Lecture 1 prelude

Before the main lecture, some intro to the course.

Our goals:

① learn some numerical methods used in CMT

② learn some of the standard CMT models

The main model we will study is the

transverse-field Ising model

$$H = -J \sum_i S_i^z S_{i+1}^z - h \sum_i S_i^x$$

To understand this we will need:

① spin-$\frac{1}{2}$ systems

② many-body states and operators

We will start the course by making sure we are all on the same page for these things, as well as some basic programming

Here are our plans:

Day 1: spin-$\frac{1}{2}$, tensor product spaces and operators acting on them

Day 2: introduce Ising model, use ED to find ground state, calculate some basic expectation values, look at energy gap

Day 3: ED for Heisenberg model, ~~introduce symmetries~~ analysis of computation time, introduce symmetries, dynamics if time permits

Day 4: Introduce MPS

Day 5: Algorithms for MPS (iTEBD & DMRG)

We'll start by understanding this H vs what you're used to.

$$H = -J \sum_i S_i^z S_{i+1}^z - h \sum_i S_i^x$$

vs

$$H = \frac{p^2}{2m} + V(r)$$

<u>Idea</u>: chain of atoms, one electron on each one

$$\Rightarrow H = \sum_i \frac{p_i^2}{2m} + V(r_i) + \sum_{i<j} V(r_i - r_j)$$

This is super hard to solve!!!

<u>Solution</u>: ① Solve each local $H = \frac{p^2}{2m} + V(r)$ separately, get usual orbitals: $s, p_x, p_y, p_z, \ldots$

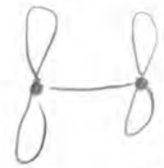
② Keep just one orbital, in this case p_z ← depends on details of atoms which one we keep

So we have

③ Assume $V(r_1 - r_2)$ really pushes electrons apart, so they stay put on their home locations

0,2

(4) Consider 2 sites



$\varphi_1(r) \quad \varphi_2(r)$

$\psi(r_1, r_2, s_1, s_2)$ must be antisymmetric

2 choices: (a) $\left(\frac{\varphi_1(r_1)\varphi_2(r_2) + \varphi_1(r_2)\varphi_2(r_1)}{\sqrt{2}}\right)\left(\frac{\uparrow\downarrow - \downarrow\uparrow}{\sqrt{2}}\right)$

(b) $\left(\frac{\varphi_1(r_1)\varphi_2(r_2) - \varphi_1(r_2)\varphi_2(r_1)}{\sqrt{2}}\right)\left(\frac{\uparrow\uparrow + \downarrow\downarrow}{\sqrt{2}}\right)$

$V(r_1 - r_2)$ makes (b) lower in energy.

The difference in energy between these two is called $\boxed{2J\left(\frac{\hbar}{2}\right)^2}$

(5) Also apply a magnetic field in $\hat{x}$ direction, $\vec{B} = B_0\hat{x}$

This produces Zeeman splitting $\Delta E = \boxed{\frac{\hbar}{2} \cdot h} = B_0 \cdot \mu_B (\#)$?

Then we get an effective model just for the spins of the e^- whose position is fixed in place. Looks like

$$H = -J \sum_i S_i^{z} S_i^{z+1} - h \sum_i S_i^{x}$$

This is the Ising model!

Now let's understand what it means mathematically

Numerical CMT

5 lecture course for Perimeter Institute summer undergrad internship program, 2020

Lecture 1: spin-$\frac{1}{2}$, tensor product spaces & operators, programming basics

Review of spin-$\frac{1}{2}$

We consider a spin-$\frac{1}{2}$ system, whose states are of the form

$$|\psi\rangle = a|\uparrow\rangle + b|\downarrow\rangle \quad \text{with} \quad |a|^2+|b|^2=1 \qquad (a,b \in \mathbb{C})$$

2-dimensional Hilbert space, (ON) basis is $\{|\uparrow\rangle, |\downarrow\rangle\}$:

$$\langle\uparrow|\uparrow\rangle = \langle\downarrow|\downarrow\rangle = 1, \quad \langle\uparrow|\downarrow\rangle = \langle\downarrow|\uparrow\rangle = 0$$

An operator $\mathcal{O}$ acting on this space is described by how it transforms the basis states:

$$\mathcal{O}|\uparrow\rangle = o_{11}|\uparrow\rangle + o_{21}|\downarrow\rangle$$

$$\mathcal{O}|\downarrow\rangle = o_{12}|\uparrow\rangle + o_{22}|\downarrow\rangle$$

