  remains. Both diagnostics agree on the position of the transition, which is a good sign, but numerically they do not behave equally well. The order-parameter curve for a finite chain of 20 spins places the transition clearly away from 0.5, and we need to go to  $L \sim 100$  before the finite-size estimate converges to the exact critical value. Exact diagonalization cannot reach the system sizes needed to resolve this clearly, while matrix product states can.

#### ✕ Computational companion

Sections “The entanglement entropy as a signal for phase transitions” and “Phase transition from the order parameter.” Sweep  $B_x$  across the transition and plot both the entanglement entropy at the central bond and  $\langle S_n^z \rangle$ . Compare how sharp the two signals are, and repeat for a smaller system to see directly the finite-size shift of the apparent transition point.

## 4.7 The Heisenberg chain at thermodynamic-limit scale

We now have the tool, which is matrix product states, and the diagnostics we need to trust it, which are the energy fluctuation and the convergence in bond dimension. Let us use both on the same kind of questions that Session 2 asked about the Heisenberg chain,  $\mathcal{H}_{\text{Heis}} = J \sum_n \mathbf{S}_n \cdot \mathbf{S}_{n+1} - B \sum_n S_n^z$ , but now at system sizes that were out of reach before.

### 4.7.1 Magnetization at zero field and around a magnetic impurity

At small field  $B$ , deep inside the gapless phase, the magnetization  $\langle S_n^z \rangle$  of a uniform Heisenberg chain stays zero at every site. The field is too weak to overcome the antiferromagnetic exchange, and translational symmetry keeps every site equivalent. This is already a nontrivial check, since it holds even though we have explicitly broken time-reversal symmetry with  $B \neq 0$ . The ground state is not yet in the regime where this symmetry breaking appears locally.

The situation changes qualitatively once we replace the uniform field by a single **magnetic impurity**, meaning that we keep  $B = 0$  everywhere except at one site,  $n = 0$ , where we apply a local field. The system responds with a nonzero magnetization  $\langle S_n^z \rangle$  that varies in space around the impurity, and *how* this response decays with the distance from the impurity is one of the clearest diagnostics we have to know if the chain is gapped or gapless. For the uniform gapless Heisenberg chain, the induced magnetization decays as a slow power law,

$$\langle S_n^z \rangle \sim \frac{1}{|n|}, \quad |n| \gg 1, \quad (64)$$

and it never quite vanishes, however far we go from the impurity. This is the signature of a gapless system. The chain has excitations at arbitrarily low energy, so a local perturbation can affect the chain arbitrarily far away with only an algebraic decay.

### 4.7.2 The correlation length of a dimerized chain from an impurity response

Now let us dimerize the exchange coupling, alternating a strong bond  $J_1$  and a weak bond  $J_2$  along the chain,  $\mathcal{H} = \sum_n J_n \mathbf{S}_n \cdot \mathbf{S}_{n+1}$  with  $J_n$  alternating between  $J_1$  and  $J_2$ . As soon as  $J_1 \neq J_2$ ,

the chain opens a gap, and if we repeat the impurity calculation we now find an exponentially decaying response,

$$\langle S_n^z \rangle \sim e^{-|n|/\xi}, \quad (65)$$

with a correlation length  $\xi$  that becomes shorter as the dimerization becomes stronger. This is a direct numerical demonstration of the physics we expected in Section 4.4. A finite gap gives a finite correlation length, and the same  $\xi$  controls both the exponential decay of the local response *and* the saturation of the entanglement entropy across any cut. To obtain a clean exponential fit, which can be clearly distinguished from the power law of the gapless case, we need chains of order 100 spins, which is an order of magnitude beyond what exact diagonalization can reach.

### 4.7.3 Excited-state magnetization profiles and the many-body gap

Beyond the ground state, we can also target a few low excited states directly and look at their magnetization profiles. In a Heisenberg chain with a small field, the ground state is the usual  $S = 0$  singlet with zero magnetization everywhere, but the first excited state has a standing-wave pattern in  $\langle S_n^z \rangle$ , with finite magnetization in some regions of the chain and the opposite sign in others. The second excited state has again zero magnetization everywhere, since it has the same time-reversal symmetry as the ground state, while the third excited state has the same standing wave as the first, related to it by time reversal. This alternation between symmetric and antisymmetric states is what we saw in the small chains of Session 2, and now we see that it remains stable at much larger  $L$ .

Finally, we can follow the many-body gap  $E_1 - E_0$  as a function of  $L$ , for both the uniform and the dimerized chain. The gap of the uniform Heisenberg chain closes as  $L \rightarrow \infty$ , consistent with the gapless behavior we found with Eq. (64), while the gap of the dimerized chain saturates to a finite value, the same value that sets the correlation length  $\xi$  in Eq. (65). To see both trends converge clearly, without being cut off by finite-size effects, we again need the large values of  $L$  that only matrix product states can give us here.

#### ✕ Computational companion

Sections “Magnetization of moderately large Heisenberg model,” “Magnetization of a large Heisenberg model with a magnetic impurity,” “Magnetization of a dimerized Heisenberg model with a magnetic impurity,” “Magnetization of many-body excitations in large quantum chains,” and “Gap of a many-body spin chain.” Reproduce the contrast between power-law and exponential decay around a magnetic impurity, look at the standing-wave profiles of the excited states, and extract the scaling of the many-body gap with  $L$  for both the pristine and the dimerized chains.

## 4.8 Fractionalization in spin- $\frac{1}{2}$ and spin-1 chains at large scale

We are now able to answer clearly a question that Session 2 could only touch with small chains. What is the real difference between the spin- $\frac{1}{2}$  and spin-1 Heisenberg models?

### 4.8.1 Non-local static correlators

A convenient and purely static probe of the gap is the non-local correlator  $\langle S_0^z S_n^z \rangle$ , which is the linear response at site  $n$  to a perturbation applied at site 0. We already saw the impurity version of this idea in Eqs. (64) and (65), and the same two behaviors appear directly in the

correlator, with a power-law decay  $\sim 1/n$  for a gapless chain and an exponential decay  $\sim e^{-n/\xi}$  for a gapped one. If we apply this to the dimerized model of the previous section with increasing dimerization strength, we see the trend directly. Stronger dimerization gives a shorter  $\xi$  and a faster exponential decay, while the undimerized limit gives back the slow power law.

Now let us apply the same correlator to the spin- $\frac{1}{2}$  and spin-1 Heisenberg models, *without* any dimerization and only with nearest-neighbor exchange,  $\mathcal{H} = J \sum_n \mathbf{S}_n \cdot \mathbf{S}_{n+1}$  for  $S = \frac{1}{2}$  and  $S = 1$  respectively. Here the system size matters a lot. If we only had exact diagonalization, which for spin-1 is limited to around  $L \sim 15$  to  $16$ , we could think that the spin-1 correlator is the *larger* of the two at those distances. But if we go to  $L \sim 40$  to  $50$  spins, the picture is completely reversed. The spin- $\frac{1}{2}$  correlator keeps decaying as a slow power law up to the largest distances, while the spin-1 correlator drops exponentially once  $n$  is larger than its correlation length, which is much shorter. This crossover only becomes visible once the system is comparable to, or larger than, this correlation length, and this is why small chains give a wrong impression. Spin-1 is gapped and spin- $\frac{1}{2}$  is not, but we need a large enough  $L$  to see it.

#### 4.8.2 Fractionalization in the spin-1 chain

The contrast is clearest in the following case. Let us take an open spin-1 chain and apply a small uniform field,  $B \sim 0.05J$ . Instead of spreading uniformly, the induced magnetization  $\langle S_n^z \rangle$  is localized almost completely at the two edges of the chain, and the bulk stays at essentially zero. Summing the magnetization over each edge region gives  $-\frac{1}{2}$  on the left and  $+\frac{1}{2}$  on the right. Each edge behaves as if it had an emergent free spin- $\frac{1}{2}$  degree of freedom, even though every microscopic spin in the chain is spin-1. This is what is called **fractionalization**, meaning that the elementary excitations of the system are not integer multiples of the microscopic spin but a real fraction of it. The simplest exactly solvable model with the same edge physics is the **AKLT point**. This is a spin-1 chain built from projected valence bonds, which is in the same phase as the Heisenberg chain and in which the emergent spin- $\frac{1}{2}$  edge states can be computed exactly, and not only observed numerically. Figure 20 shows how it is built and where the edge spins come from. At  $L = 50$  the two edge moments still visibly leak into the bulk, and only at  $L = 100$  do we see them clearly localized at the two ends with essentially nothing in between. This confirms that in the thermodynamic limit the spin-1 Heisenberg chain has a fully gapped bulk and a pair of free spin- $\frac{1}{2}$  edge modes. This is the Haldane phase, which is one of the simplest examples of a symmetry-protected topological phase in one dimension.

