

# PHYS 130C

## Part 1: Quantum Many-Body Physics

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### Qubits, Bosons and Fermions

#### ■ Introduction

#### ■ What are Quantum Many-Body Systems?

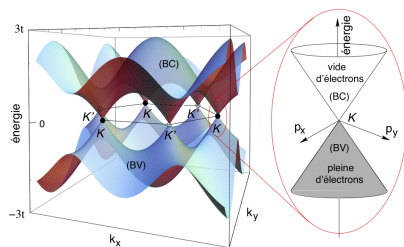
**Quantum many-body systems** are physical systems made up of a *large number of interacting* constituents, governed by the laws of *quantum* mechanics.

- *Electrons* in a solid, (CMP)
- *Ultra-cold atoms* in an optical lattice, (AMO)
- *Elementary particles* in a collider, (HEP)
- *Qubits* in a quantum computer. (QI)

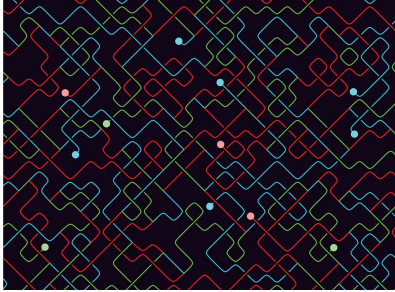
When many particles are **interacting** together, their **collective behavior** often leads to complex **emergent phenomena** that are dramatically different from just a few particles in isolation.

#### ■ What Make Them Interesting?

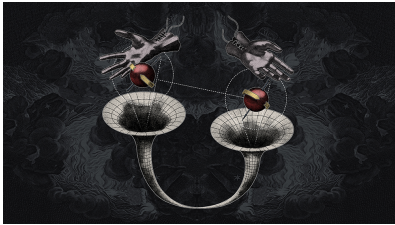
- **Everything can be Emergent**
  - Emergent **Particle**: Dirac fermions in graphene



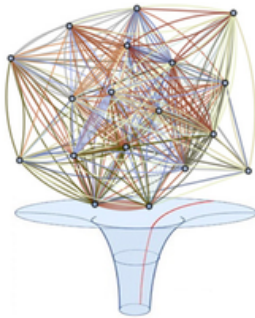
- Emergent **Force**: Gauge force in quantum magnets



- Emergent **Spacetime**: ER = EPR



- Emergent **Gravity**: SYK model



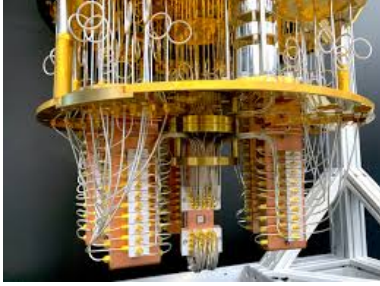
Conclusion: Despite the seemingly simple building blocks, many-body systems can display phenomena that are rich, surprising, and deeply beautiful.

- **Connection to Real-World Technology**

- **High-temperature superconductor**: strongly-correlated collective phenomenon of interacting electrons



- **Quantum computation**: store and process information by quantum many-body entanglement



- **Mathematical and Conceptual Beauty**
  - Topological phases of matter
  - Renormalization group (RG) theory
  - Quantum entanglement and tensor network
  - Emergent gauge theories
  - Holography and AdS/CFT correspondence

## ■ Qubits

### ■ Single Qubit

A **single qubit** is the simplest quantum system, representing the quantum analog of a classical bit (a *two-state* system). Unlike a classical bit, which can only be either 0 or 1, a qubit can be in a *superposition* of both states simultaneously.

#### • Quantum States

- A **pure state** of a qubit is represented by a *vector* in a 2-dimensional Hilbert space, spanned by the **basis states**  $|0\rangle$  and  $|1\rangle$ , which can be represented as one-hot vectors:

$$|0\rangle \simeq \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle \simeq \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (1)$$

- A generic state of a qubit is a *linear combination* of the basis states

$$|\psi\rangle = \psi_0 |0\rangle + \psi_1 |1\rangle \simeq \begin{pmatrix} \psi_0 \\ \psi_1 \end{pmatrix}, \quad (2)$$

where  $\psi_0, \psi_1 \in \mathbb{C}$  and  $|\psi_0|^2 + |\psi_1|^2 = 1$ .

#### • Physical Observables

- In quantum mechanics, physical observables are represented by **Hermitian operators**. The only observable for a single qubit is its **spin** or polarization, often measured along different axis.
- The **Pauli matrices** are basis of Hermitian operators, corresponding to the spin observable along three orthogonal axes.

$$\begin{aligned}
 X &:= |1\rangle\langle 0| + |0\rangle\langle 1| \simeq \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \\
 Y &:= i|1\rangle\langle 0| - i|0\rangle\langle 1| \simeq \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \\
 Z &:= |0\rangle\langle 0| - |1\rangle\langle 1| \simeq \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
 \end{aligned}$$

It is also useful to introduce the identity operator

$$I := |0\rangle\langle 0| + |1\rangle\langle 1| \simeq \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{4}$$

such that any Hermitian observable  $O$  can be written as

$$O = cI + xX + yY + zZ, \tag{5}$$

with  $c, x, y, z \in \mathbb{R}$ .

**Disclaimer:** different notations of Pauli operators

- Quantum information:  $X, Y, Z$  and  $I$ ;
- Condensed matter physics:  $\sigma = (\sigma^x, \sigma^y, \sigma^z) = (\sigma^1, \sigma^2, \sigma^3)$  and  $\sigma^0$ .
- **Measuring** a qubit in the **computational basis** ( $Z$  eigen basis) means measuring its  $Z$  observable.

If the qubit is in the state  $|\psi\rangle = \psi_0|0\rangle + \psi_1|1\rangle$ , measuring in the computational basis will:

- yield  $|0\rangle$  with probability  $|\psi_0|^2$ ,
- yield  $|1\rangle$  with probability  $|\psi_1|^2$ .

## ■ Two Qubits

A *composite system* of **two qubits** is described by a 4-dimensional Hilbert space, as the **tensor product** of the two individual qubit Hilbert spaces.

### • Quantum States

- Each qubit has *two* basis states:  $|0\rangle$  and  $|1\rangle$ , so two qubits have *four* **basis states**, arranged as follows:

	qubit 2
	$ 0\rangle \quad  1\rangle$
qubit 1	$ 0\rangle \quad  00\rangle \quad  01\rangle$
	$ 1\rangle \quad  10\rangle \quad  11\rangle$

We can choose to represent them as one-hot vectors:

0	1	2	3
$ 00\rangle$	$ 01\rangle$	$ 10\rangle$	$ 11\rangle$
⊞	⊞	⊞	⊞

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

This is also called the **computational basis** ( $Z_1$  and  $Z_2$  eigen basis).

- The mathematical construction of  $|01\rangle$  is a *tensor product* of  $|0\rangle$  and  $|1\rangle$  states, denoted as

$$|01\rangle = |0\rangle \otimes |1\rangle. \quad (7)$$

How to make sense of  $\otimes$  ?

- *Practically*, tensor product of two vectors means

$$\begin{array}{ccc} |0\rangle & \otimes & |1\rangle \\ \Downarrow & & \Downarrow \\ \begin{pmatrix} 1 \\ 0 \end{pmatrix} & \otimes & \begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{array} = \begin{array}{ccc} |01\rangle \\ \Downarrow \\ \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \end{array} \quad (8)$$

- *Formally*, **tensor product** is a *binary operation* that is *linear* in both factors:

$$\begin{aligned} & (\alpha_0 |0\rangle + \alpha_1 |1\rangle) \otimes (\beta_0 |0\rangle + \beta_1 |1\rangle) \\ &= \alpha_0 \beta_0 |0\rangle \otimes |0\rangle + \alpha_0 \beta_1 |0\rangle \otimes |1\rangle + \alpha_1 \beta_0 |1\rangle \otimes |0\rangle + \alpha_1 \beta_1 |1\rangle \otimes |1\rangle \\ &\stackrel{\text{short}}{=} \alpha_0 \beta_0 |00\rangle + \alpha_0 \beta_1 |01\rangle + \alpha_1 \beta_0 |10\rangle + \alpha_1 \beta_1 |11\rangle. \end{aligned} \quad (9)$$

The only way to implement this algebra correctly on the vector level is to require the tensor product be computed as (see also Eq. (8))

$$\boxed{\begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix} \otimes \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix} = \begin{pmatrix} \alpha_0 \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix} \\ \alpha_1 \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} \alpha_0 \beta_0 \\ \alpha_0 \beta_1 \\ \alpha_1 \beta_0 \\ \alpha_1 \beta_1 \end{pmatrix}.} \quad (10)$$

- Rules of tensor product on basis vectors

$$\begin{aligned} |a\rangle \otimes |b\rangle &= |ab\rangle, \\ \langle a| \otimes \langle b| &= \langle ab|, \end{aligned} \quad (11)$$

$$\begin{aligned} (|a\rangle \langle b|) \otimes (|c\rangle \langle d|) &= |ac\rangle \langle bd|, \\ \langle ac|bd\rangle &= (\langle a| \otimes \langle c|) (|b\rangle \otimes |d\rangle) = \langle a|b\rangle \langle c|d\rangle. \end{aligned} \quad (12)$$

## • Physical Observables

- Introduce the Pauli operators  $X_1, Y_1, Z_1$  for the first qubit, and  $X_2, Y_2, Z_2$  for the second qubit, any *physical observable* of a two-qubit system is described by a *Hermitian operator* as a linear combination of the followings:

- **Trivial observable:**

$$\mathbb{1} = I \otimes I. \quad (13)$$

- **Single-qubit observables:**

$$\begin{aligned} \text{qubit 1: } X_1 &= X \otimes I, Y_1 = Y \otimes I, Z_1 = Z \otimes I, \\ \text{qubit 2: } X_2 &= I \otimes X, Y_2 = I \otimes Y, Z_2 = I \otimes Z. \end{aligned} \quad (14)$$

- **Two-qubit observables** (joint measurements):

$$\begin{array}{c|c|c} X_1 & X_2 & X_1 Y_2 \\ \hline Y_1 & X_2 & Y_1 Y_2 \\ \hline Z_1 & X_2 & Z_1 Y_2 \end{array} \quad (15)$$

For example, by  $Z_1 Y_2$ , one means:

$$Z_1 Y_2 = (Z \otimes I)(I \otimes Y) = Z \otimes Y. \quad (16)$$

Altogether there are 16 *basis observables*.

- The **tensor product** of operator is defined as

$$\begin{aligned} A &= \sum_{ab} |a\rangle A_{ab} \langle b|, B = \sum_{cd} |c\rangle B_{cd} \langle d|, \\ \Rightarrow A \otimes B &= \sum_{abcd} |a\rangle \otimes |c\rangle A_{ab} B_{cd} \langle b| \otimes \langle d|. \end{aligned} \quad (17)$$

Practically, it is computed as

$$\begin{aligned} Z \otimes Y &\simeq \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ &= \begin{pmatrix} 1 \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} & 0 \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ 0 \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} & -1 \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & -i & 0 \end{pmatrix}. \end{aligned} \quad (18)$$

In *Mathematica*, you can use `KroneckerProduct` to calculate tensor product of matrices, such as:

```
KroneckerProduct[PauliMatrix[3], PauliMatrix[2]] // MatrixForm
```

**Exc  
1**

Represent the Hamiltonian  $H = X_1 X_2 + Y_1 Y_2 + Z_1 Z_2$  as a  $4 \times 4$  matrix in the computational basis. Diagonalize the matrix to find the eigen energies and corresponding eigen states.