This can be represented as a matrix, with $|\uparrow\rangle$ and $|\downarrow\rangle$ represented as coordinate vectors:

$$|\uparrow\rangle \rightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\downarrow\rangle \rightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Adjoints are

$$\langle\uparrow| \to (1\ 0)\ ,\ \langle\downarrow| \to (0\ 1)$$

Check orthonormality:

$$\langle\uparrow|\uparrow\rangle = (1\ 0)\begin{pmatrix}1\\0\end{pmatrix} = 1 = (0\ 1)\begin{pmatrix}0\\1\end{pmatrix} = \langle\downarrow|\downarrow\rangle \checkmark$$
$$\langle\uparrow|\downarrow\rangle = (1\ 0)\begin{pmatrix}0\\1\end{pmatrix} = 0 = (0\ 1)\begin{pmatrix}1\\0\end{pmatrix} = \langle\downarrow|\uparrow\rangle \checkmark$$

What does O look like in this representation?

Consider matrix M acting on $\begin{pmatrix}1\\0\end{pmatrix}$:

$$\begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22}\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}m_{11}\\m_{21}\end{pmatrix} = m_{11}\begin{pmatrix}1\\0\end{pmatrix} + m_{21}\begin{pmatrix}0\\1\end{pmatrix}$$

In other words

$$M = \begin{pmatrix} M\cdot\begin{pmatrix}1\\0\end{pmatrix} & M\cdot\begin{pmatrix}0\\1\end{pmatrix}\end{pmatrix}$$

So O is $\begin{pmatrix} o_{11} & o_{12} \\ o_{21} & o_{22}\end{pmatrix}$

We are especially interested in <u>Hermitian operators</u>, since they are observables.

If $O^\dagger = O$, then $O = \begin{pmatrix} o_{11} & o_{21}^R - i o_{21}^I \\ o_{21}^R + i o_{21}^I & o_{22}\end{pmatrix}$ where all 6 numbers are in $\mathbb{R}$

$[o_{21} = o_{12}^*]$

<u>This can be written as:</u>

$$\frac{o_{11}+o_{22}}{2}\cdot\begin{pmatrix}1&0\\0&1\end{pmatrix} + \frac{o_{11}-o_{22}}{2}\begin{pmatrix}1&0\\0&-1\end{pmatrix} + \underset{\uparrow \atop \frac{o_{12}+o_{21}}{2}}{o_{12}^R}\begin{pmatrix}0&1\\1&0\end{pmatrix} + \underset{\uparrow \atop \frac{o_{21}-o_{12}}{2i}}{o_{21}^I}\begin{pmatrix}0&-i\\i&0\end{pmatrix}$$

ie every Hermitian operator is of the form

$$a \cdot Id_2 + b \cdot \sigma^z + c \cdot \sigma^x + d \cdot \sigma^y$$

where

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

Now let's put these back in the original representation.

eg $\sigma^z \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $\sigma^z \begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ $\Rightarrow$ $\sigma^z |\uparrow\rangle = |\uparrow\rangle$, $\sigma^z |\downarrow\rangle = -|\downarrow\rangle$

Overall we have:

$$\boxed{Id: \begin{matrix} |\uparrow\rangle \mapsto |\uparrow\rangle \\ |\downarrow\rangle \mapsto |\downarrow\rangle \end{matrix}, \quad \sigma^z: \begin{matrix} |\uparrow\rangle \mapsto |\uparrow\rangle \\ |\downarrow\rangle \mapsto -|\downarrow\rangle \end{matrix}, \quad \sigma^x: \begin{matrix} |\uparrow\rangle \longmapsto |\downarrow\rangle \\ |\downarrow\rangle \longmapsto |\uparrow\rangle \end{matrix}, \quad \sigma^y: \begin{matrix} |\uparrow\rangle \longmapsto i|\downarrow\rangle \\ |\downarrow\rangle \mapsto -i|\uparrow\rangle \end{matrix}}$$

At this point, I want to emphasize that the fundamental objects are the states and operators, not their vectors and matrix representations.

- For example, I could choose instead $|\uparrow\rangle \to \begin{pmatrix} 0 \\ 1 \end{pmatrix}$, $|\downarrow\rangle \to \begin{pmatrix} 1 \\ 0 \end{pmatrix}$.