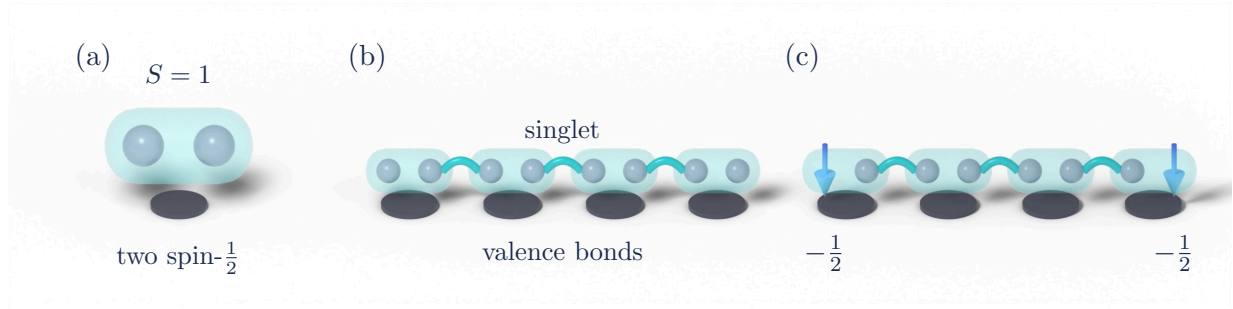


**Figure 20:** The AKLT construction of the spin-1 chain. (a) Each spin-1 is written as two spin- $\frac{1}{2}$  inside one capsule, which is the projector that keeps only their symmetric states with total spin 1. (b) The right half of each site forms a singlet with the left half of the next site, so every bond has one valence bond and the bulk has no free moment. (c) The outer halves of the two end sites have no partner, and they are the free spin- $\frac{1}{2}$  at the edges. A small field polarizes them, so the two edge regions have moments of  $-\frac{1}{2}$  and  $+\frac{1}{2}$ , which is half of what a spin-1 can have, while the bulk stays at zero.

We can see the same physics again, even more directly, in the **dynamical** correlator  $\langle S_n^+(t) S_n^-(0) \rangle$  as a function of both position  $n$  and energy  $\omega$ , which is the same kind of quantity that we used in Session 2 to obtain excitation spectra. In the bulk of the spin-1 chain, creating a spin excitation costs a finite energy, which is the bulk gap we just discussed. However, at the two edges the dynamical correlator has spectral weight at essentially *zero* energy, meaning that an edge spin can be flipped at no energy cost. This zero-energy edge response is the direct spectral signature of the free spin- $\frac{1}{2}$  edge modes. Again, it only becomes sharp and clear once the chain is long enough,  $L \sim 40$  spin-1's or more, so that the two edges are decoupled from each other and from any remaining contribution of the bulk.

#### ✕ Computational companion

Sections “Non-local static correlators in a large system,” “Fractionalization in the  $S = 1$  Heisenberg model,” and “Non-local correlator in the  $S = 1/2$  and  $S = 1$  Heisenberg models.” Plot  $\langle S_0^z S_n^z \rangle$  on a log scale for the spin- $\frac{1}{2}$  and spin-1 chains, and see how the contrast between power-law and exponential decay only becomes clear once  $L$  is large enough. Then compare the localization of the spin-1 edge magnetization at  $L = 50$  and at  $L = 100$ , and finally look at the dynamical correlator to see the zero-energy edge excitation directly. Note that for this last comparison the notebook attaches an explicit spin- $\frac{1}{2}$  to each end of the spin-1 chain, so that the emergent edge modes can combine with them into a conventional total spin that is not fractional.

## Closing summary

- Matrix product states write the exponentially many wavefunction coefficients  $C(s_1, \dots, s_L)$  as a chain of small matrices, Eq. (52), and the number of parameters grows only linearly in  $L$  and quadratically in the bond dimension  $\chi$ , Eq. (53).
- This ansatz is only as good as the entanglement of the target state allows. The Schmidt decomposition shows that the bond dimension bounds the entanglement entropy across any cut,  $S_A \leq \ln \chi$ , Eq. (62).
- Ground states of gapped, local, one-dimensional Hamiltonians obey an area law, meaning that their entanglement entropy saturates, or at criticality grows at most logarithmically, instead of growing with system size. This is why a moderate  $\chi$  that does not depend on  $L$  is enough in 1D, and why the same ansatz becomes exponentially expensive in two dimensions.

- Energy fluctuations, Eq. (54), allow us to check convergence without knowing the exact answer. Open boundary conditions roughly halve the entanglement entropy compared with periodic ones, so the required  $\chi$  is roughly its square root.
- The entanglement entropy is also a physical diagnostic. It has its peak exactly at the quantum phase transition of the transverse-field Ising model, which is clearly resolved once  $L$  is close to the thermodynamic limit.
- Repeating the study of the Heisenberg chain of Session 2 at 40 to 100 spins and more turns qualitative hints into sharp and converged results. We find power-law versus exponential correlators, a many-body gap that closes versus one that saturates, and a clear separation between the gapless spin- $\frac{1}{2}$  chain and the gapped, fractionalized spin-1 chain with its emergent spin- $\frac{1}{2}$  edge modes.

Matrix product states solved our  $2^L$  problem for spin chains, but everything we did here was written in the spin language of Session 2. In the next session we go back to the fermions of Session 3 and connect them to spins through the Jordan-Wigner mapping, which we only mentioned in Section 4.6.1. We will also present the general tensor-network algorithm, which is the variational sweep that produces the matrices  $M_n^{s_n}$  that we have used in this session without showing how to obtain them.

# PHYS-E0510 – Advanced Computational Methods in Physics D

## Session 5

### Matrix Product States for Fermionic Models

**Companion notebook:** `mps_many_body_fermionic.ipynb`    **Prerequisites:** Sessions 3 and 4 (exact diagonalization directly in the fermionic basis, and matrix product states for spin chains)

## Contents and goals

Let us first recall where we stopped. In Session 3 we did our many-body calculations again, directly in the fermionic basis and without any restriction to product states, and this worked well. We recovered the exact charge-density-wave transition of spinless fermions and the spin-charge separation in the Hubbard model. However, we found the same limitation that we always find with exact diagonalization, since the Hilbert space grows as  $2^L$  for spinless fermions and as  $4^L$  for the Hubbard chain, so for the Hubbard chain we could only reach about half the length that we could reach for spins. In Session 4 we introduced the solution to this problem, which is matrix product states, but we only used them for *spin* Hamiltonians. In this session we will connect the two. We will solve interacting *fermionic* Hamiltonians with tensor networks, for system sizes of a hundred sites or more. The way we do this is by first mapping them to spin Hamiltonians with the Jordan-Wigner transformation, and then using all the MPS tools that we already built. First, we will repeat the spinless and Hubbard results of Session 3 at a size where the physics is clear. Then we will introduce two new diagnostics, which are pairing correlators and the correlation entropy. At the end we will see the general tensor-network algorithm that we have been using since Session 4 without looking at how it works.

## Learning outcomes

By the end of this session, you should be able to do the following.

- Map a fermionic Hamiltonian to an equivalent spin Hamiltonian with the Jordan-Wigner transformation, and explain why nearest-neighbor hopping needs no explicit string.
- Use MPS for system sizes of  $\sim 100$  sites to locate a quantum phase transition that exact diagonalization could not resolve sharply.
- Compute pairing correlators, including how they are enhanced toward a behavior similar to Cooper pairs for attractive interactions, and use the correlation entropy to judge how far a ground state is from a mean-field description with a single Slater determinant.
- Describe with diagrams how the DMRG sweep optimizes an MPS one tensor at a time, and place MPS and DMRG within the larger family of tensor-network methods, such as PEPS and MERA.