By definition, operator tensor product has the following properties:

$$(A \otimes B)(C \otimes D) = (A B) \otimes (C D), \quad (20)$$

$$(\alpha A + \beta B) \otimes C = \alpha A \otimes C + \beta B \otimes C, \quad (21)$$

$$A \otimes (\beta B + \gamma C) = \beta A \otimes B + \gamma A \otimes C,$$

$$\text{Tr}(A \otimes B) = (\text{Tr } A)(\text{Tr } B). \quad (22)$$

## ■ Many Qubits

A  $N$ -qubit system is described by a  $2^N$ -dimensional Hilbert space, as tensor product of  $N$  single-qubit Hilbert spaces:

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3 \otimes \dots \otimes \mathcal{H}_N. \quad (23)$$

- **Quantum States:** a generic many-qubit quantum state

$$|\psi\rangle = \sum_{a_1 a_2 \dots} \psi_{a_1 a_2 \dots} |a_1 a_2 \dots\rangle = \sum_{[a]} \psi_{[a]} |[a]\rangle. \quad (24)$$

**Notation:** bundled index  $[a] = a_1 a_2 \dots a_N$ , with  $a_i = 0, 1$ , and

$$|[a]\rangle = |a_1\rangle \otimes |a_2\rangle \otimes \dots \otimes |a_N\rangle. \quad (25)$$

- **Physical Observables**

- A generic operator takes the form of

$$\begin{aligned} O &= \sum_{a_1 a_2 \dots} \sum_{b_1 b_2 \dots} |a_1 a_2 \dots\rangle O_{a_1 a_2 \dots, b_1 b_2 \dots} \langle b_1 b_2 \dots| \\ &= \sum_{[a],[b]} |[a]\rangle O_{[a],[b]} \langle [b]|. \end{aligned} \quad (26)$$

- Any operator  $O$  can be decomposed to a linear combination of **Pauli operators**  $P$  with some coefficients  $o_P$ ,

$$O = \sum_P o_P P, \quad (27)$$

where  $P$  takes the form of

$$P = P_1 \otimes P_2 \otimes \dots \otimes P_N, \quad (28)$$

with  $P_i \in \{I, X, Y, Z\}$ .

- There are all together  $4^N$  Pauli operators (including identity) for a  $N$ -qubit system.
- They form a set of *complete* and *orthogonal operator basis*.
- All Pauli operators can be *generated* by  $X_i$  and  $Z_i$ , constructed as

$$\begin{aligned} & \textit{ith factor} \\ & \downarrow \\ X_i &= \dots \otimes I \otimes I \otimes X \otimes I \otimes I \otimes \dots, \\ Z_i &= \dots \otimes I \otimes I \otimes Z \otimes I \otimes I \otimes \dots, \end{aligned}$$

(29)

or defined by the following **algebraic definitions**:

$$\begin{aligned}
X_i^2 &= Z_i^2 = \mathbf{1}, \\
X_i Z_i &= -Z_i X_i, \\
X_i Z_j &= Z_j X_i \text{ (for } i \neq j\text{)}.
\end{aligned}
\tag{30}$$

for all  $i, j \in \{1, 2, \dots, N\}$ .

- What about  $Y_i$ ? - It is simply defined as  $Y_i := i X_i Z_i$ .
- Such that any Pauli operator can be written as

$$P_{\xi, \zeta} = i^{\xi \cdot \zeta} \prod_i X_i^{\xi_i} \prod_i Z_i^{\zeta_i}, \tag{31}$$

uniquely labeled by two *binary vectors*  $\xi = (\xi_1, \xi_2, \dots, \xi_N)$  and  $\zeta = (\zeta_1, \zeta_2, \dots, \zeta_N)$  with  $\xi_i, \zeta_i = 0, 1$ . The factors of  $i$  are taken care of by  $i^{\xi \cdot \zeta}$ , where  $\xi \cdot \zeta$  means the dot product of the binary vectors.

Exc  
2

Check that the following four operators all commute:

$$X_1 X_2 X_4, Z_1 Z_2 X_3 X_4, Y_1 X_2 Y_3 Z_4, X_1 Z_2 Z_4,$$

using their operator algebra, without relying on explicit matrix representations.

HW  
1

Consider a four-qubit system, initially prepared in the *ground state*  $|\psi\rangle$  of the following Hamiltonian

$$H = -Z_1 X_2 Z_3 - Z_2 X_3 Z_4 - Z_3 X_4 Z_1 - Z_4 X_1 Z_2.$$

- On state  $|\psi\rangle$ , measure the 1st and 3rd qubits in  $X$  basis, suppose the outcome for the 1st qubit is  $X_1 = -1$ , what should be the measurement outcome of  $X_3$ ?
- After the measurement, suppose the system collapses to a new state  $|\phi\rangle$ . Compute the expectation value of  $X_2 X_4$  and  $Z_2 Z_4$  on the state  $|\phi\rangle$ .

## ■ Bosons

### ■ Single-Mode Bosons

**Bosons** are *identical particles* that can occupy a single-particle mode by any *natural number*  $n = 0, 1, 2, \dots$

- **Quantum states:** Boson occupation states

$$\begin{aligned}
|0\rangle & \text{ vacuum (empty)} \\
|1\rangle & \text{ one boson occupied} \\
|2\rangle & \text{ two bosons occupied} \\
& \vdots \\
|n\rangle & n \text{ bosons occupied} \\
& \vdots
\end{aligned}$$

- They are distinct *eigenstates* of the **boson number operator**  $\hat{n}$ ,



$$\hat{n} |n\rangle = n |n\rangle, \quad (33)$$

where  $n \in \mathbb{N}$  is the corresponding *eigenvalue*.

- They form a complete set of **orthonormal basis**,

$$\langle n|n'\rangle = \delta_{nn'}. \quad (34)$$

- They can be represented as **one-hot vectors**:

$$|0\rangle \simeq \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix}, |1\rangle \simeq \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix}, |2\rangle \simeq \begin{pmatrix} 0 \\ 0 \\ 1 \\ \vdots \end{pmatrix}, \dots \quad (35)$$

**Comment:** These vectors are infinite dimensional, because the Hilbert space dimension is infinite. In practice, we can (artificially) choose to *truncate* the Hilbert space dimension to some finite *maximal* boson number  $n_{\max}$  (if we don't care about states with that many bosons, as they are too high in energy).

- Any quantum state of single-mode bosons must be a *linear superposition* of the boson occupation states

$$|\psi\rangle = \sum_{n \in \mathbb{N}} \psi_n |n\rangle. \quad (36)$$

### • Boson Operators

- **Boson creation operator:**  $b^\dagger \leftrightarrow$  **Boson annihilation operator:**  $b$   
They are Hermitian conjugate to each other.

- Actions on boson occupation states

$$\begin{aligned} b^\dagger |n\rangle &= \sqrt{n+1} |n+1\rangle, \\ b |n\rangle &= \sqrt{n} |n-1\rangle. \end{aligned} \quad (37)$$

**Interpretation:** creation operator raise the boson number by one, and annihilation operator lowers the boson number by one, BUT there are *square root factors* (also known as *boson enhancement factors*) in the front.

- **Boson number operator** can be expressed as

$$\hat{n} = b^\dagger b. \quad (38)$$

**Exc**  
**3**

Using Eq. (37) to show that Eq. (38) can reproduce Eq. (33) consistently.

- **Boson commutation relation**

$$\begin{aligned} [b, b] &= [b^\dagger, b^\dagger] = 0, \\ [b, b^\dagger] &= \mathbf{1}. \end{aligned} \quad (40)$$

**Note:** commutator  $[A, B] := AB - BA$ .

In fact, this should be treated as the algebraic *definition* of the boson creation and annihilation operators.

**Exc  
4**

Use Eq. (37) to check that Eq. (40) holds for any state as operator identities.

- Boson operators can be represented as matrices

$$b^\dagger \simeq \begin{pmatrix} 0 & & & \\ \sqrt{1} & 0 & & \\ & \sqrt{2} & 0 & \\ & & \ddots & \ddots \end{pmatrix}, \quad b \simeq \begin{pmatrix} 0 & \sqrt{1} & & \\ & 0 & \sqrt{2} & \\ & & 0 & \ddots \\ & & & \ddots \end{pmatrix}, \quad (42)$$

such that the number operator is diagonal as expected

$$b^\dagger b \simeq \begin{pmatrix} 0 & & & \\ & 1 & & \\ & & 2 & \\ & & & \ddots \end{pmatrix}. \quad (43)$$

**Comment:** These are infinite dimensional matrices, due to infinite dimensional Hilbert space. In practice, we can truncate them to finite dimension by setting a (artificial) maximal boson number  $n_{\max}$ .

## ■ Multi-Mode Bosons

Bosons can also occupy *multiple* single-particle modes. Here a particular **single-particle mode** can refer to any of the following:

- a *momentum* eigenstate (a plane wave) for bosons to follow,
- a *position* eigenstate (a site on an optical lattice) for atoms to stay,
- a *cavity* eigenstate (a wave mode) for photons to populate,
- a *polarization* mode (transverse/longitudinal) for phonon to take ...

Different single-particle modes will be labeled by different **mode quantum number**  $\alpha$  (mode index).

- **Quantum States:** *Tensor product* of boson occupation states

$$|[n]\rangle = \bigotimes_i |n_i\rangle = |n_1\rangle \otimes |n_2\rangle \otimes |n_3\rangle \otimes \dots, \quad (44)$$

where  $n_i \in \mathbb{N}$  is the number of bosons occupying the  $i$ th mode.

$[n] = n_1 n_2 n_3 \dots$  denotes the sequence of boson occupation numbers.

- They are *joint* eigenstates of **boson number operators**  $\hat{n}_i$

$$\forall i: \hat{n}_i |[n]\rangle = n_i |[n]\rangle. \quad (45)$$

- They form a complete set of **orthonormal basis**,

$$\langle [n] |[n']\rangle = \prod_i \delta_{n_i n'_i}. \quad (46)$$

- Any quantum many-body state of multi-mode bosons must be a *linear superposition* of these boson occupation states.

## • Boson Operators

- For each mode  $i$ , define

**Boson creation** operator:  $b_i^\dagger \leftrightarrow$  **Boson annihilation** operator:  $b_i$

- Actions on boson occupation states

$$\begin{aligned} b_i^\dagger |\dots n_{i-1} n_i n_{i+1} \dots\rangle &= \sqrt{n_i + 1} |\dots n_{i-1} (n_i + 1) n_{i+1} \dots\rangle, \\ b_i |\dots n_{i-1} n_i n_{i+1} \dots\rangle &= \sqrt{n_i} |\dots n_{i-1} (n_i - 1) n_{i+1} \dots\rangle. \end{aligned} \quad (47)$$

**Comment:** the boson creation/annihilation operator only acts on the tensor product Hilbert space of its own mode, and has no side effect on other modes.