  Then the 4 matrices are

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

  These have changed, even though the actual operators have not.
  This is a change of basis

- Example 2: we can also try a less trivial change of basis and find a new representation

  eg $|\rightarrow\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$

  $|\leftarrow\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle - |\downarrow\rangle)$

  ① Check ON basis: $\langle\rightarrow|\rightarrow\rangle = \frac{1}{2}(\langle\uparrow|\uparrow\rangle + \langle\downarrow|\downarrow\rangle + \langle\uparrow|\downarrow\rangle + \langle\downarrow|\uparrow\rangle) = 1$ ✓

  $\langle\rightarrow|\leftarrow\rangle = \frac{1}{2}(\langle\uparrow|\uparrow\rangle - \langle\downarrow|\downarrow\rangle + \langle\downarrow|\uparrow\rangle - \langle\uparrow|\downarrow\rangle) = 0$ ✓

  ⋮ ok ✓

② Find actions of operators

eg $$Id\,|\rightarrow\rangle = \tfrac{1}{\sqrt{2}}\left(Id\,|\uparrow\rangle + Id\,|\downarrow\rangle\right) = \tfrac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right) = |\rightarrow\rangle$$

$$\sigma_x\,|\leftarrow\rangle = \tfrac{1}{\sqrt{2}}\left(\sigma_x|\uparrow\rangle - \sigma_x|\downarrow\rangle\right) = \tfrac{1}{\sqrt{2}}\left(|\downarrow\rangle - |\uparrow\rangle\right) = -|\leftarrow\rangle$$

$$\sigma_y\,|\rightarrow\rangle = \tfrac{1}{\sqrt{2}}\left(\sigma_y|\uparrow\rangle + \sigma_y|\downarrow\rangle\right) = \tfrac{1}{\sqrt{2}}\left(i|\downarrow\rangle - i|\uparrow\rangle\right) = -i|\leftarrow\rangle$$

etc

<u>Result</u>:

Id: $|\rightarrow\rangle \mapsto |\rightarrow\rangle$, $|\leftarrow\rangle \mapsto |\leftarrow\rangle$, σ^z: $|\rightarrow\rangle \mapsto |\leftarrow\rangle$, $|\leftarrow\rangle \mapsto |\rightarrow\rangle$, σ^x: $|\rightarrow\rangle \mapsto |\rightarrow\rangle$, $|\leftarrow\rangle \mapsto -|\leftarrow\rangle$, σ^y: $|\rightarrow\rangle \mapsto -i|\leftarrow\rangle$, $|\leftarrow\rangle \mapsto i|\rightarrow\rangle$

Then let $|\rightarrow\rangle \rightarrow \begin{pmatrix}1\\0\end{pmatrix}$

$|\leftarrow\rangle \rightarrow \begin{pmatrix}0\\1\end{pmatrix}$

so the operators are represented by

$$\underset{Id}{\begin{pmatrix}1&0\\0&1\end{pmatrix}},\ \underset{\sigma^z}{\begin{pmatrix}0&1\\1&0\end{pmatrix}},\ \underset{\sigma^x}{\begin{pmatrix}1&0\\0&-1\end{pmatrix}},\ \underset{\sigma^y}{\begin{pmatrix}0&i\\-i&0\end{pmatrix}}$$

The matrices have changed, but the <u>physical objects</u>, the operators, have not.

Here I want to pause the main story and show how to implement this change of basis directly in the matrix language.

Look at <u>eg</u> σ^z:

if $\begin{pmatrix}1\\0\end{pmatrix} = |\uparrow\rangle$, $\begin{pmatrix}0\\1\end{pmatrix} = |\downarrow\rangle$, $\sigma^z = \begin{pmatrix}1&0\\0&-1\end{pmatrix}$

To get the first col of the new matrix when $\begin{pmatrix}1\\0\end{pmatrix} = |\rightarrow\rangle$, $\begin{pmatrix}0\\1\end{pmatrix} = |\leftarrow\rangle$,

want to do the following steps: ~~$\begin{pmatrix}1\\0\end{pmatrix}$ → ① → ② apply σ^z → ③ rewrite w/ new $\begin{pmatrix}1\\0\end{pmatrix}$, $\begin{pmatrix}0\\1\end{pmatrix}$~~

① $\begin{pmatrix}1\\0\end{pmatrix}_{\substack{new\\basis}} = \frac{1}{\sqrt2}(|\uparrow\rangle + |\downarrow\rangle) = \frac{1}{\sqrt2}\begin{pmatrix}1\\1\end{pmatrix}_{\substack{old\\basis}}$ Rewrite as a vector in the old basis, so you can apply old σ^z matrix

② apply σ^z: $\begin{pmatrix}1&0\\0&-1\end{pmatrix}_{old} \cdot \begin{pmatrix}1\\1\end{pmatrix}_{old}/\sqrt2 = \begin{pmatrix}1\\-1\end{pmatrix}_{old}/\sqrt2$

③ transform back to new basis. Here it's easy to see it by eye, it's just $\begin{pmatrix}0\\1\end{pmatrix}_{new}$

~~$\begin{pmatrix}a\\b\end{pmatrix}_{old}$ means $\langle\uparrow|\psi\rangle = a$, $\langle\downarrow|\psi\rangle = b$~~

So in the new basis, the 1st col of $\sigma^z = \begin{pmatrix}0\\1\end{pmatrix}$

Now let's write ① and ③ as matrix multiplication

① new basis → old basis.