## 5.1 The Jordan-Wigner mapping from spins to fermions

### 5.1.1 Spin models and fermionic models

The first question we want to answer is almost a philosophical one. Are spin models and fermionic models in fact the same thing? At first sight they look like different kinds of objects. A fermionic

Hamiltonian is built from operators  $c_i^\dagger, c_i$  that anticommute on different sites,  $\{c_i, c_j^\dagger\} = \delta_{ij}$ , while a spin- $\frac{1}{2}$  Hamiltonian is built from operators  $S_i^x, S_i^y, S_i^z$  that *commute* on different sites and only have a nontrivial algebra on the same site. Tensor networks, in the way we built them in Session 4, are bosonic objects, since an MPS is a product of matrices, one per site, and nothing in this construction knows about fermionic minus signs. So if we want to use MPS to solve fermionic Hamiltonians, which is what we want to do in this session, we first need a dictionary that turns a fermionic Hamiltonian into an equivalent spin Hamiltonian.

### 5.1.2 Matching the local Hilbert spaces

The first step is easy. A single fermionic site has exactly two states, empty  $|0\rangle$  and occupied  $|1\rangle = c^\dagger |0\rangle$ , because  $c^\dagger c^\dagger = 0$  forbids double occupancy. A single spin- $\frac{1}{2}$  also has exactly two states,  $|\downarrow\rangle$  and  $|\uparrow\rangle$ . So let us identify them site by site,

$$|0\rangle \leftrightarrow |\downarrow\rangle, \quad |1\rangle \leftrightarrow |\uparrow\rangle, \quad (66)$$

and in the same way identify the operators that move between them. The operator  $c^\dagger$  takes an empty site to an occupied one, in the same way as  $S^+$  takes down to up, so we would like to write  $c^\dagger \leftrightarrow S^+$  and  $c \leftrightarrow S^-$ . Since  $n = c^\dagger c$  is 0 or 1 while  $S^z$  is  $\mp\frac{1}{2}$ , we also have

$$S_i^z = n_i - \frac{1}{2}. \quad (67)$$

So far this looks like a clean bijection between the two Hilbert spaces. However, there is a point that we did not discuss yet, which is that fermionic operators on different sites *anticommute*, while spin operators on different sites *commute*. This mismatch is not a technical detail, and it means that the naive identification  $S_i^\pm \stackrel{?}{=} c_i^\dagger$  cannot be right as it is. Panel (a) of Figure 21 shows the matching of the two local spaces, and the other two panels show the correction that we will now construct.

### 5.1.3 The string operator

Let us see the mismatch explicitly, since it is the reason for this whole section. We take the naive guess  $\tilde{S}_i^+ \equiv c_i^\dagger$ ,  $\tilde{S}_j^- \equiv c_j$  for  $i \neq j$ . Then

$$\tilde{S}_i^+ \tilde{S}_j^- = c_i^\dagger c_j, \quad \tilde{S}_j^- \tilde{S}_i^+ = c_j c_i^\dagger = -c_i^\dagger c_j, \quad (68)$$

where the last step is the fermionic anticommutation relation for  $i \neq j$ . So the naive guess gives two operators that *anticommute*,  $\tilde{S}_i^+ \tilde{S}_j^- = -\tilde{S}_j^- \tilde{S}_i^+$ . Real spin operators on different sites must instead *commute*,  $S_i^+ S_j^- = S_j^- S_i^+$ , because they belong to independent two-level systems that are joined with an ordinary tensor product. This is the mismatch between anticommutation and commutation that we found above, and it means that we need to add something to the naive guess that fixes the sign.

To fix the sign, we order the sites along the chain, and we define, for every site  $i$ , the operator

$$K_i \equiv \prod_{j < i} (1 - 2n_j), \quad (69)$$

which is the parity of the number of fermions to the left of site  $i$ , meaning that  $K_i = +1$  if an even number of sites to the left are occupied and  $K_i = -1$  if this number is odd. This operator

is what is called the **Jordan-Wigner string**. Since  $K_i$  is built only from number operators  $n_j = c_j^\dagger c_j$ , which are quadratic in fermionic operators,  $K_i$  commutes with any fermionic operator on a different site, because the two sign changes cancel, even though it looks like a long and complicated string of anticommuting objects. It is also Hermitian and unitary,  $K_i^2 = 1$ . With this, the correct dictionary is

$$S_i^+ = c_i^\dagger K_i, \quad S_i^- = c_i K_i, \quad S_i^z = n_i - \frac{1}{2}. \quad (70)$$

We can check by direct computation, using  $K_i^2 = 1$  and the fact that  $K_i$  commutes with operators on other sites, that Eq. (70) gives exactly the correct spin algebra, which is  $[S_i^\alpha, S_j^\beta] = 0$  for  $i \neq j$  and the usual  $\mathfrak{su}(2)$  algebra on the same site. So the string is necessary, and it is the one piece of bookkeeping that gives consistent operator algebras to a fermionic Hilbert space and to a spin Hilbert space, which are the same vector space.

#### 5.1.4 Why nearest-neighbor hopping barely notices the string

This mapping is useful in practice, and not only a mathematical curiosity, because of what happens for nearest-neighbor terms. Let us take  $i < j$  and write the general spin bilinear  $S_i^+ S_j^-$  in terms of fermions. We write  $K_j = K_i(1 - 2n_i) \prod_{i < k < j} (1 - 2n_k)$  and use  $K_i^2 = 1$  together with the operator identity  $c_i^\dagger(1 - 2n_i) = c_i^\dagger$ . This identity holds because  $c_i^\dagger n_i = 0$ , meaning that we cannot create a particle on a site that is already occupied. A short calculation then gives

$$S_i^+ S_j^- = c_i^\dagger c_j \prod_{i < k < j} (1 - 2n_k), \quad i < j. \quad (71)$$

So in general, moving an electron from  $j$  to  $i$  requires a whole string of  $S^z$  operators on every site in between. However, let us look at the special case  $j = i + 1$ . In this case the product in Eq. (71) runs over an empty range and is equal to 1, so

$$S_i^+ S_{i+1}^- = c_i^\dagger c_{i+1}. \quad (72)$$

The string cancels completely. We can check directly, with the same identities, that  $S_{i+1}^- S_i^+$  gives the same operator, which confirms that these two spin operators commute as they must. So *nearest-neighbor* hopping maps to a local spin term without a string, while longer-range hopping does not. This is the reason why the Jordan-Wigner transformation works so well with one-dimensional tensor-network methods for nearest-neighbor models. The models for which we build MPS Hamiltonians never need the string explicitly, since the string only guarantees the consistency of the mapping and never enters the Hamiltonian that we give to the solver.

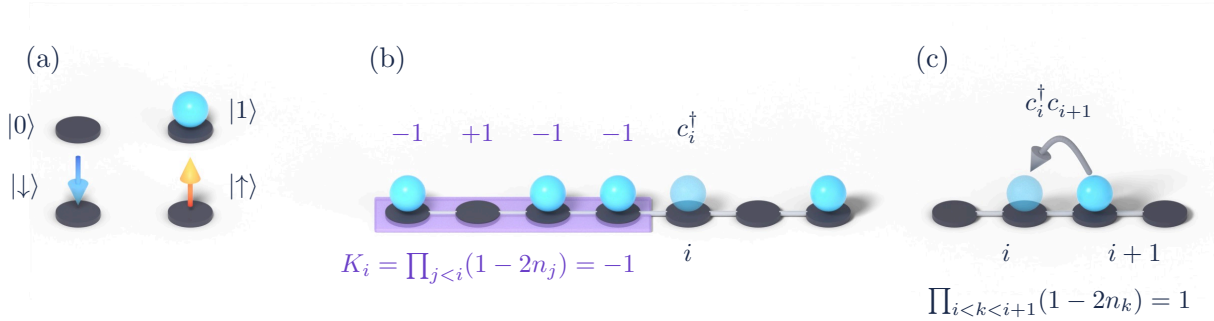


**Figure 21:** The Jordan-Wigner string, and why it usually does not appear. (a) The local Hilbert spaces matched site by site. A spinless fermionic site, behind, is either empty or occupied, and a spin- $\frac{1}{2}$ , in front, points either down or up, so  $|0\rangle \leftrightarrow |\downarrow\rangle$  and  $|1\rangle \leftrightarrow |\uparrow\rangle$  is a clean bijection. The picture cannot show the mismatch that the rest of the section corrects, which is that operators on different fermionic sites anticommute, while spin operators on different sites commute. (b) The dictionary of Eq. (70) attaches the parity factor  $K_i = \prod_{j < i} (1 - 2n_j)$  to  $c_i^\dagger$ , which puts an electron on the ghosted site. Every shaded site to the left of  $i$  contributes  $-1$  if it is occupied and  $+1$  if it is empty, so for the three electrons to its left  $K_i = -1$ . This string to the left of the site is what corrects the mismatch. (c) On a nearest-neighbor bond the product in Eq. (71) runs over the empty range  $i < k < i+1$ , so the string is 1 and the spin bilinear reduces to the bare hop of the electron from  $i+1$  to  $i$ . This is why the models for which we build matrix product state Hamiltonians never meet the string explicitly.