- **Boson number operator** of mode  $i$  can be express as

$$\hat{n}_i = b_i^\dagger b_i. \quad (48)$$

- **Boson commutation relations**

$$\begin{aligned} [b_i, b_j] &= [b_i^\dagger, b_j^\dagger] = 0, \\ [b_i, b_j^\dagger] &= \delta_{ij} \mathbf{1}. \end{aligned} \quad (49)$$

These relations should be considered as the algebraic *definition* of the boson creation and annihilation operator for multiple modes.

## ■ Fermions

### ■ Single-Mode Fermions

**Fermions** are *identical particles* that can occupy a single-particle mode by only *zero* or *one* particle, i.e.  $n = 0, 1$  — a rule known as the **Pauli exclusion principle**.

- **Quantum states:** Fermion occupation states

$|0\rangle$  vacuum (empty)

$|1\rangle$  one fermion occupied

and no more state. The Hilbert space dimension is 2.

- They are still distinct *eigenstates* of the **fermion number operator**  $\hat{n}$ ,

$$\hat{n} |n\rangle = n |n\rangle. \quad (50)$$

Just now the *eigenvalue* can only be  $n = 0, 1$ .

- They form a complete set of **orthonormal basis**, and can be represented as one-hot vectors:

$$|0\rangle \simeq \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |1\rangle \simeq \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (51)$$

**Question:** This looks just the same as a *single qubit*, right?

**Answer:** Yes, indeed, a single-mode fermion and a single qubit are *equivalent* quantum systems. But multi-mode fermions and multi-qubit system will be *different*, as we will see.

## • Fermion Operators

- **Fermion creation operator:**  $c^\dagger \leftrightarrow$  **Fermion annihilation operator:**  $c$   
They are Hermitian conjugate to each other.

- Actions on fermion occupation states

$$\begin{aligned} c^\dagger |0\rangle &= |1\rangle, & c^\dagger |1\rangle &= 0; \\ c |0\rangle &= 0, & c |1\rangle &= |0\rangle. \end{aligned} \quad (52)$$

**Note:** be careful to distinguish the *vacuum state*  $|0\rangle$  (meaning that there is such a state, and the state contains no particle) and the *zero vector*  $0$  (meaning that there is no such a state). In quantum mechanics, a 0 probability amplitude indicates the state is *impossible*.

- **Empty state can not be empty:** it is *impossible* to remove a fermion from the vacuum state, because there was no fermion there. Therefore, we have

$$c |0\rangle = 0. \quad (53)$$

- **Filled state can not be filled:** it is *impossible* to add a second fermion to a mode when it is already occupied by one fermion — the Pauli exclusion principle. Therefore, we have

$$c^\dagger |1\rangle = 0. \quad (54)$$

Interestingly, Eq. (52) can be summarized in two lines

$$\begin{aligned} c^\dagger |n\rangle &= \sqrt{1-n} |1-n\rangle, \\ c |n\rangle &= \sqrt{n} |1-n\rangle. \end{aligned} \quad (55)$$

**Interpretation:**  $n \leftrightarrow 1-n$  toggles between  $n = 0$  and  $n = 1$  state, as expected. The peculiar

- **Fermion number operator** can be expressed as

$$\hat{n} = c^\dagger c. \quad (56)$$

**Exc 5**

Use Eq. (55) to show that Eq. (56) can reproduce Eq. (33) consistently.

- **Fermion anticommutation relation**

$$\begin{aligned} \{c, c\} = \{c^\dagger, c^\dagger\} &= 0, \\ \{c, c^\dagger\} &= \mathbf{1}. \end{aligned} \quad (58)$$

**Note:** anticommutator  $\{A, B\} := AB + BA$ .

In fact, this should be treated as the algebraic *definition* of the fermion creation and annihilation operators.

**Exc 6**

Use Eq. (55) to check that Eq. (58) holds for any state as operator identities.

- For a single mode, fermion operators have simple  $2 \times 2$  matrix representations in the  $\{|0\rangle, |1\rangle\}$  basis

$$c^\dagger \simeq \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad c \simeq \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad (61)$$

such that the number operator is diagonal as expected

$$c^\dagger c \simeq \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \quad (62)$$

- **Jordan-Wigner transformation:** If the fermion occupation states are mapped to the qubit states, fermion operators can also be represented as Pauli operators, as

$$c^\dagger = \frac{X - iY}{2}, \quad c = \frac{X + iY}{2}, \quad c^\dagger c = \frac{I - Z}{2}. \quad (63)$$

## ■ Multi-Mode Fermions

Fermions can also occupy *multiple* single-particle modes, labeled by different **mode quantum number**  $i$  (mode index).

- **Quantum States:** *Tensor product* of fermion occupation states

$$|[n]\rangle = \bigotimes_i |n_i\rangle = |n_1\rangle \otimes |n_2\rangle \otimes |n_3\rangle \otimes \dots, \quad (64)$$

where  $n_i \in \mathbb{N}$  is the number of fermions occupying the  $i$ th mode.

$[n] = n_1 n_2 n_3 \dots$  denotes the sequence of fermion occupation numbers.

- They are *joint* eigenstates of **fermion number operators**  $\hat{n}_i$

$$\forall i: \hat{n}_i |[n]\rangle = n_i |[n]\rangle. \quad (65)$$

- They form a complete set of **orthonormal basis**,

$$\langle [n] |[n']\rangle = \prod_i \delta_{n_i n'_i}. \quad (66)$$

- Any quantum many-body state of multi-mode fermions must be a *linear superposition* of these fermion occupation states.

### • Fermion Operators

- For each mode  $i$ , define

**Fermion creation** operator:  $c_i^\dagger \leftrightarrow$  **Fermion annihilation** operator:  $c_i$

- Actions on fermion occupation states

$$\begin{aligned} c_i^\dagger |\dots n_{i-1} n_i n_{i+1} \dots\rangle &= (-)^{\sum_{j<i} n_j} \sqrt{1-n_i} |\dots n_{i-1} (1-n_i) n_{i+1} \dots\rangle, \\ c_i |\dots n_{i-1} n_i n_{i+1} \dots\rangle &= (-)^{\sum_{j<i} n_j} \sqrt{n_i} |\dots n_{i-1} (1-n_i) n_{i+1} \dots\rangle. \end{aligned} \quad (67)$$

**Comment:** the fermion creation/annihilation operator *not only* acts on its own mode. There is an important **fermion sign** that depends on the *parity* of the number of fermions occupying the *preceding* modes (for this to make sense, a canonical ordering of single-particle mode is required), because each exchange of two fermions will change the sign of the whole many-body state — a defining feature of fermions.

- **Fermion number operator** of mode  $i$  can be express as

$$\hat{n}_i = c_i^\dagger c_i. \quad (68)$$

- **Fermion commutation relations**

$$\begin{aligned} \{c_i, c_j\} &= \{c_i^\dagger, c_j^\dagger\} = 0, \\ \{c_i, c_j^\dagger\} &= \delta_{ij} \mathbf{1}. \end{aligned} \quad (69)$$

These relations should be considered as the algebraic *definition* of the boson creation and annihilation operator for multiple modes.

Eq. (69) implies the following rules:

- **No double action:** double creation or annihilation of fermions on the same mode  $i$  is forbidden

$$\begin{aligned} c_i c_i &= 0, \\ c_i^\dagger c_i^\dagger &= 0. \end{aligned} \quad (70)$$

- **Exchange minus sign:** exchanging two fermion operations of different modes ( $i \neq j$ ) will generate a minus sign (the fermion sign)

$$\begin{aligned}
c_i c_j &= -c_j c_i, \\
c_i^\dagger c_j^\dagger &= -c_j^\dagger c_i^\dagger, \\
c_i^\dagger c_j &= -c_j c_i^\dagger, \\
c_i c_j^\dagger &= -c_j^\dagger c_i.
\end{aligned} \tag{71}$$

- **Matter and anti-matter:**  $c_i^\dagger c_i$  counts the *number* of **particles** in the mode  $i$ , whereas  $c_i c_i^\dagger$  counts the *number* of **anti-particles** in the same mode:

$$c_i c_i^\dagger = \mathbf{1} - c_i^\dagger c_i. \tag{72}$$

state	particle	anti-particle	$c_i^\dagger c_i$	$c_i c_i^\dagger$
$ 0\rangle_i$	empty	occupied	0	1
$ 1\rangle_i$	occupied	empty	1	0

**Slogan:** where no particle is found, an anti-particle is bound.

operator	particle	anti-particle
creation	$c_i^\dagger$	$c_i$
annihilation	$c_i$	$c_i^\dagger$
number	$c_i^\dagger c_i$	$c_i c_i^\dagger$

It turns out that all **matter** in our universe are made of **fermions** (leptons and quarks), so **every matter has its anti-matter partner** — a profound symmetry encoded in the quantum mechanical rules of fermion operators.

These rules provides a better understanding of how fermion creation and annihilation operators acts on fermion occupation states:

- Consider a fermion system of 5 single-particle modes, the *vacuum* state is denoted as (modes are arranged from left to right)

$$|00000\rangle := |0\rangle_1 \otimes |0\rangle_2 \otimes |0\rangle_3 \otimes |0\rangle_4 \otimes |0\rangle_5. \tag{73}$$

- Any fermion occupation state can be constructed by applying fermion *creation operators* on the vacuum state

$$\begin{aligned}
|10000\rangle &= c_1^\dagger |00000\rangle, \\
|01000\rangle &= c_2^\dagger |00000\rangle, \\
|00100\rangle &= c_3^\dagger |00000\rangle, \\
|10100\rangle &= c_1^\dagger c_3^\dagger |00000\rangle, \\
|10110\rangle &= c_1^\dagger c_3^\dagger c_4^\dagger |00000\rangle.
\end{aligned} \tag{74}$$

- If we add fermions one by one to the system, the order matters:

Starting from the vacuum state,

- add fermion on mode 1 then mode 3 then mode 4:

$$\begin{aligned}
& |00\ 000\rangle \\
& \rightarrow c_1^\dagger |00\ 000\rangle = |10\ 000\rangle \\
& \rightarrow c_3^\dagger |10\ 000\rangle = c_3^\dagger c_1^\dagger |00\ 000\rangle = -c_1^\dagger c_3^\dagger |00\ 000\rangle = -|10\ 100\rangle \\
& \rightarrow -c_4^\dagger |10\ 100\rangle = -c_4^\dagger c_1^\dagger c_3^\dagger |00\ 000\rangle = -c_1^\dagger c_3^\dagger c_4^\dagger |00\ 000\rangle = -|10\ 110\rangle
\end{aligned} \tag{75}$$

- add fermion on mode 1 then mode 4 then mode 3:

$$\begin{aligned}
& |00\ 000\rangle \\
& \rightarrow c_1^\dagger |00\ 000\rangle = |10\ 000\rangle \\
& \rightarrow c_4^\dagger |10\ 000\rangle = c_4^\dagger c_1^\dagger |00\ 000\rangle = -c_1^\dagger c_4^\dagger |00\ 000\rangle = -|10\ 010\rangle \\
& \rightarrow -c_3^\dagger |10\ 010\rangle = -c_3^\dagger c_1^\dagger c_4^\dagger |00\ 000\rangle = c_1^\dagger c_3^\dagger c_4^\dagger |00\ 000\rangle = |10\ 110\rangle
\end{aligned} \tag{76}$$

The resulting states are differed by a minus sign, due to the exchange of fermions between mode 3 and 4 effectively comparing the two processes.