The first column is: what happens to $\begin{pmatrix}1\\0\end{pmatrix}_{new}$

$\begin{pmatrix}1\\0\end{pmatrix}_{new} \to \frac{1}{\sqrt2}\begin{pmatrix}1\\1\end{pmatrix}_{old}$

2nd col: what happens to $\begin{pmatrix}0\\1\end{pmatrix}_{new}$? $\mapsto \frac{1}{\sqrt2}\begin{pmatrix}1\\-1\end{pmatrix}_{old}$

So matrix is $\frac{1}{\sqrt2}\begin{pmatrix}1&1\\1&-1\end{pmatrix}$

1st col: write new $\begin{pmatrix}1\\0\end{pmatrix}$ in terms of old $\begin{pmatrix}1\\0\end{pmatrix}, \begin{pmatrix}0\\1\end{pmatrix}$

2nd col: write new $\begin{pmatrix}0\\1\end{pmatrix}$ in terms of old $\begin{pmatrix}1\\0\end{pmatrix}, \begin{pmatrix}0\\1\end{pmatrix}$

③ old basis → new basis.

$\frac{1}{\sqrt2}\begin{pmatrix}1&1\\1&-1\end{pmatrix}$

1st col: old $\begin{pmatrix}1\\0\end{pmatrix}$ in terms of new $\begin{pmatrix}1\\0\end{pmatrix}, \begin{pmatrix}0\\1\end{pmatrix}$

2nd col: old $\begin{pmatrix}0\\1\end{pmatrix}$ in terms of new $\begin{pmatrix}1\\0\end{pmatrix}, \begin{pmatrix}0\\1\end{pmatrix}$

Put it all together: $\sigma^x_{new} = \left[\frac{1}{\sqrt2}\begin{pmatrix}1&1\\1&-1\end{pmatrix}\right]\cdot\begin{pmatrix}1&0\\0&-1\end{pmatrix}\cdot\left[\frac{1}{\sqrt2}\begin{pmatrix}1&1\\1&-1\end{pmatrix}\right]\begin{pmatrix}1&0\\0&1\end{pmatrix}$

Annotated

V

$$\begin{pmatrix}0&1\\1&0\end{pmatrix} = \left[\frac{1}{\sqrt{2}}\begin{pmatrix}1&1\\1&-1\end{pmatrix}\right]\cdot\begin{pmatrix}1&0\\0&-1\end{pmatrix}\left[\frac{1}{\sqrt{2}}\begin{pmatrix}1&1\\1&-1\end{pmatrix}\right]\begin{pmatrix}1&0\\0&1\end{pmatrix}$$

get 2nd col by acting on $\binom{0}{1}_{new}$

σ^z_{new}

σ^z_{old}

write new vector in terms of old ones

get 1st col by acting on $\binom{1}{0}_{new}$

apply σ^z in old basis

transform back to new basis

Some notes:
- matrix on the right is the identity so it can be dropped.
- Write it as $\mathcal{O}_{new} = V^{\dagger}\cdot\mathcal{O}_{old}\cdot V\cdot Id$
- columns of V are the new basis vectors in terms of the old ones.
- the matrices for the two basis transformations are Hermitian conjugates because:
  - if you apply both in succession you must get back the original vector, so they are inverses
  - the basis being orthonormal means that

    $V^{\dagger}V = VV^{\dagger} = Id$

[Note: if you ever use a non-ON basis, this procedure will still work but $V^{\dagger} \to \tilde{V} \neq V^{\dagger}$]

~~Next up is our first programming exercise~~

Note that $H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$ is called the "Hadamard gate" in quantum computing literature. As we've just seen, it performs a change of basis between

$\begin{pmatrix} 1 \\ 0 \end{pmatrix} = |\uparrow\rangle$ where $\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ called "z basis" because σ^z is diagonal

$\begin{pmatrix} 0 \\ 1 \end{pmatrix} = |\downarrow\rangle$ $\qquad \sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

and

$\begin{pmatrix} 1 \\ 0 \end{pmatrix} = |\rightarrow\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$ where $\sigma^z = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ called "x basis"

$\begin{pmatrix} 0 \\ 1 \end{pmatrix} = |\leftarrow\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle - |\downarrow\rangle)$ $\qquad \sigma^x = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

Next up is our first programming exercise.

Goals:
- learn to use Jupyter notebook
- learn how to create arrays and matrices
- matrix multiplication and eigenvalue decomposition
- test Hadamard change of basis