### 5.1.5 The practical recipe

Putting all this together, the scheme that we use for the rest of this session has four steps. First, we start from an interacting fermionic Hamiltonian. Second, we rewrite it site by site and bond by bond as an equivalent spin Hamiltonian using Eq. (70), which for nearest-neighbor models has no explicit strings. Third, we solve this *artificial* spin Hamiltonian, which does not look physical, with the MPS tools of Session 4. Fourth, we map the expectation values back to the fermionic language with the same dictionary in reverse. In practice, once this is set up, we can think of it as a many-body solver for interacting fermions and forget about the string. This is what the `fermionchain` class of `dmrgpy` does internally for every calculation in the companion notebook, which uses open boundary conditions everywhere. This matters because the cancellation of the string for nearest-neighbor hopping in Section 5.1 relies on a fixed ordering of the sites from left to right. On a periodic chain, the bond that closes the ring is not nearest-neighbor in this ordering, and it gets an explicit string that depends on the filling, which is one more reason to use open chains.

For a Hubbard-type model with spin, each site has two fermionic flavors,  $c_{i\uparrow}^\dagger$  and  $c_{i\downarrow}^\dagger$ , so the recipe above needs one more choice. Before we can apply Eq. (70), we need an explicit ordering of all the  $2L$  orbitals along a single one-dimensional string. The natural option is to interleave them site by site,  $\uparrow_1, \downarrow_1, \uparrow_2, \downarrow_2, \dots$ , so that operators on the same site stay next to each other. The other option is to put all the up spins first and all the down spins after them,  $\uparrow_1, \dots, \uparrow_L, \downarrow_1, \dots, \downarrow_L$ , which keeps the hopping of each spin sector local but turns the onsite  $U$  term into a long string. Both orderings are exact, and `dmrgpy` chooses one for us internally, so keep in mind that this choice exists when you see a spinful Jordan-Wigner string written somewhere else.

## 5.2 The spinless interacting chain at large scale

### 5.2.1 The model and its two limits

Let us now use these tools for a model that we already know well from Session 3, which is spinless fermions with nearest-neighbor hopping and nearest-neighbor repulsion,

$$\mathcal{H}_{\text{CDW}} = -t \sum_i \left( c_i^\dagger c_{i+1} + \text{h.c.} \right) + V \sum_i n_i n_{i+1}. \quad (73)$$

We already know its two limits. At  $V = 0$  it is a free-fermion metal, and for  $V \rightarrow \infty$  it becomes a charge density wave, with one electron on every other site. What exact diagonalization could not tell us clearly is where between these two limits the transition happens, because  $L \lesssim 16$  is too small to see a sharp thermodynamic phase transition. MPS will answer this question for us.

### 5.2.2 The equivalence with the XXZ chain

Before the numerics, let us look at the Jordan-Wigner image of Eq. (73), because it connects us again to a model from Session 2. Using Eq. (70) and (71) for neighboring sites, the hopping term becomes  $-t(S_i^+ S_{i+1}^- + \text{h.c.}) = -2t(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y)$ . The density term is diagonal and easy to translate,  $n_i n_{i+1} = S_i^z S_{i+1}^z + \frac{1}{2}(S_i^z + S_{i+1}^z) + \frac{1}{4}$ . Summed over the whole chain, the linear term  $\frac{1}{2} \sum_i (S_i^z + S_{i+1}^z)$  is equal to  $V S_{\text{tot}}^z$ , up to the two boundary sites that do not cancel. This is a uniform field that commutes with the hopping in the bulk and only shifts the energy at fixed filling, meaning at fixed  $S_{\text{tot}}^z$ . The remaining  $O(1)$  boundary field on the first and last site does not commute with the hopping in the bulk, but it is a boundary effect that does not change the transition in the bulk, so we drop it here, and we are left with

$$\mathcal{H}_{\text{CDW}} \longleftrightarrow \sum_i \left[ -2t (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) + V S_i^z S_{i+1}^z \right] + \text{const.} \quad (74)$$

This is the **XXZ chain** with anisotropy  $\Delta \equiv V/(2t)$ . Its exact Bethe-ansatz solution puts the transition between a gapless easy-plane phase and a gapped Néel-ordered phase exactly at the isotropic Heisenberg point  $\Delta = 1$ , which is at  $V = 2t$ . We should keep this number in mind, since we will find it again numerically. Panel (a) of Figure 22 shows the dictionary on a single bond, where the hop of an electron is the flip-flop of an up and a down spin, and two neighboring electrons are two neighboring up spins.

### 5.2.3 Charge order from a pinning field

A Hamiltonian with translational symmetry cannot spontaneously break this symmetry in a finite calculation, since the ground state stays a symmetric superposition of the two CDW patterns. For this reason, here and also in the mean-field discussion of Session 1, we add an infinitesimal seed that breaks the symmetry, and we see whether the bulk amplifies it or screens it. Let us take a chain of  $L = 100$  sites, add a small pinning term that favors a bit less charge on the first site and a bit more on the last one, and look at the resulting charge profile  $\langle n_i \rangle$ .

For strong interaction,  $V = 40t$ , the pinning is enough for the whole chain to lock into the charge-ordered pattern, with high and low density alternating from one edge to the other. This tells us clearly that we are inside the symmetry-broken phase. For moderate interaction,  $V = t$ , the result is completely different. The charge oscillates near the pinned edge, but the amplitude of the oscillation decays as we move into the bulk, and in the middle of the chain the density has

gone back to the uniform value  $\langle n_i \rangle = \frac{1}{2}$ . In other words, the bulk screens the perturbation, which is the signature of a phase that does *not* break translational symmetry, even though  $V = t$  is a sizeable interaction. Panel (b) of Figure 22 shows the two profiles next to each other.

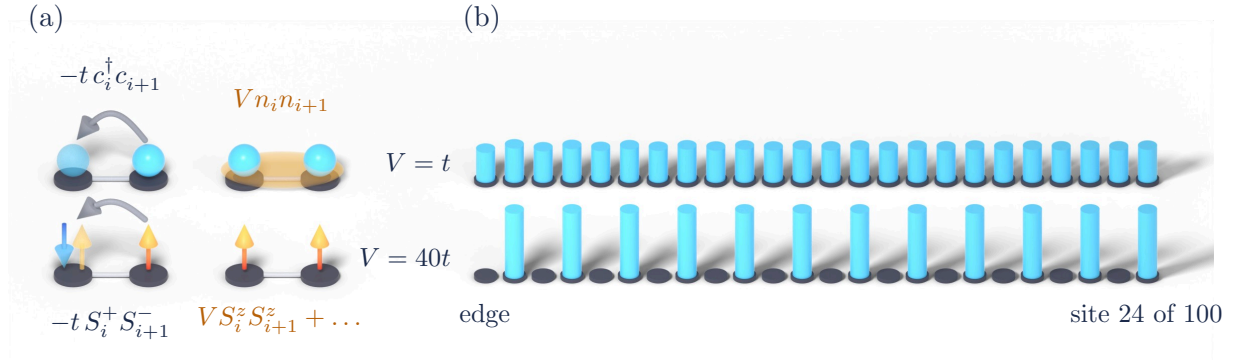


**Figure 22:** The spinless chain as the XXZ chain, and charge order from a pinning field. (a) The dictionary of Eq. (74) on one bond, with fermions behind and spins in front. The hop of an electron from  $i + 1$  to  $i$  is the flip-flop  $S_i^+ S_{i+1}^-$ , where the ghosts mark where the electron and the up spin end up. The repulsion of two neighboring electrons, which is the energy cost in amber, is the Ising term  $V S_i^z S_{i+1}^z$  together with the uniform field that we drop at fixed filling. (b) The density  $\langle n_i \rangle$  on the first 24 of the  $L = 100$  sites, shown as columns whose height is the density. It is computed with the density matrix renormalization group at  $\chi = 20$  and with the pinning  $m(n_1 - n_L)$ ,  $m = 0.1t$ , of the notebook, and the sweeps start from the charge pattern that the pinning favors. For  $V = t$ , behind, the pinned edge leaves an oscillation of a few percent that dies out into the bulk, meaning that the bulk screens the seed, while for  $V = 40t$ , in front, every site is full or empty from the edge on, meaning that the bulk amplifies it.