Now we have a better understanding of the fermion sign factor  $(-)^{\sum_{j<i} n_j}$  in Eq. (67), as the creation or annihilation operator has to commute through the existing creation operators on all the proceeding modes to reach its mode position in order to act on the vacuum state canonically to reconstruct the fermion occupation state.

## ■ Jordan-Wigner Transformation

Jordan-Wigner transformation is an exact mapping between **qubit** systems and **fermion** systems.

### • State correspondence

- Qubit:  $|a_1\ a_2\ \dots\rangle$  with  $a_i = 0, 1$  — the  $i$ th qubit in the 0 or 1 state.
- Fermion:  $|n_1\ n_2\ \dots\rangle$  with  $n_i = 0, 1$  — the  $i$ th mode being *empty* or *occupied*.

- **Operator correspondence:** The fermion operators can be written in terms of Pauli operators as

$$\boxed{
\begin{aligned}
c_i &= \prod_{j<i} Z_j \frac{X_i + i Y_i}{2}, \\
c_i^\dagger &= \prod_{j<i} Z_j \frac{X_i - i Y_i}{2}.
\end{aligned}
} \tag{77}$$

**Exc 7** Verify that the construction Eq. (77) satisfies the fermion anticommutation relation Eq. (69), therefore justified to be called fermion operators.

- The product  $\prod_{j<i} Z_j$  is called the **Jordan-Wigner string**, a *non-local* operator necessary to ensure the correct fermion anticommutation relation is reproduced.

**Comment:** The **non-locality** of the Jordan-Wigner string has sparked deep reflection



among some physicists.

- If we simply accept the **anticommutation relations** of fermionic operators as the *defining property* of fermions, then we can build a quantum many-body theory of fermions, without questioning their origin.
- However, if we consider the universe to be, at the fundamental level, a **quantum computer**—where every **physical phenomenon** ultimately arises from some *computable quantum algorithm* on foundational qubits—then it becomes difficult to imagine why all *matter particles* in the universe, as *fermions*, would have to be realized in such a complex, non-local manner. This line of thought has led to the discovery of **topological order**, a theoretical framework that provides a *local physical origin* for the non-local nature of fermions.
- **Matrix representation:** Despite of the complexity, Eq. (77) actually provides a systematic method to *represent* fermion operators as *matrices*, given that we know how to represent each Pauli matrix and how to tensor product them together.

Use Jordan-Wigner transformation to rewrite the following Hamiltonian of a *fermion* system to the Hamiltonian of a *qubit* system:

HW  
2

$$H = -t \sum_i (c_{i+1}^\dagger c_i + h.c.) + V \sum_i (n_i - 1/2)(n_{i+1} - 1/2),$$

where  $n_i = c_i^\dagger c_i$  and *h.c.* denotes the Hermitian conjugate of the term. Assume that the system is defined on an infinite 1D lattice. Express the qubit Hamiltonian in terms of Pauli operators.

## Quantum Many-Body Problems

### ■ Overview

### ■ What are the Problems?

**Quantum many-body problem** is the problem of predicting how *physical properties* of quantum many-body systems *respond* to the tuning *parameters*, environmental *noises*, *measurements* or quantum *operations*.

A traditional task is

**Ground state problem:** predict how *ground state* properties respond to *Hamiltonian* parameters.

- Input: **Hamiltonian**  $H(\mathbf{g})$ , parametrized by  $\mathbf{g} = (g_1, g_2, \dots)$ ,
- Output: **ground state**  $|\Psi_0\rangle$  of  $H(\mathbf{g})$  for any  $\mathbf{g}$ , i.e.,

$$|\Psi_0\rangle = \underset{|\Psi\rangle}{\operatorname{argmin}} \langle \Psi | H(\mathbf{g}) | \Psi \rangle, \quad (85)$$

such that given any observable  $O$ , one can predict its ground state expectation value  $\langle O \rangle = \langle \Psi_0 | O | \Psi_0 \rangle$ .

- Why care about *ground state*? — The ground state reveals properties of many-body systems at **low temperature**, which are crucial for understanding **quantum phases** (quantum magnet, superconductor, superfluid, topological insulator) and **quantum phase transitions**.

## ■ What are the Challenges?

- **Quantum Entanglement:** When particles *interact* with each other, they become quantum *entangled* with each other. *Entangled* quantum systems are fundamentally *non-decomposable* due to non-local quantum information sharing among all the entangled parties.
- **Curse of Dimensionality:** The *Hilbert space dimension* of quantum many-body system grows *exponentially* with the *number* of particles (or qubits) [Recall:  $N$ -qubit system Hilbert space dimension is  $2^N$ ], making it exponentially hard to solve for the ground state (or even just to write down the solution).

## ■ Exact Diagonalization: A Brute-Force Approach

### □ Algorithm

- Input: **Hamiltonian**  $H$  (we will omit its parameters for now).
- Step 1: represent the Hamiltonian  $H$  as a *matrix*.
- Step 2: solve the eigen problem to find the *eigenvalues* (energy levels) and *eigenvectors* (corresponding states) of  $H$

$$H |\Psi_n\rangle = E_n |\Psi_n\rangle. \tag{86}$$

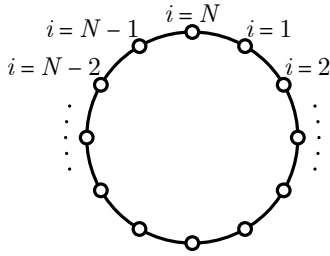
- Step 3: find the *lowest* energy eigenvalue  $E_0$ , and pick out its *corresponding* eigenstate  $|\Psi_0\rangle$ .
- Output:  $|\Psi_0\rangle$  will be a **ground state** of  $H$ .

### □ Explanation

## ■ Transverse-Field Ising Model

### ■ Model Hamiltonian

Consider a 1D lattice of  $N$  qubits arranged in a ring (i.e., assuming *periodic* boundary condition)



- **Hamiltonian**

$$H = -J \sum_{i=1}^N Z_i Z_{i+1} - h \sum_{i=1}^N X_i, \quad (89)$$

with the understanding that  $Z_{i+N} = Z_i$  under periodic boundary condition.

- **Parameters:**

- **Ising coupling** strength  $J$ : large  $J$  favors all qubits to be either all 0 or all 1, such that  $Z_i Z_{i+1} = +1$  for all neighbors, such that the Ising energy is minimized.
- **Transverse field** strength  $h$ : large  $h$  favors all qubits to be in superposition states  $|+\rangle \propto |0\rangle + |1\rangle$ , such that  $X_i = +1$  for all qubits independently, such that the transverse field energy is minimized.

However, only their ratio  $J/h$  matters, as the overall energy scale can always be redefined.

- **$\mathbb{Z}_2$  Ising Symmetry**

**Symmetry:**  $\mathbb{Z}_2$  Ising (spin flip) symmetry, implemented by the following unitary operator

$$U = \prod_{i=1}^N X_i. \quad (90)$$

- Under  $\mathbb{Z}_2$  symmetry transformation,

$$\begin{aligned} Z_i &\rightarrow U Z_i U^\dagger = -Z_i, \\ X_i &\rightarrow U X_i U^\dagger = X_i, \end{aligned} \quad (91)$$

the Ising spin operator  $Z_i$  gets a minus sign (spin flipped), but the Hamiltonian  $H$  in Eq. (89) remains unchanged.

- In other words, the system is **symmetric**  $\Leftrightarrow$  the Hamiltonian  $H$  commutes with the symmetry operator  $U$

$$[H, U] = 0, \quad (92)$$

for *any* parameters  $J$  and  $h$  in  $H$ .

- The symmetry is named by the mathematical structure of a  $\mathbb{Z}_2$  **group**, which consists of two group elements  $\mathbb{Z}_2 = \{1, U\}$ , with the following *group multiplication* rules

$$\begin{array}{c|cc} \cdot & 1 & U \\ \hline 1 & 1 & U \\ U & U & 1 \end{array} \cong \begin{array}{c|cc} + & 0 & 1 \\ \hline 0 & 0 & 1 \\ 1 & 1 & 0 \end{array},$$

which is isomorphic to the *mod-2 addition* of  $\mathbb{Z}_2$  integers  $\{0, 1\}$  (hence the name).

## ■ Two Limits

- **Strong coupling** limit  $J/h \rightarrow \infty$ : **ferromagnetic, ordered** phase.

- **Ground states:** *two* fold degenerated

$$|\Psi_0\rangle \in \text{span} \{|000 \dots\rangle, |111 \dots\rangle\}. \quad (93)$$

No matter which state we choose, the ground state will *spontaneously break* the  $\mathbb{Z}_2$  symmetry.

- **Spontaneous symmetry breaking:** the Hamiltonian  $H$  has a symmetry, but all its short-range-entangled ground states necessarily breaks the symmetry.

- If a *discrete* symmetry group  $G$  is spontaneously broken to its subgroup  $G'$ , the **ground state degeneracy** (GSD) will be given by

$$\text{GSD} = \frac{|G|}{|G'|}, \quad (94)$$

where  $|G|$  denotes the order (number of elements) of a group  $G$ .

$\Rightarrow$  In our case,  $\mathbb{Z}_2 \rightarrow \mathbb{Z}_1$ ,  $\text{GSD} = 2/1 = 2$ .

- **Weak coupling** limit  $J/h \rightarrow 0$ : **paramagnetic, disordered** phase.

- **Ground state:** unique

$$|\Psi_0\rangle = |+++ \dots\rangle = \frac{1}{2^{N/2}} \sum_{[a]} |[a]\rangle, \quad (95)$$

as an *equal-amplitude* superposition of all possible Ising (bit-string) configurations

$[a] = a_1 a_2 \dots$  ( $a_i = 0, 1$ ).

- **Symmetric:** the  $\mathbb{Z}_2$  symmetry is preserved (no symmetry breaking).

The two limits are in *distinct* phases, because whether or not the  $\mathbb{Z}_2$  symmetry is spontaneously broken has an yes-or-no answer.

**Question:** how does the system transition between these two phases?

## ■ Representing the Hamiltonian

Let us try to do some numerics. We start by telling the computer what is our Hamiltonian, and represent each term in the Hamiltonian as a matrix.