#### ✕ Computational companion

Section “Charge expectation value for weak and strong interactions.” Plot  $\langle n_i \rangle$  along the  $L = 100$  chain for  $V = 40t$  and  $V = t$ , and confirm the two behaviors described above, which are saturated order in the first case and a decaying edge oscillation in the second. Section “Charge density in the presence of an impurity” lets you repeat almost the same diagnostic with the perturbation placed inside the chain instead of at the edge. Moving it to the middle is a good way to convince yourself that the effect is a bulk property and not an artifact of the boundary.

#### 5.2.4 The phase transition at $V_c$

We can make the qualitative picture above quantitative by changing  $V$  continuously and following the bulk charge imbalance as a function of  $V$ , or equivalently the site density deep in the chain, far from the pinning. Below a critical value, the bulk density stays flat at  $\langle n \rangle = \frac{1}{2}$  regardless of how strongly we pin the edges. Above it, the bulk itself develops a finite charge imbalance, and the pinning field is only needed to select which of the two equivalent sublattices orders. Numerically this happens at  $V_c \approx 2t$ , in agreement with the exact XXZ result that we derived in Eq. (74). This is a quantum phase transition in the thermodynamic limit, which is a nonanalyticity of the ground state as a function of  $V$  at zero temperature. Exact diagonalization with the  $L \sim 12$  to 14 of Session 3 could not resolve it sharply, and the transition only becomes sharp at the  $L \sim 100$  scale that MPS gives us.

### ✕ Computational companion

Section “Phase transition in a repulsive fermionic model.” Change  $V$  and locate where the bulk density departs from 0.5, and check that this matches  $V_c \approx 2t$ . Then repeat the whole calculation with a much smaller chain,  $L = 10$ , and see how much less sharp the transition becomes. This shows directly why we needed to go beyond exact diagonalization.

## 5.3 Correlators as a diagnostic of the phases

Pinning fields and density profiles are intuitive, but they need an explicit term that breaks the symmetry. A cleaner diagnostic, without any field, comes from nonlocal correlation functions, and it generalizes something that we already used for the Heisenberg model in Session 2.

### 5.3.1 The nonlocal particle-particle correlator

We define the single-particle correlator between the first site and site  $n$ ,

$$C(n) \equiv \langle c_1^\dagger c_n \rangle. \quad (75)$$

Physically, this is what a Kubo-formula response calculation would give if we pinned site 1 with an infinitesimal field and measured the induced amplitude at site  $n$ . So it contains the same physics as the pinning-field experiment of Section 5.2, but in a single object without any field. In a gapless metallic phase,  $C(n)$  decays only as a power law,  $C(n) \sim n^{-\alpha}$ , because there are excitations at arbitrarily low energy that keep correlations alive at arbitrarily long distance. This is the same phenomenology that we found for the gapless quantum magnet in Session 2. In a gapped insulating phase, on the other hand,  $C(n)$  decays exponentially,

$$C(n) \sim e^{-n/\xi}, \quad (76)$$

where  $\xi$  is the **correlation length**, which is set by the energy gap. A finite energy is needed to create an excitation, and this finite energy cost is what kills correlations beyond a finite distance.

For the model of Eq. (73), both  $V = 0$  and  $V = t$  give a power-law decay, which is a straight line on a log-log plot, while  $V = 6t$ , deep in the charge-ordered phase, gives instead a straight line on a *log-linear* plot, meaning an exponential decay. This is the same contrast between the  $V = 0/1$  metal and the  $V = 6$  insulator that we already expected qualitatively in Section 5.2, and now it is completely quantitative.

### ✕ Computational companion

Section “Non-local static correlators for the particle-particle response of a large interacting fermionic model.” Plot  $\ln|C(n)|$  against  $n$  for a few values of  $V$ , and confirm that the metal gives a slowly varying curve, which is a power law, while the CDW gives a straight line, which is an exponential decay with slope  $-1/\xi$ .

### 5.3.2 Pairing correlators and the Cooper-pair susceptibility

Everything so far involved moving a single electron. Let us now ask a different question, which is how much the ground state wants to create or destroy a *pair* of electrons at the same time. We

define the local bond-pair annihilation operator  $\Delta_i \equiv c_i c_{i+1}$  and its correlator,

$$P(i, j) \equiv \langle \Delta_j^\dagger \Delta_i \rangle = \langle c_{j+1}^\dagger c_j^\dagger c_{i+1} c_i \rangle. \quad (77)$$

This is a new object, with no analogue in Session 3, where we never asked two-particle questions of this kind. It is a four-point correlator, also called a two-particle correlator, and it measures how correlated the destruction of a pair near  $i$  is with the creation of a pair near  $j$ . By the same Kubo-formula argument as before, it is what determines the linear response of the system to an external pairing field, which is what is called its **Cooper-pair susceptibility**.

For the repulsive model of Eq. (73),  $P(i, j)$  decays faster than in the noninteracting case. Repulsion discourages two electrons from being close to each other, so it *quenches* pairing fluctuations. If instead we change the sign of the interaction and make it attractive,  $V < 0$ , the correlator decays more slowly than in the noninteracting case, meaning that the system is more willing to host a fluctuating pair. This is the microscopic seed of Cooper pairing and superconductivity, which is the same attractive channel that we mentioned in Session 1 but did not study further. So repulsive interactions suppress pair correlations, and attractive interactions enhance them.

#### ✕ Computational companion

Section “Non-local pairing fluctuations of an attractive fermionic model.” Compare  $P(i, j)$  for  $V = 0$ , a repulsive  $V > 0$  and an attractive  $V < 0$ , and confirm that repulsion makes the pairing correlator decay faster than in the free case, while attraction makes it decay slower.

## 5.4 Spin-charge separation in the Hubbard model at large scale

### 5.4.1 The Hubbard chain and its two kinds of excitations

Let us now include spin again and go back to the Hubbard model,

$$\mathcal{H}_{\text{Hub}} = -t \sum_{i\sigma} \left( c_{i\sigma}^\dagger c_{i+1,\sigma} + \text{h.c.} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (78)$$

In Session 3 we already saw, with exact diagonalization on small chains, that at strong  $U$  this model shows **spin-charge separation**. The individual electron cannot be split, but the collective low-energy excitations of the many-body ground state can. Charge excitations are gapped, since it costs a finite energy  $\sim U$  to move a charge across the Mott-insulating background. Spin excitations are instead gapless, because at half filling and strong  $U$  the Hubbard model maps to the Heisenberg antiferromagnet of the superexchange derivation of Session 1, and the Heisenberg model is a gapless quantum magnet with fractional spin- $\frac{1}{2}$  spinon excitations, as we studied directly in Session 2. What large system sizes give us here is that we can see this contrast not as a hint in a few energy levels, but as two very different decay laws in real space.

### 5.4.2 Charge gap from the particle-particle correlator

As in Section 5.3, we follow  $C(n) = \langle c_{1\sigma}^\dagger c_{n\sigma} \rangle$ . At  $U = 0$  the chain is a free-fermion metal and  $C(n)$  decays as a slow power law. When we turn on  $U$ , the decay becomes faster and faster, and once  $U$  is large enough to open the Mott gap,  $C(n)$  decays exponentially, with a correlation

length that becomes shorter as  $U$  grows. This is the signature of the charge gap that we are looking for.

#### ✕ Computational companion

Section “Non-local static correlators for the particle-particle response of a large Hubbard model” and, next to it, “Spin and charge correlator in the Hubbard model.” Plot  $\ln |C(n)|$  for increasing  $U$  and confirm the crossover from power-law to exponential decay, which is the charge gap seen in real space.

### 5.4.3 Gapless spin excitations from the spin-spin correlator

Let us now build the analogous correlator for spin instead of charge,  $\langle \mathbf{S}_1 \cdot \mathbf{S}_n \rangle$ . Since  $S_i^z = \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow})$  and  $S_i^+ = c_{i\uparrow}^\dagger c_{i\downarrow}$ , this is a *biquadratic* object in the fermionic operators, meaning a product of two fermion bilinears rather than a single one, but it is computed in the same way once it is written in the underlying MPS. The result is the mirror image of the charge correlator. At  $U = 0$  the spin correlator decays quickly, but as  $U$  grows it becomes *more* long-ranged, which is the opposite trend to the charge correlator. This is spin-charge separation written as two decay rates. Repulsion opens a gap in the charge sector while it keeps, and even enhances, the spin correlations, which is consistent with the mapping to a gapless Heisenberg spin chain at strong  $U$ .

#### ✕ Computational companion

Section “Spin-Spin non-local correlator of the Hubbard model.” Plot  $\ln |\langle \mathbf{S}_1 \cdot \mathbf{S}_n \rangle|$  for increasing  $U$  and confirm the opposite trend to the charge correlator, which is that the decay gets *slower* as  $U$  grows. Try also an attractive  $U$ , and think about why the roles of the spin and charge sectors should be exchanged in that case.

### 5.4.4 Pairing correlators in the Hubbard model

Finally, we define the onsite singlet pair operator  $\Delta_i^{\text{onsite}} \equiv c_{i\downarrow} c_{i\uparrow}$ , which is a different pairing channel from the nearest-neighbor bond operator  $\Delta_i$  of Section 5.3, and its correlator  $\langle (\Delta_j^{\text{onsite}})^\dagger \Delta_i^{\text{onsite}} \rangle$ . This is the direct analogue for the Hubbard model of the pairing susceptibility that we built in Section 5.3. The qualitative conclusion is the same as before, since repulsive  $U$  suppresses the pairing correlator with respect to the noninteracting case, while attractive  $U$  enhances it. With the two Hubbard results of this section, we have now seen the full statement that we announced at the beginning of the section. Repulsion opens a gap in the charge sector, leaves the spin sector gapless or even enhances it, and at the same time quenches pairing, which is the opposite of what an attractive interaction would do.

#### ✕ Computational companion

Section “Pairing correlators in the Hubbard model.” Repeat the comparison between repulsive and attractive interactions from the spinless case, now for the onsite singlet pairing correlator, and check that the same qualitative behavior appears.

## 5.5 The correlation entropy and the validity of mean-field theory

### 5.5.1 The need for a many-body description

In Sessions 4 and 5 we have assumed, without saying it, that we *need* the full many-body machinery and that mean-field theory is never enough. But is this always true? We now have a tool that answers this question directly from the exact ground state, without running a separate mean-field calculation and comparing energies by hand.

### 5.5.2 Definition via the correlation matrix

Let us take the same nonlocal correlator that we have used during the whole session,  $C_{ij} \equiv \langle c_i^\dagger c_j \rangle$ , but now we do not look at it as a single number for fixed  $i = 1$ . Instead, we look at it as an  $L \times L$  Hermitian matrix, which is called the **correlation matrix**. We diagonalize it,  $C = \sum_k \nu_k |k\rangle \langle k|$ , with real eigenvalues  $\nu_k$ .

Let us first assume that the ground state is a Slater determinant,  $|\Psi\rangle = \prod_{n \in \text{occ}} c_{a_n}^\dagger |\Omega\rangle$ , which is the kind of state that mean-field theory builds. In the single-particle basis that diagonalizes the mean-field orbitals,  $C_{ij}$  is diagonal, with a 1 for every occupied orbital and a 0 for every empty one, so  $C^2 = C$ . This means that the correlation matrix of a Slater determinant is a *projector*, and a projector has eigenvalues that are exactly 0 or 1, since  $\nu_k^2 = \nu_k$  forces  $\nu_k \in \{0, 1\}$ . This gives us a clean test. If every eigenvalue of  $C$  is exactly 0 or 1, the state is a single Slater determinant, or is equivalent to one, and mean-field theory can reach it exactly.

For a correlated ground state,  $C^2 \neq C$  in general, and the eigenvalues  $\nu_k$  are spread continuously over  $[0, 1]$  instead of sitting at the two endpoints. We can quantify how far we are from the product-state limit with an entropy that is built in the same way as a binary Shannon entropy for each occupation probability  $\nu_k$ ,

$$S_{\text{corr}} = - \sum_k \left[ \nu_k \ln \nu_k + (1 - \nu_k) \ln(1 - \nu_k) \right]. \quad (79)$$

Every term in the sum vanishes when  $\nu_k \in \{0, 1\}$  and is strictly positive otherwise, so  $S_{\text{corr}} = 0$  if and only if the ground state is exactly a Slater determinant. The larger  $S_{\text{corr}}$  is, the further the true ground state is from anything that a single mean-field calculation could produce, regardless of how it was initialized. Figure 23 shows the eigenvalues  $\nu_k$  as the fillings of cups, for a Slater determinant and for a correlated ground state.

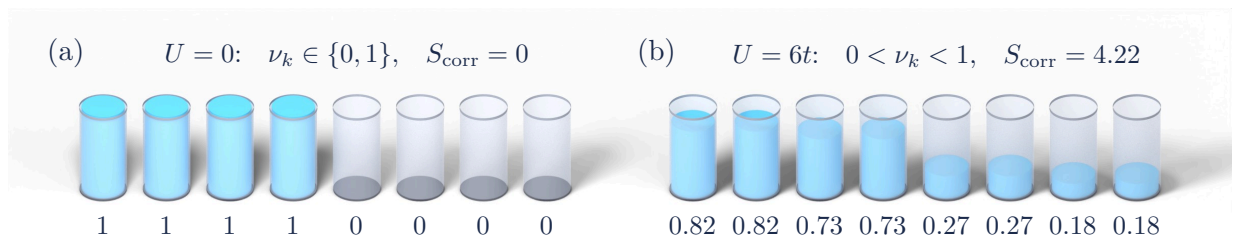


**Figure 23:** The eigenvalues of the correlation matrix, with one cup per natural orbital  $|k\rangle$  filled to  $\nu_k$ . (a) A Slater determinant, which is the four-site Hubbard chain of the notebook at  $U = 0$  and half filling. Every cup is full or empty, so every term of Eq. (79) vanishes and  $S_{\text{corr}} = 0$ . (b) The same chain at  $U = 6t$ , from exact diagonalization. The eight eigenvalues come in spin pairs, 0.82, 0.73, 0.27 and 0.18, no cup is full or empty, and  $S_{\text{corr}} = 4.22$ , meaning that no single Slater determinant reproduces this ground state. What  $S_{\text{corr}}$  measures is how far the cups are from being full or empty.

### 5.5.3 Applied to the spinless chain

Let us apply Eq. (79) to the model of Eq. (73). We already know that both of its limits are in fact product states. At  $V = 0$  the ground state is the filled Fermi sea, which is a Slater determinant by construction. At  $V \rightarrow \infty$  the ground state is the perfect charge-density-wave pattern, with one electron on a site, none on the next one and so on, which is also exactly a single Slater determinant, only in real space instead of momentum space. So  $S_{\text{corr}} \rightarrow 0$  at both ends. In between, and in particular close to the critical point  $V \approx 2t$  that we found in Section 5.2, the correlation entropy has a clear peak. This is the regime where the ground state is most entangled and furthest from a description with a single Slater determinant, and it coincides with the quantum phase transition itself, since critical points are in general where correlations, and therefore entanglement, are strongest.

#### ✕ Computational companion

Section “The correlation entropy of an interacting fermionic model.” Plot  $S_{\text{corr}}$  as a function of  $V$  and confirm that it vanishes both at  $V = 0$  and at large  $V$ , with a peak near  $V \approx 2t$ . Then make the system smaller and see how the height and the position of the peak change. This connects directly to the finite-size effects that we already saw for the phase transition itself.