- Let us first pick a finite *system size*  $N$ , and enumerate *terms* in our Hamiltonian.

```
Block[{N = 4, J, h, H},
  H = -J Sum[RotateLeft[PadLeft[P["Z"], "Z"], N, "I"], i], {i, N}] -
    h Sum[RotateLeft[PadLeft[P["X"], N, "I"], i], {i, N}]
  -h (P[I, I, I, X] + P[I, I, X, I] + P[I, X, I, I] + P[X, I, I, I]) -
    J (P[I, I, Z, Z] + P[I, Z, Z, I] + P[Z, I, I, Z] + P[Z, Z, I, I])
```

- As a **symbolic programming language**, *Mathematica* allows us to manipulate mathematical symbols directly, which makes it well-suited for *algebraic manipulation, equation solving, and calculus*.

- The key mechanism for the symbolic processing is its **rule-based replacement** system, which works by defining *rules* that determines how symbols are *matched* and *replaced* according to specific patterns.

Here is how it works:

- First define a rule set called “represent”, that replaces *I, X, Y, Z* by their corresponding Pauli matrices.

```
Block[{represent},
  represent = {
    "I" → SparseArray@PauliMatrix[0],
    "X" → SparseArray@PauliMatrix[1],
    "Y" → SparseArray@PauliMatrix[2],
    "Z" → SparseArray@PauliMatrix[3]};
  MatrixForm /@ {"I", "X", "Y", "Z"} //. represent]
```

$$\left\{ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\}$$

- Then extend the rule set by rules for Pauli operators

```
Block[{represent},
  represent = { ... +,
    P[a_] ⇒ a,
    P[a_, b_] ⇒ KroneckerProduct[a, P[b]]};
  MatrixForm /@ {P["X"], P["Z"], "Z", P["X", "I", "Z"]} //. represent]
```

$$\left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \end{pmatrix} \right\}$$

Putting together the above constructions, we can represent the transverse-field Ising model Hamiltonian as a matrix for any given parameters  $J$  and  $h$ .

$$\begin{pmatrix} -4J & -h & -h & 0 & -h & 0 & 0 & 0 & -h & 0 & 0 & 0 & 0 & 0 & 0 \\ -h & 0 & 0 & -h & 0 & -h & 0 & 0 & 0 & -h & 0 & 0 & 0 & 0 & 0 \\ -h & 0 & 0 & -h & 0 & 0 & -h & 0 & 0 & 0 & -h & 0 & 0 & 0 & 0 \\ 0 & -h & -h & 0 & 0 & 0 & 0 & -h & 0 & 0 & 0 & -h & 0 & 0 & 0 \\ -h & 0 & 0 & 0 & 0 & -h & -h & 0 & 0 & 0 & 0 & 0 & -h & 0 & 0 \\ 0 & -h & 0 & 0 & -h & 4J & 0 & -h & 0 & 0 & 0 & 0 & 0 & -h & 0 \\ 0 & 0 & -h & 0 & -h & 0 & 0 & -h & 0 & 0 & 0 & 0 & 0 & -h & 0 \\ 0 & 0 & 0 & -h & 0 & -h & -h & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -h \\ -h & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -h & -h & 0 & -h & 0 & 0 \\ 0 & -h & 0 & 0 & 0 & 0 & 0 & 0 & -h & 0 & 0 & -h & 0 & -h & 0 \\ 0 & 0 & -h & 0 & 0 & 0 & 0 & 0 & -h & 0 & 4J & -h & 0 & 0 & -h \\ 0 & 0 & 0 & -h & 0 & 0 & 0 & 0 & -h & -h & 0 & 0 & 0 & 0 & -h \\ 0 & 0 & 0 & 0 & -h & 0 & 0 & 0 & -h & 0 & 0 & 0 & 0 & -h & -h \\ 0 & 0 & 0 & 0 & 0 & -h & 0 & 0 & 0 & -h & 0 & 0 & -h & 0 & -h \\ 0 & 0 & 0 & 0 & 0 & 0 & -h & 0 & 0 & 0 & -h & 0 & -h & 0 & -h \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -h & 0 & 0 & 0 & -h & 0 & -h & -4J \end{pmatrix}$$

## ■ Solving the Eigen Problem

- **Eigen solver.** For numerical matrix, the eigen problems can be solved by an algorithm called **Arnoldi iteration**. One can request the number of eigen values and states to be calculated.
- **Parametrization.** For this purpose, we substitute numerical values for  $J$  and  $h$ . Since only  $J/h$  matters, we can choose to parametrize them as

$$J = g, \quad h = 1 - g, \tag{96}$$

with  $g \in [0, 1]$ , such that there is only a single parameter to tune, and the overall energy scale is bounded between  $\pm N$ .

```
Block[{N = 4, g = 0., H, represent, Es, Ψs},
  represent = {...} + ;
  H[J_, h_] := ReplaceRepeated[...], + ;
  {Es, Ψs} = Eigensystem[N@H[g, 1 - g], 2, Method → {"Arnoldi", "Shift" → -N - 0.1}]
  {{-4., -2.},
  {{0.25, 0.25, 0.25, 0.25, 0.25, 0.25, 0.25, 0.25, 0.25, 0.25, 0.25, 0.25, 0.25, 0.25, 0.25},
  {0.009913, 0.300151, -0.293983, -0.00374487, 0.198388,
  0.488626, -0.105508, 0.18473, -0.18473, 0.105508, -0.488626,
  -0.198388, 0.00374487, 0.293983, -0.300151, -0.009913}}}
```

Let us visualize the lowest two states as a function of  $J/h$ .

$$\begin{array}{l} J/h = \infty \\ \hline -4. 0.252648 \text{ |0000\rangle} + 0.967558 \text{ |1111\rangle} \\ -4. 0.967558 \text{ |0000\rangle} - 0.252648 \text{ |1111\rangle} \end{array}$$

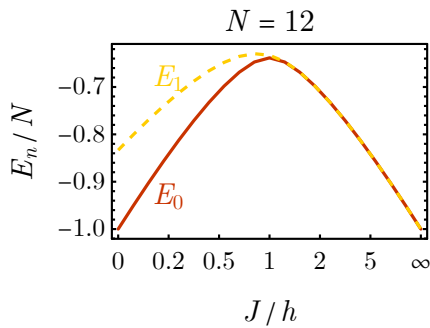
- Strictly speaking, the ground state degeneracy splits as long as the system is tuned away from the  $J/h \rightarrow \infty$  limit. However, the splitting is small in the strong coupling regime.
- It seems that the ground state interpolates between the two limits continuously.

Question: Where is the phase transition?

**Phases and phase transitions** are only well-defined in the *thermodynamic limit* ( $N \rightarrow \infty$ ).  $\Rightarrow$  We should study how physical properties scales with system size  $N$ .

## ■ Energy Gap Scaling

The energy density  $E_n/N$  of the lowest two energy level v.s. the  $J/h$  parameter, showing how the ground state degeneracy splits.

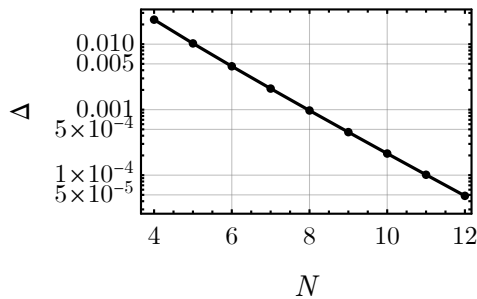


Define the energy gap

$$\Delta = E_1 - E_0. \quad (97)$$

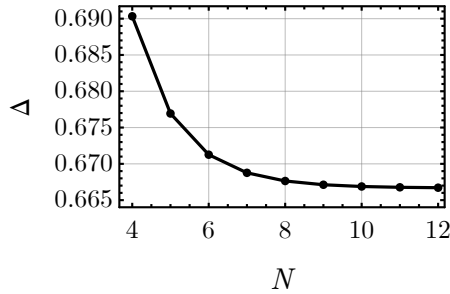
- In the **symmetry breaking** phase (strong coupling), e.g.  $J/h = 2$ , the energy gap decays to zero with system size  $N$  exponentially

$$\Delta \sim e^{-\alpha N}. \quad (98)$$



- In the **symmetric** phase (weak coupling), e.g.  $J/h = 1/2$ , the energy gap tends to a constant in the large  $N$  limit.

$$\Delta \sim \text{const.} \quad (99)$$



## ■ Physical Observables

What can we learn from the ground state  $|\Psi_0\rangle$  itself? We can study various physical observables

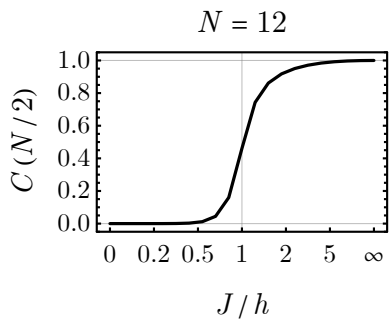
$$\langle O \rangle := \langle \Psi_0 | O | \Psi_0 \rangle. \quad (100)$$

- **Correlation function:** used to indicate the ordered phase.

$$C(d) = \langle Z_i Z_{i+d} \rangle. \quad (101)$$

It characterizes the correlation between Ising spins  $Z_i$  and  $Z_{i+d}$  separated by distance  $d$  on the lattice. Strong correlation indicates the spins are ordered.

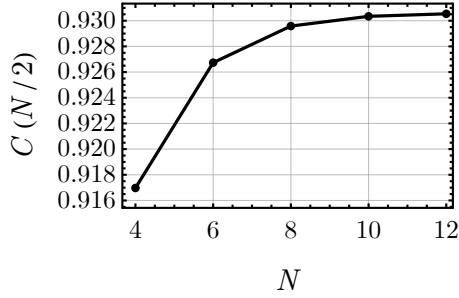
- Long-distance correlation function v.s.  $J/h$  ratio, indicating phase transition (transition gets sharper as  $N \rightarrow \infty$ )



- In the **symmetry breaking** phase (strong coupling), e.g.  $J/h = 2$ , the correlation function approaches to *constant* at long range

$$C(d) \sim \text{const.} \quad (102)$$

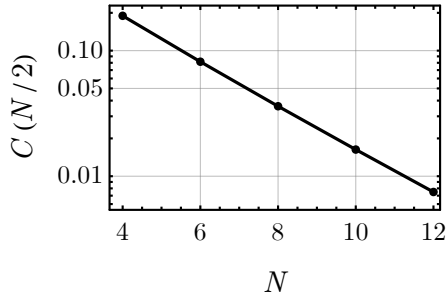




- In the **symmetric** phase (weak coupling), e.g.  $J/h = 1/2$ , the correlation function decays to zero *exponentially* with the distance  $d$ .

$$C(d) \sim e^{-d/\xi}, \quad (103)$$

the decay length scale  $\xi$  is called the **correlation length**.