### 5.5.4 Driving a quantum magnet toward its mean-field solution

We can make this diagnostic even more concrete by building, in a single Hamiltonian, a controlled crossover between a strongly correlated state and a mean-field one. Let us take the Hubbard model and add exactly the staggered mean-field magnetic term that the self-consistent loop of Session 1 would have generated by itself, which is the same staggered field that we switched on in Session 3,

$$\mathcal{H} = \mathcal{H}_{\text{Hub}} + J_z \sum_i (-1)^i S_i^z. \quad (80)$$

At  $J_z = 0$  this is the ordinary Hubbard model, which at strong  $U$  and half filling behaves like a gapless quantum antiferromagnet. This state is similar to a spin liquid, in the sense that the local magnetization vanishes everywhere by symmetry, even though the spin-spin correlations are long-ranged. When we turn on  $J_z$ , we explicitly push the ground state toward the symmetry-broken state with staggered magnetization that mean-field theory would give us directly. And indeed, as  $J_z$  grows, the correlation entropy of Eq. (79) decreases systematically. The ground state is pushed by hand toward the kind of product-like, symmetry-broken state to which a self-consistent mean-field calculation would converge by itself. This brings us back to Session 1. In Session 3 we saw the magnetization grow with this same field, and now we can also see quantitatively how much entanglement is lost in the product-state simplification that mean-field theory always makes, and so when it is a good approximation and when it is not.

#### ✕ Computational companion

Section “From a quantum magnet to a symmetry broken mean field magnet.” Change the staggered field  $J_z$  and look at how the local staggered magnetization grows and the correlation entropy decreases. Then increase  $U$ , check how the correlation entropy at  $J_z = 0$  changes, and think about why a stronger  $U$  should push the system further from a mean-field description, or closer to it.

### ✕ Computational companion

The notebook also contains three sections that go beyond these notes and develop the same tools further. Section “Energy of interacting spinless fermions as a function of the system size” looks again at how the finite-size scaling of the ground-state energy lets you extrapolate to the thermodynamic limit. Section “Magnetic correlations in a dimerized Hubbard model” asks how alternating strong and weak bonds change the spin correlator that we built in Section 5.4. Section “Correlation entropy of the Anderson model” applies the correlation entropy of Section 5.5 to a single correlated impurity coupled to a metallic host, and follows how the entropy is distributed in space around the impurity. They are natural extensions to try once you have worked through the sections above.

## 5.6 The general tensor-network algorithm

We have now used matrix product states a lot, during two full sessions, without looking at how the ground-state search is actually done. Let us finish by doing this.

### 5.6.1 Diagrammatic notation

It helps a lot to draw tensors instead of writing out their indices. A scalar is a dot with no legs, a vector is a dot with one leg, a matrix is a dot with two legs, and a general rank-three tensor is a dot with three legs, with one leg per index. Contracting an index between two tensors, meaning summing over it, is drawn by joining the corresponding legs into a single line. For instance, a matrix-vector multiplication is a dot with two legs joined to a dot with one leg along one shared leg, which leaves one free leg, so the result is a vector again, as it should be. An MPS is then a one-dimensional chain of such dots. Each site has one *physical* leg, of dimension 2 for a spin- $\frac{1}{2}$  or, after Jordan-Wigner, for a spinless-fermion site, and two *bond* legs of dimension  $\chi$  that connect it to its left and right neighbors,

$$|\Psi\rangle = \sum_{\{s_i\}} M_1^{s_1} M_2^{s_2} \cdots M_L^{s_L} |s_1 s_2 \cdots s_L\rangle, \quad (81)$$

where each  $M_i^{s_i}$  is a  $\chi \times \chi$  matrix, with a row and a column vector at the two ends, and the matrix product along the chain is exactly the string of joined bond legs in the diagram. The bond legs have no physical meaning by themselves. They are the bookkeeping that allows a single tensor to encode the entanglement between the two halves of the chain that it separates, with the bound  $S_A \leq \ln \chi$ , which is the entanglement-entropy bound that we derived in Session 4.

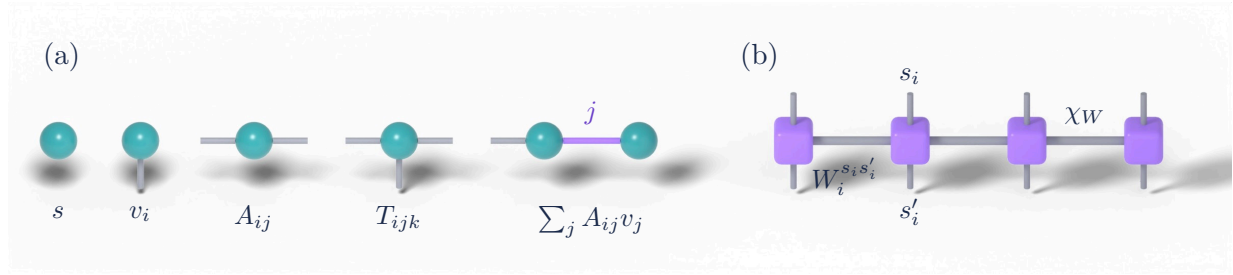


**Figure 24:** Diagrammatic notation for tensors, and the matrix product operator. (a) A dot with one leg per index. A scalar  $s$  has no legs, a vector  $v_i$  has one, a matrix  $A_{ij}$  has two and a rank-three tensor  $T_{ijk}$  has three. Summing over an index shared by two tensors is drawn by joining the corresponding legs, here the leg  $j$  of a matrix and of a vector, so what is left has one free leg and is a vector again, exactly as it should be for a matrix-vector multiplication. (b) A matrix product operator, which is the operator version of the matrix product state that we used in Session 4. Each site tensor  $W_i^{s_i s'_i}$  has two physical legs, one up for the row index  $s_i$  and one down for the column index  $s'_i$ , in addition to the two internal bond legs, here of dimension  $\chi_W$ , and the tensors at the ends have a single bond leg. For a nearest-neighbor Hamiltonian these internal bonds only need to carry a few states, which is enough to encode  $\mathcal{H}$  exactly and not approximately.

### 5.6.2 Matrix product operators

Hamiltonians need the same treatment. A **matrix product operator (MPO)** is the operator version of an MPS. Instead of one physical leg per site we now have two, one for the row index and one for the column index of the local operator, together with the same two internal bond legs as before,

$$\mathcal{H} = \sum_{\{s_i, s'_i\}} W_1^{s_1 s'_1} W_2^{s_2 s'_2} \cdots W_L^{s_L s'_L} |s_1 \cdots s_L\rangle \langle s'_1 \cdots s'_L|. \quad (82)$$

For a nearest-neighbor Hamiltonian such as  $\mathcal{H}_{\text{Heis}} = J \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1}$ , this internal bond dimension, which we call  $\chi_W$ , can be made very small. It only needs to be large enough to store whether nothing has happened yet, whether an  $S^x$ ,  $S^y$  or  $S^z$  was just placed and waits for its partner on the next site, or whether the interaction has already been closed. So a few internal states per bond are enough to represent the exact Hamiltonian, and not an approximation to it. Panel (b) of Figure 24 shows this chain of operator tensors.

### 5.6.3 Contraction and compression when applying $\mathcal{H}$ to a state

The operation that we need again and again is  $\mathcal{H}|\Psi\rangle$ . In diagrams, this means joining the physical legs of the MPO to the physical legs of the MPS, one site at a time, and merging the two bond legs that now run in parallel between neighboring sites, one from the MPS and one from the MPO, into a single wider bond. The result is again an MPS, but with bond dimension  $\chi\chi_W$ , which is the product of the two bond dimensions that we started with. This is the practical cost of contraction. Every time we act with  $\mathcal{H}$ , the bond dimension grows, and if we did this many times without doing anything else, it would grow exponentially and we would lose the whole advantage of using an MPS. The solution is the same tool that we already used for state compression in Session 4, which is a singular value decomposition on every bond, where we keep only the largest  $\chi$  singular values and discard the rest. This is equivalent to keeping the  $\chi$  largest eigenvalues of the reduced density matrix across that bond. Because the entanglement in a gapped one-dimensional

system saturates at a finite value, this truncation introduces only a small and controllable error, and it is the most important practical operation behind every tensor-network calculation that we have run in this session.