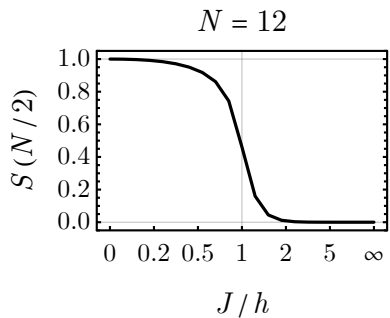


- **String operator**: used to indicate the disordered phase.

$$S(d) = \left\langle \prod_{j=i}^{i+d-1} X_j \right\rangle. \quad (104)$$

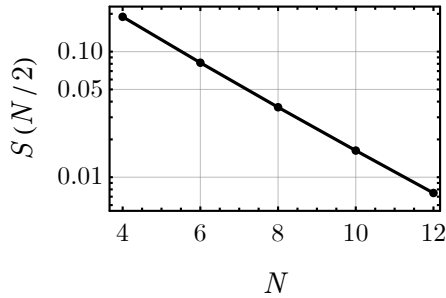
String operator is a segment of *symmetry operator* of length  $d$ , which flips all the Ising spins in the segment. Its expectation value measure the *probability* to see the segment of spin being flipped under *quantum fluctuation* in the ground state. In the symmetric (disordered) phase, such probability should be high.

- Long-range string operator v.s.  $J/h$  ratio, indicating phase transition (transition gets sharper as  $N \rightarrow \infty$ )



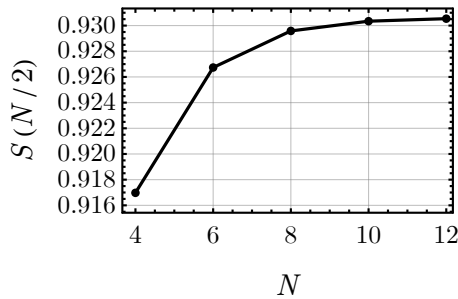
- In the **symmetry breaking** phase (strong coupling), e.g.  $J/h = 2$ , the string operator decays to zero *exponentially* with the distance  $d$ .

$$S(d) \sim e^{-d/\xi}. \tag{105}$$



- In the **symmetric** phase (weak coupling), e.g.  $J/h = 1/2$ , the string operator approaches to *constant* at long range.

$$S(d) \sim \text{const.} \tag{106}$$



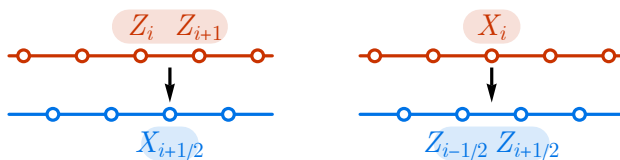
The above numerical result strongly suggests that there is a correspondence between  $C(d)$  and  $S(d)$  as we interchange  $J$  and  $h$ .

### ■ Kramers-Wannier Duality

**Kramers-Wannier duality** is an *operator mapping*, under which

$$\begin{aligned} Z_i Z_{i+1} &\rightarrow X_{i+1/2}, \\ X_i &\rightarrow Z_{i-1/2} Z_{i+1/2}. \end{aligned}$$

(107)



- It maps the Pauli operators acting the *original* qubits (in red) to the Pauli operators acting a *new* set of qubits (in blue) on the *dual lattice* (shifted by 1/2 lattice constant).
- Requirements:

- The **algebraic relations** (such as commutation relations) among these operators are *preserved* under the mapping.
- The **locality** of the Hamiltonian is also preserved.

In fact, the Hamiltonian Eq. (89) gets mapped to

$$H = -J \sum_{i=1}^N X_{i+1/2} - h \sum_{i=1}^N Z_{i-1/2} Z_{i+1/2}, \quad (108)$$

on the dual lattice, effectively *interchange* the roles of  $J$  and  $h$ .

$$\begin{array}{ll} J/h & \leftrightarrow & h/J \\ \text{lattice} & \leftrightarrow & \text{dual-lattice} \\ \text{order} & \leftrightarrow & \text{disorder} \\ C(d) & & S(d) \\ \text{disorder} & \leftrightarrow & \text{order} \\ S(d) & & C(d) \end{array}$$

**Exc 8** Show that the correlation function  $C(d)$  and string operator  $S(d)$  maps to each other under Kramers-Wannier duality.

- **Implication:** under Kramers-Wannier duality, the ordered (disordered) phase of the original Ising model maps to the disordered (ordered) phase of the dual Ising model, but both models are *identical*, so if there is a single phase transition separating the ordered and disordered phases, it must happen at

$$J/h = 1. \quad (111)$$

This is the **critical point** of the transverse-field Ising model.

## ■ Bose-Hubbard Model

### ■ Model Hamiltonian

Consider a 1D lattice of  $N$  sites with *periodic* boundary condition.

- **Hamiltonian**

$$H = -t \sum_{i=1}^N (b_{i+1}^\dagger b_i + h.c.) + \frac{U}{2} \sum_{i=1}^N n_i(n_i - 1) - \mu \sum_{i=1}^N n_i, \quad (112)$$

where

- $b_i^\dagger$  and  $b_i$  are **boson creation** and **annihilation** operators on site- $i$ , with  $b_{i+N} = b_i$  given the periodic boundary condition,

- $n_i = b_i^\dagger b_i$  denotes the **boson number operator** (we will omit the hat of  $\hat{n}$  for simplicity).
- Parameters:
  - **Hopping amplitude**  $t$ : measures boson *mobility* on the lattice.  $b_{i+1}^\dagger b_i$  describes the process of moving a boson from site- $i$  to the neighboring site- $(i+1)$ , and the Hermitian conjugate term  $b_i^\dagger b_{i+1}$  describes the reverse process.
  - **On-site interaction** strength  $U$ : also known as the **Hubbard interaction**, can be *attractive* ( $U < 0$ ) or *reclusive* ( $U > 0$ ).  $n_i(n_i - 1)/2$  counts the *number of pairs* that can form among  $n_i$  bosons on a site, as interaction is *pair-wise*.
  - **Chemical potential**  $\mu$ : adjust to set the number of particles.

**Remark:** If we fix the total boson number  $N_b$  (i.e., assuming a canonical ensemble), we can drop the chemical potential term.

## ■ U(1) Symmetry

The Hamiltonian enjoys a continuous U(1) symmetry, implemented by the following unitary operator

$$U(\theta) = e^{i\theta N_b}, \quad (113)$$

where  $N_b$  is the U(1) **charge operator** that generates the unitary, and is given by

$$N_b = \sum_i n_i, \quad (114)$$

which is also the operator of total boson number in the system.

- Under the U(1) **symmetry transformation**,

$$\begin{aligned} b_i &\rightarrow U(\theta) b_i U(\theta)^\dagger = e^{-i\theta} b_i, \\ b_i^\dagger &\rightarrow U(\theta) b_i^\dagger U(\theta)^\dagger = e^{i\theta} b_i^\dagger. \end{aligned} \quad (115)$$

**Exc  
9**

Prove Eq. (115) given the definition Eq. (113).

The Bose-Hubbard model Hamiltonian  $H$  in Eq. (112) is invariant under such opposite phase rotations of the boson creation and annihilation operators (as they always appear in pairs in  $H$ ).

- The U(1) symmetry is associated with the *conservation law* of the **boson number conservation**, as the symmetry implies

$$[H, N_b] = 0. \quad (119)$$

the charge operator  $N_b$  will not evolve in time, and is therefore *conserved*.

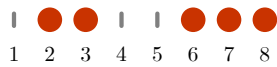
- Because  $N_b$  is conserved, we can always restrict the Hilbert space to a fixed eigen-subspace of  $N_b$ , such that  $N_b$  becomes a *number* (the eigenvalue) other than an *operator*.

## ■ Hilbert Space

Suppose the system has totally  $N_b$  **number of bosons**, and the lattice has  $N$  **number of sites**, the many-body Hilbert space dimension is

$$D_b = \frac{(N_b + N - 1)!}{N_b! (N - 1)!}, \quad (120)$$

the number of ways to distribute  $N_b$  identical bosons across  $N$  lattice sites = ways to insert  $(N - 1)$  dividers between  $N_b$  balls in a row.



- Following the above idea, all basis states can be enumerated given  $N$  and  $N_b$ . Here is a simple example:

$$\{ |0, 0, 3\rangle, |0, 1, 2\rangle, |0, 2, 1\rangle, |0, 3, 0\rangle, \\ |1, 0, 2\rangle, |1, 1, 1\rangle, |1, 2, 0\rangle, |2, 0, 1\rangle, |2, 1, 0\rangle, |3, 0, 0\rangle \}$$

- The Hilbert space dimension grows *exponentially* with system size  $N$  at any *fixed density*  $N_b/N$ . — Exactly solving the problem is hard for large systems.

## ■ Representing the Hamiltonian

- We can use *Mathematica* to quickly build a symbolic system to implement the action of boson creation and annihilation operators on boson occupation states.

$$\begin{aligned} \mathbf{b}[1] @ |0, 0, 0\rangle &\rightarrow 0 \\ \mathbf{b}^\dagger[1] @ |0, 0, 0\rangle &\rightarrow |1, 0, 0\rangle \\ \mathbf{b}^\dagger[2] @ * \mathbf{b}[3] @ |0, 4, 3\rangle &\rightarrow \sqrt{15} |0, 5, 2\rangle \\ \mathbf{b}^\dagger[2] @ * \mathbf{b}[2] @ |0, 2, 1\rangle + 2 |0, 3, 0\rangle &\rightarrow 2 |0, 2, 1\rangle + 6 |0, 3, 0\rangle \end{aligned}$$

- This enables us to apply the Hamiltonian Eq. (112) to each basis state and compute the resulting state.

$$\begin{aligned}
H@|0, 0, 3\rangle &\rightarrow 3 U |0, 0, 3\rangle - \sqrt{3} t |0, 1, 2\rangle - \sqrt{3} t |1, 0, 2\rangle \\
H@|0, 1, 2\rangle &\rightarrow -\sqrt{3} t |0, 0, 3\rangle + U |0, 1, 2\rangle - 2 t |0, 2, 1\rangle - t |1, 0, 2\rangle - \sqrt{2} t |1, 1, 1\rangle \\
H@|0, 2, 1\rangle &\rightarrow -2 t |0, 1, 2\rangle + U |0, 2, 1\rangle - \sqrt{3} t |0, 3, 0\rangle - \sqrt{2} t |1, 1, 1\rangle - t |1, 2, 0\rangle \\
H@|0, 3, 0\rangle &\rightarrow -\sqrt{3} t |0, 2, 1\rangle + 3 U |0, 3, 0\rangle - \sqrt{3} t |1, 2, 0\rangle \\
H@|1, 0, 2\rangle &\rightarrow -\sqrt{3} t |0, 0, 3\rangle - t |0, 1, 2\rangle + U |1, 0, 2\rangle - \sqrt{2} t |1, 1, 1\rangle - 2 t |2, 0, 1\rangle \\
H@|1, 1, 1\rangle &\rightarrow -\sqrt{2} t |0, 1, 2\rangle - \sqrt{2} t |0, 2, 1\rangle - \\
&\quad \sqrt{2} t |1, 0, 2\rangle - \sqrt{2} t |1, 2, 0\rangle - \sqrt{2} t |2, 0, 1\rangle - \sqrt{2} t |2, 1, 0\rangle \\
H@|1, 2, 0\rangle &\rightarrow -t |0, 2, 1\rangle - \sqrt{3} t |0, 3, 0\rangle - \sqrt{2} t |1, 1, 1\rangle + U |1, 2, 0\rangle - 2 t |2, 1, 0\rangle \\
H@|2, 0, 1\rangle &\rightarrow -2 t |1, 0, 2\rangle - \sqrt{2} t |1, 1, 1\rangle + U |2, 0, 1\rangle - t |2, 1, 0\rangle - \sqrt{3} t |3, 0, 0\rangle \\
H@|2, 1, 0\rangle &\rightarrow -\sqrt{2} t |1, 1, 1\rangle - 2 t |1, 2, 0\rangle - t |2, 0, 1\rangle + U |2, 1, 0\rangle - \sqrt{3} t |3, 0, 0\rangle \\
H@|3, 0, 0\rangle &\rightarrow -\sqrt{3} t |2, 0, 1\rangle - \sqrt{3} t |2, 1, 0\rangle + 3 U |3, 0, 0\rangle
\end{aligned}$$

- We can collect coefficients in front of the basis states and organize them into the matrix representation.

$$\begin{pmatrix}
3 U & -\sqrt{3} t & 0 & 0 & -\sqrt{3} t & 0 & 0 & 0 & 0 & 0 \\
-\sqrt{3} t & U & -2 t & 0 & -t & -\sqrt{2} t & 0 & 0 & 0 & 0 \\
0 & -2 t & U & -\sqrt{3} t & 0 & -\sqrt{2} t & -t & 0 & 0 & 0 \\
0 & 0 & -\sqrt{3} t & 3 U & 0 & 0 & -\sqrt{3} t & 0 & 0 & 0 \\
-\sqrt{3} t & -t & 0 & 0 & U & -\sqrt{2} t & 0 & -2 t & 0 & 0 \\
0 & -\sqrt{2} t & -\sqrt{2} t & 0 & -\sqrt{2} t & 0 & -\sqrt{2} t & -\sqrt{2} t & -\sqrt{2} t & 0 \\
0 & 0 & -t & -\sqrt{3} t & 0 & -\sqrt{2} t & U & 0 & -2 t & 0 \\
0 & 0 & 0 & 0 & -2 t & -\sqrt{2} t & 0 & U & -t & -\sqrt{3} t \\
0 & 0 & 0 & 0 & 0 & -\sqrt{2} t & -2 t & -t & U & -\sqrt{3} t \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -\sqrt{3} t & -\sqrt{3} t & 3 U
\end{pmatrix}$$

## ■ Solving the Eigen Problem

For a small system, we can diagonalize the Bose-Hubbard model Hamiltonian exactly and find the ground state at different  $U/t$  ratio.

Consider **repulsive** Hubbard interaction ( $U > 0$ ):

$$U/t = 0.0$$

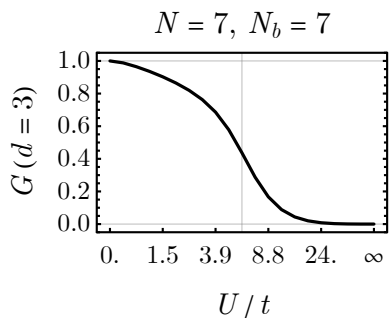
$$\begin{aligned}
&+0.196 |\bullet\bullet\bullet\bullet\bullet\rangle \\
&+0.139 |\circ\bullet\bullet\bullet\bullet\rangle + (19 \text{ terms}) \\
&+0.098 |\circ\circ\bullet\bullet\bullet\rangle + (29 \text{ terms}) \\
&+0.08 |\circ\circ\circ\bullet\bullet\rangle + (29 \text{ terms}) \\
&+0.057 |\circ\circ\circ\circ\bullet\rangle + (19 \text{ terms}) \\
&+0.04 |\circ\circ\circ\circ\bullet\rangle + (19 \text{ terms}) \\
&+0.018 |\circ\circ\circ\circ\circ\rangle + (4 \text{ terms})
\end{aligned}$$

- **Weak Interaction** regime (small  $U/t$ )
  - Bosons are **delocalized** across the entire lattice. Each boson can be found anywhere in the system, independent of the other bosons.
- **Strong Interaction** regime (large  $U/t$ )
  - Bosons are **localized**. Each boson is confined to a lattice site, due to the strong on-site repulsive interaction that prevents bosons from hopping to neighboring sites.
  - There is an **energy gap** to boson excitations.
- There is a **quantum phase transition** separating the weak and strong interacting phases, known as the **Kosterlitz-Thouless (KT) transition**. [2016 Nobel Prize in Physics]

## ■ Physical Observables

- **Boson Correlation**

$$G(d) = \langle b_i^\dagger b_{i+d} \rangle. \quad (121)$$



- **Weak interacting** phase: boson correlation  $G(d)$  decays in a *power law* (algebraically) with the distance  $d$

$$G(d) \sim d^{-\alpha}. \quad (122)$$

- **Strong interacting** phase: boson correlation  $G(d)$  decays *exponentially* with the distance  $d$

$$G(d) \sim e^{-d/\xi}. \quad (123)$$

- Our current **exact diagonalization** approach will not be able to further study these behaviors and pin down the KT transition, because the system size we can achieve is too small. Yet, it still provides us qualitative understanding of helpful physical pictures.

## ■ Sachdev-Ye-Kitaev Model

### ■ Majorana Fermion

**Majorana fermions** are fermions that are *their own antiparticles*. They are generated by Hermitian fermion operators  $\chi^\dagger = \chi$ .

- **Real and Imaginary Decomposition:** Majorana fermions can be thought as the “real part” and “imaginary part” of the traditional fermion operator

$$\begin{cases} c_i = \frac{1}{2} (\chi_{2i-1} + i \chi_{2i}) \\ c_i^\dagger = \frac{1}{2} (\chi_{2i-1} - i \chi_{2i}) \end{cases} \begin{cases} \chi_{2i-1} = c_i^\dagger + c_i \\ \chi_{2i} = i(c_i^\dagger - c_i) \end{cases} \quad (124)$$

- These Majorana fermion operators still acts on the states in the same fermion many-body Hilbert space. They are just linear combination of  $c_i$  and  $c_i^\dagger$ .
- **Anti-commutation Relations:** Majorana fermion operators  $\chi_i$  are defined by the following algebraic property:

$$\{\chi_i, \chi_j\} = 2 \delta_{ij}. \quad (125)$$

This is also the defining property of the **Clifford algebra** generators.

- **Jordan-Wigner Transformation:** Majorana fermion operator can be systematically represented as Pauli matrices

$$\chi_{2i-1} = \prod_{j<i} Z_j X_i, \quad \chi_{2i} = \prod_{j<i} Z_j Y_i. \quad (126)$$

## ■ Model Hamiltonian

The **Sachdev-Ye-Kitaev (SYK) model** describes a system of  $N$  Majorana modes with *random, all-to-all interactions*.

$$H = \sum_{1 \leq i < j < k < l \leq N} J_{ijkl} \chi_i \chi_j \chi_k \chi_l, \quad (127)$$

where

- $\chi_i$  are **Majorana fermion** operators,
- $J_{ijkl}$  are **random coupling constants** drawn from independent identical Gaussian distributions, with

$$\overline{J_{ijkl}} = 0, \quad \overline{J_{ijkl}^2} = \frac{2}{N^3}. \quad (128)$$

The SYK model serves as a bridge between different fields of physics, offering insights into *quantum chaos, strongly correlated systems, and black hole* physics.

## ■ $\mathbb{Z}_2^F$ Symmetry

Any Hamiltonian of fermion system must at least respect the  $\mathbb{Z}_2^F$  **fermion parity** symmetry, which is implemented by the following unitary operator



$$\boxed{(-)^F = (-1)^{\sum_i n_i},} \quad (129)$$

where

- $n_i = c_i^\dagger c_i$  is the fermion number operator,
- $\sum_i n_i$  counts the total number of fermions in the system,
- $(-)^F = +1$  on those states with *even* number of fermions and  $-1$  on those states with *odd* number of fermions, hence the name fermion *parity*.
- Fermion parity operator is a two-fold operator (like an Ising symmetry)

$$(-)^F (-)^F = \mathbb{1}. \quad (130)$$

therefore, the symmetry group is  $\mathbb{Z}_2$ . (A superscript  $F$  is usually put on  $\mathbb{Z}_2^F$  to indicate the **F**ermion parity symmetry — a fundamental symmetry unique to fermion systems).

- Under **fermion parity transformation**: all fermion operators *changes sign*

$$\begin{aligned} c_i &\rightarrow (-)^F c_i (-)^F = -c_i, \\ c_i^\dagger &\rightarrow (-)^F c_i^\dagger (-)^F = -c_i^\dagger, \\ \chi_i &\rightarrow (-)^F \chi_i (-)^F = -\chi_i. \end{aligned} \quad (131)$$

But since each term in the Hamiltonian always contains *even* number of fermion operators, the fermion parity symmetry is always respected.

**Exc**  
**10**

Prove Eq. (131) given the definition Eq. (129).

- **Fermion parity conservation**: as a result, the Hamiltonian commutes with the fermion parity operator

$$\boxed{[H, (-)^F] = 0,} \quad (136)$$

such that the fermion parity is always *conserved* in fermion systems.

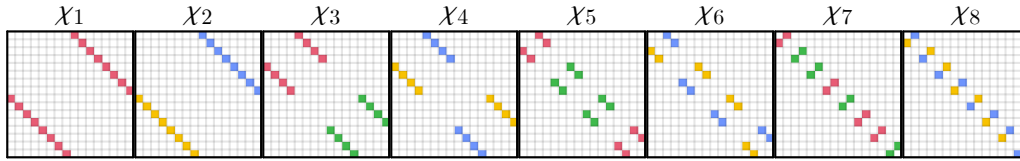
- **Jordan-Wigner Transformation**: the fermion parity operator can be represented as

$$\boxed{(-)^F = \prod_i Z_i.} \quad (137)$$

It indeed anti-commutes with all fermion operators, as expected.

## ■ Matrix Representations

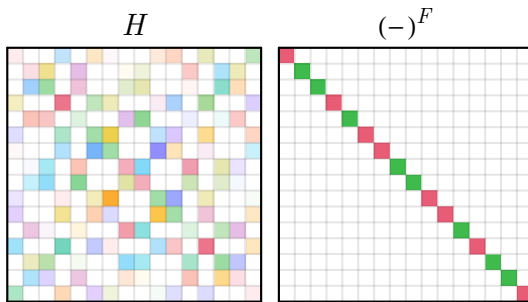
- First we can construct the matrix representation for Majorana fermion operators using **Jordan-Wigner transformation** Eq. (126).



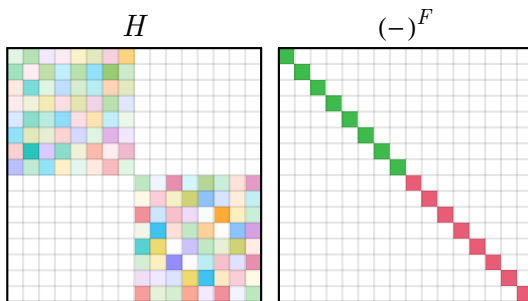
Legend: each pixel corresponds to a matrix element.

Color code: ■ = 1, ■ =  $i$ , ■ =  $-1$ , ■ =  $-i$ ,  = 0.