#### 5.6.4 The DMRG sweep as a variational search

Finally, how do we actually find the ground state, and not only apply  $\mathcal{H}$  once? We treat the MPS as a variational ansatz and minimize the energy functional directly. We introduce a Lagrange multiplier  $\lambda$  to enforce normalization, so we want a stationary point of

$$f[\{M\}] = \langle \Psi[\{M\}] | \mathcal{H} | \Psi[\{M\}] \rangle - \lambda (\langle \Psi[\{M\}] | \Psi[\{M\}] \rangle - 1). \quad (83)$$

The key simplification, and the reason why this problem can be solved at all, is that  $|\Psi\rangle$  is *linear* in any single one of its tensors  $M_i^{s_i}$  once all the others are fixed. We set  $\partial f / \partial M_i^{s_i} = 0$  at fixed neighbors and contract all the tensors that we are not currently changing, on both the bra and the ket side, together with the Hamiltonian MPO. This reduces the whole exponentially large problem to a small effective eigenvalue equation that lives only on the local space at site  $i$ , which is the product of the physical space and the two bond spaces,

$$H_{\text{eff}}(i) M_i^{s_i} = \lambda M_i^{s_i}. \quad (84)$$

We diagonalize this small dense matrix, whose size is set by  $\chi$  and not by the full  $2^L$ -dimensional Hilbert space, and we keep the lowest eigenvector as the new  $M_i^{s_i}$ . Then we move to site  $i + 1$ , build its effective Hamiltonian again with the tensor at  $i$  that we just updated, and repeat. We sweep all the way to the right end of the chain and back to the left, and we repeat this sweep until the energy stops changing. This procedure is the **density matrix renormalization group (DMRG)** algorithm. In this sense, variational MPS optimization and DMRG are the same procedure, reached from two different starting points.

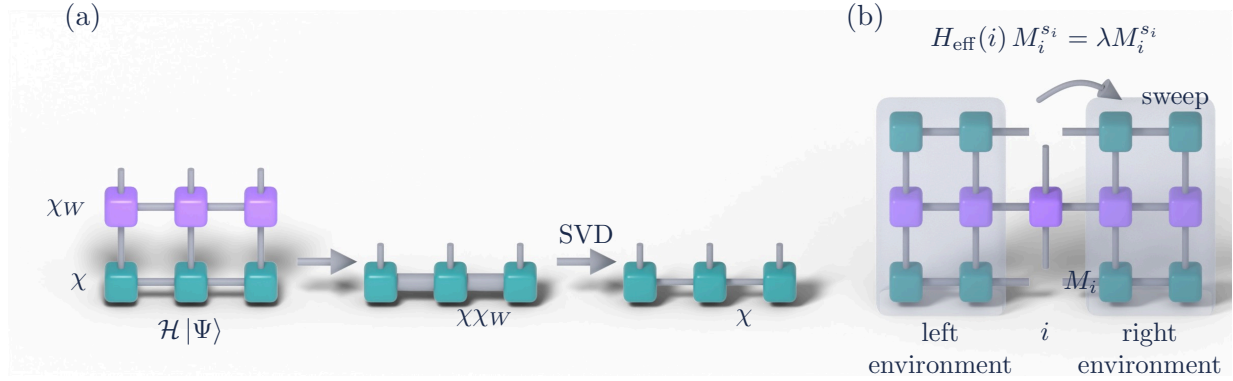


**Figure 25:** The two operations from which every calculation in these two sessions is built, with the tensors of the state in teal and those of the operator in violet. (a) Acting with  $\mathcal{H}$ , drawn by joining the column legs of the matrix product operator to the physical legs of the state one site at a time, with the legs of the state drawn pointing up so that the two chains stack. The two bond legs that now run in parallel, of dimensions  $\chi$  and  $\chi_W$ , merge into a single one of dimension  $\chi\chi_W$ , drawn thick. So the result is again a matrix product state, only with a larger bond dimension, and a singular value decomposition on every bond that keeps the largest  $\chi$  values compresses it back. (b) The variational ground-state search. The state, the operator and the conjugate state are stacked, and everything except site  $i$  is contracted into a left and a right environment, which are the shaded blocks. The tensors of the state and of its conjugate at  $i$  are left out, so what remains is  $H_{\text{eff}}(i)$  with the open legs on which  $M_i^{s_i}$  sits. This reduces the exponentially large problem to the small eigenvalue problem  $H_{\text{eff}}(i)M_i^{s_i} = \lambda M_i^{s_i}$  at that one site. Solving it, moving one site over and repeating, back and forth along the chain, is the DMRG sweep.

### 5.6.5 PEPS and MERA beyond matrix product states

Matrix product states are the simplest tensor-network architecture, with one tensor per site along a line, and this simplicity is the reason why they work so well in one dimension. The entanglement across any cut of a gapped 1D chain saturates, so a finite bond dimension is enough. The natural generalization to two dimensions is a **projected entangled pair state (PEPS)**, which gives every site one bond leg per lattice neighbor instead of only two. This allows it to capture the larger area-law entanglement of 2D systems, but there is a price, since we lose the cheap and exact contraction that we used during the whole session. Contracting a 2D tensor network exactly is computationally hard in general, and PEPS calculations rely on additional approximate contraction schemes. Critical, scale-invariant 1D systems give a related problem even in one dimension, since their entanglement grows logarithmically with subsystem size instead of saturating. This is the regime for which the **multiscale entanglement renormalization ansatz (MERA)** was built, which is a hierarchical network of alternating disentangling and coarse-graining tensors, organized in layers that follow the scale invariance of the critical point itself. We will not develop either of these further in this course, but it is useful to know that they exist. MPS is the first and most tractable member of a much larger family of variational tensor architectures, where each member gives more entanglement capacity at the cost of a harder optimization problem.

### Closing summary

- The Jordan-Wigner mapping identifies the fermionic and spin- $\frac{1}{2}$  local Hilbert spaces site by site, and fixes the resulting mismatch between anticommutation and commutation with

a string operator  $K_i$ . Nearest-neighbor fermionic hopping maps to a spin term without a string, which is the reason why MPS methods for 1D nearest-neighbor models fit fermionic chains so naturally.

- Mapping the fermionic Hamiltonian to its Jordan-Wigner spin image and solving it with MPS allows us to repeat the spinless CDW transition and the Hubbard spin-charge separation of Session 3 at  $L \sim 100$ . At this size the results are sharp and clear, and they are not blurred by the limit of exact diagonalization, which is  $L \sim 20$  for spinless fermions and half of that for the Hubbard chain. The transition of the spinless chain at  $V_c \approx 2t$  matches the exact XXZ result.
- Nonlocal particle-particle correlators distinguish gapless phases, with a power-law decay, from gapped phases, with an exponential decay. Pairing correlators, which are a new four-point diagnostic, show that repulsive interactions quench Cooper-pair fluctuations while attractive interactions enhance them, in both the spinless and the Hubbard models.
- The correlation matrix built from these correlators has eigenvalues in  $[0, 1]$ , which are exactly 0 or 1 only for a Slater determinant. The resulting correlation entropy measures how far a ground state is from any mean-field description. It has a peak at the phase transition of the spinless chain, and it decreases smoothly as a staggered field drives the Hubbard model toward its mean-field, symmetry-broken solution.
- The general tensor-network algorithm represents states as MPS and operators as MPOs. Applying  $\mathcal{H}$  makes the bond dimension grow, and this growth is controlled by a truncation based on the SVD. The variational ground-state search reduces, tensor by tensor, to a sequence of small effective eigenvalue problems that are solved by sweeping back and forth along the chain, which is the DMRG algorithm. PEPS and MERA extend the same idea to two dimensions and to critical systems, respectively, and they are beyond the scope of this course.
- Looking back at the whole course, mean-field theory, in Session 1, gives us a cheap approximation with polynomial cost that can fail qualitatively whenever the true ground state is entangled. Exact diagonalization, in Sessions 2 and 3, removes this failure completely but only for small systems, since the Hilbert space grows exponentially. Matrix product states, in Sessions 4 and 5, recover the exact many-body answer, including the entanglement, at the large system sizes that are meaningful for the thermodynamic limit. At these sizes the physics, such as phase transitions, fractionalization and spin-charge separation, becomes clear, and the cost stays polynomial as long as the entanglement stays bounded. This progression, from product states, to unrestricted but very small Hilbert spaces, to states with bounded entanglement at large sizes, is the main idea that connects the whole course.