- Then we generate random coupling constant tensor  $J_{ijkl}$  by **random sampling**, and construct the SYK Hamiltonian  $H$  by **tensor contraction**.



- Some matrix elements in  $H$  are always 0, why?
- Inspect the **fermion parity** operator  $(-)^F$ . It becomes clear that those matrix elements in  $H$  are forbidden by the  $\mathbb{Z}_2^F$  symmetry, as they correspond to transitions between states of *different* fermion parities (thereby violating the fermion parity conservation).
- If we rearrange the basis state by **fermion parity** into *even* and *odd* parity subspaces, the Hamiltonian will be transformed to the **block diagonal form**.



- The *block diagonal* structure reduces the **computational complexity** for exact diagonalization, as it enables us to diagonalize each block *independently*. — The complexity is reduced to  $1/8 + 1/8 = 1/4$  of the original task.

## ■ Quantum Chaos

**Chaos** was originally introduced to describes *classical dynamics* that exhibit *extreme sensitivity* to *initial conditions*, where a small difference in starting points leads to vastly different outcomes over time. This is often called the “**butterfly effect**.”

- Examples of **Classical Chaos**:
  - **Weather Systems**: long-term weather forecast is almost impossible.
  - **Double Pendulum**: a simple pendulum is periodic, but you can't predict the behavior of a pendulum hanging below another one.
  - **Three-Body Problem** (in classical gravity): there is a famous Chinese science fiction [by Cixin Liu] about it ...
- **Key Takeaway**: *unpredictable* and *random* behavior can emerge in *deterministic* systems due to sensitivity to initial conditions.

**Quantum Chaos** is the study of *chaotic behaviors* in *quantum* systems, where traditional notions of classical chaos, like the butterfly effect, take on new forms.

- Naively, quantum system should not exhibit chaos: because the **time-evolution equation** is *linear*, *small* changes in the initial state *remain small*.
- Instead, quantum chaos manifests through other features, such as
  - **Energy-level statistics**, [1][2]
  - Eigenstate thermalization hypothesis (ETH) and volume-law entanglement entropy,
  - Local operator growth and quantum information scrambling.

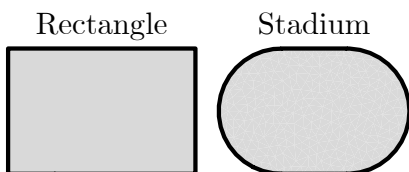
[1] E. Wigner, *Characteristic Vectors of Bordered Matrices with Infinite Dimensions*, Ann. Math. **62**, 548 (1955).

[2] F. J. Dyson, *Statistical Theory of the Energy Levels of Complex Systems. I*, J. Math. Phys. (N.Y.) **3**, 140 (1962).

## ■ Energy-Level Statistics (Billiard)

**Classical billiard** is a *point particle* moving without friction on a table  $\Omega$ , enclosed by *rigid boundaries*, such that the particle bouncing around by *elastic collisions* with the boundaries, conserving energy.

- **Rectangle** shape: the motion will be very regular (**integrable**). (the horizontal and vertical motions are decoupled, and both are periodic)
- **Stadium** shape: the motion will be **chaotic**.



**Quantum billiard** amounts to solving the **Schrödinger equation** within the billiard table region  $\Omega$ .

$$-\frac{1}{2} \nabla^2 \psi_n(\mathbf{x}) = E_n \psi_n(\mathbf{x}), \quad (138)$$

where

- $\psi_n(\mathbf{x})$  is the eigen wave function, restricted in  $\mathbf{x} \in \Omega$  (with the Dirichlet boundary condition  $\psi_n(\mathbf{x} \in \partial\Omega) = 0$ ),
- $E_n$  is the corresponding eigen energy (**energy level**).

Suppose the energy levels have been ordered

$$E_0 \leq E_1 \leq E_2 \leq \dots \leq E_n \leq E_{n+1} \leq \dots, \quad (139)$$

we can define

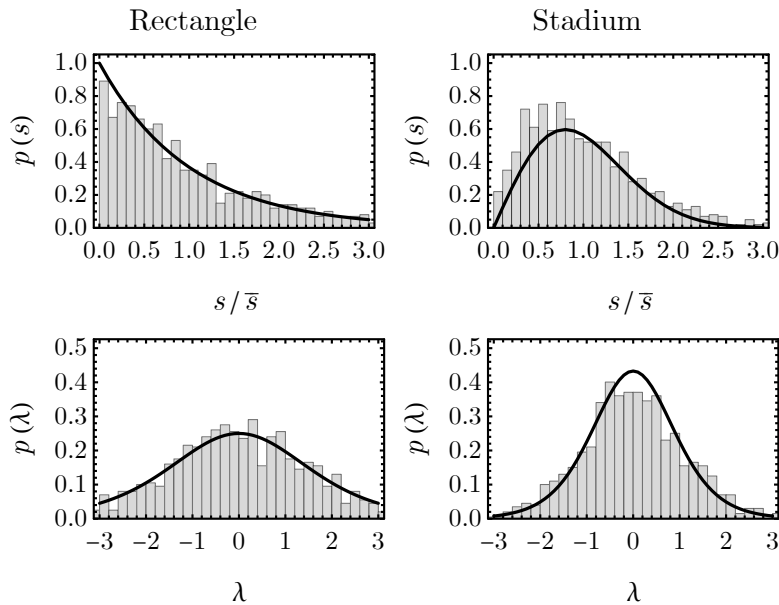
- the **energy level spacing**

$$s_n := E_{n+1} - E_n, \quad (140)$$

- the **log level spacing ratio** (to construct a dimensionless scale)

$$\lambda_n := \log\left(\frac{s_{n+1}}{s_n}\right). \quad (141)$$

These variables will look pretty random across the spectrum, but we can collect their statistics, and study their **probability distribution**. Following are statistics of the lowest 1000 energy levels.



- Rectangle case: the classical dynamics is **integrable**, the energy levels will be *uncorrelated*, and the level statistics  $p(s)$  follows **Poisson distribution**, correspondingly the distribution  $p(\lambda)$  will be *boarder*.

- What is Poisson distribution? Sample  $N$  *independent, uniformly* distributed random *real* numbers from  $[0, N]$ , sort them, and calculate the spacings  $s$  between consecutive values. In the *large- $N$  limit*, the spacings  $s$  will follow the Poisson distribution

$$p(s) = e^{-s}. \quad (142)$$

- Stadium case: the classical dynamics is **chaotic**, the energy levels are *correlated* with **level repulsion**, and the level statistics  $p(s)$  follows **Wigner-Dyson distribution** (more specifically the GOE distribution here), correspondingly the distribution  $p(\lambda)$  will be more *concentrated*.

- What are Wigner-Dyson distributions? Sample *independent Gaussian* random numbers to construct  $N \times N$  *Hermitian* matrices, and calculate the spacings  $s$  between consecutive *eigenvalues*. In the large- $N$  limit, the spacing  $s$  will follow the Wigner-Dyson distribution

$$p(s) \propto s^\beta e^{-\alpha s^2}, \quad (143)$$

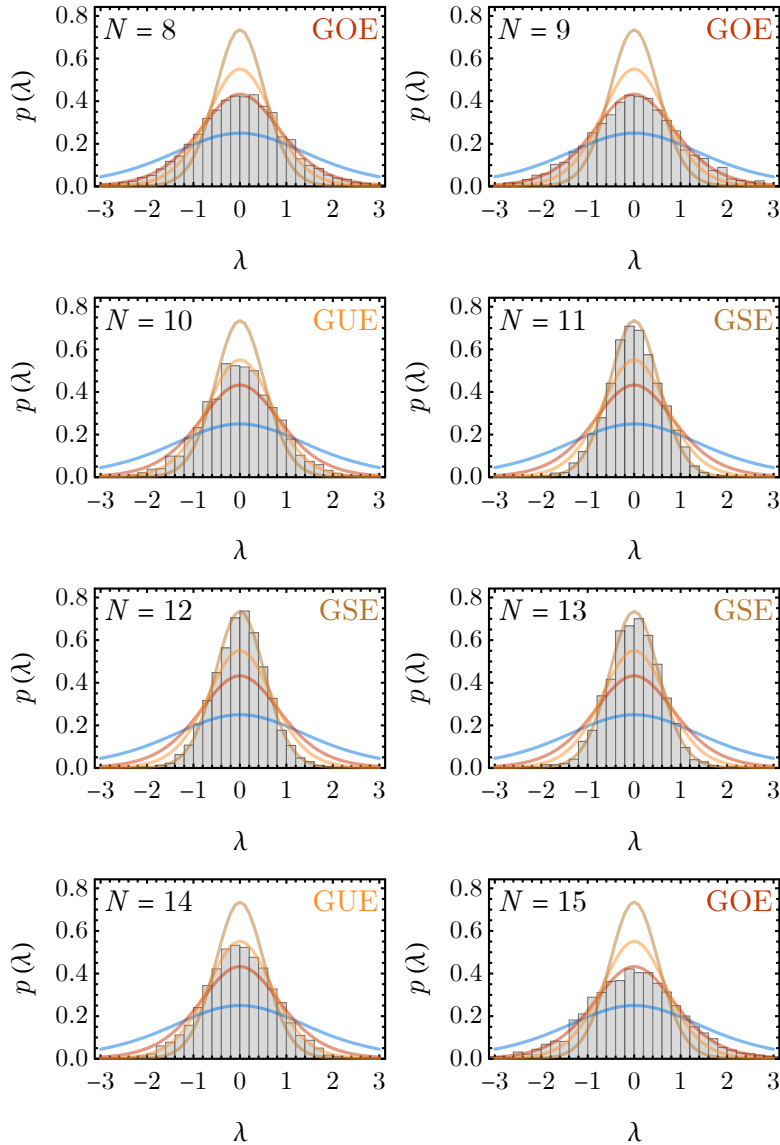
where  $\beta$  depends on whether the *matrix elements* are:

- **real** - Gaussian Orthogonal Ensemble (GOE):  $\beta = 1$ ,
- **complex** - Gaussian Unitary Ensemble (GUE):  $\beta = 2$ ,
- **quaternion** - Gaussian Symplectic Ensemble (GSE):  $\beta = 4$ .

## ■ Energy-Level Statistics (SYK)

Collect the energy-level statistics analysis to the SYK model. Focus on the distribution  $p(\lambda)$  of **log level spacing ratio** (as it has greater distinctiveness)

Legends :      
Poisson   GOE GUE GSE  
Wigner-Dyson



- For various different **Majorana mode number**  $N$ , the SYK model always exhibits the **Wigner-Dyson level statistics**, indicating **quantum chaotic** behavior.
- Interestingly, the distribution cycles through the three Gaussian ensembles (GOE, GUE, GSE) with respect to  $N$  with a period 8, a phenomenon that is profoundly related to the **quantum anomaly** associated with the  $\mathbb{Z}_2^F$  and time-reversal symmetry of the SYK model. [3]

[3] Yi-Zhuang You, Andreas W. W. Ludwig, Cenke Xu. *Sachdev-Ye-Kitaev Model and Thermalization on the Boundary of Many-Body Localized Fermionic Symmetry Protected Topological States*. arXiv:1602.06964