Title: Summer Undergrad 2020 - Numerical Methods (A) - Lecture 3

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Collection: Summer Undergrad 2020 - Numerical Methods

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Abstract: Exact diagonalization part 1: solve two-site Ising model, find energies, expectation values, etc.; Find matrices for N-site Ising model

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Note Jun 1, 2020 (2)
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Two-site Ising model (cont.)

$$H = -J\underbrace{\left(\sigma_0^z \otimes \sigma_1^z\right)}_{\begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & 1 \end{pmatrix}} - h\underbrace{\left(\sigma_0^x \otimes Id_1 + Id_0 \otimes \sigma_1^x\right)}_{\begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}}$$

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Two limits

$h = 0$ $\quad H = -J\,\sigma_0^z \otimes \sigma_1^z$

eig states: $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$, $E = -J$

$|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, $E = J$

$J = 0$ $\quad H = h(\sigma_0^x + \sigma_1^x)$

eig states: $|\rightarrow\rightarrow\rangle$, $E = -2h$

$|\rightarrow\leftarrow\rangle$

$|\leftarrow\rightarrow\rangle$, $E = 0$

$|\leftarrow\leftarrow\rangle$, $E = 2h$

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$|\leftarrow\leftarrow\rangle$, $E=2h$

Goal: • Find eigenstates/energies for any J, h

• Find some properties of GS

Expectation values

$\langle \sigma_0^z \otimes Id_1 + Id_0 \otimes \sigma_1^z \rangle$: tendency

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Expectation values

- $\underbrace{\langle \sigma_0^z \otimes Id_1 + Id_0 \otimes \sigma_1^z \rangle}_{\langle \sigma_0^z + \sigma_1^z \rangle}$: tendency of spins to point along z in a particular direction

eg $|\psi\rangle = |\uparrow\uparrow\rangle$ $\quad \langle \sigma_0^z + \sigma_1^z \rangle = 2$

$|\psi\rangle = |\uparrow\downarrow\rangle$ $\quad \langle \sigma_0^z + \sigma_1^z \rangle = 0$

- $\langle \sigma_0^z \otimes \sigma_1^z \rangle$: measures tendency of

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$\langle \sigma_0^z + \sigma_1^z \rangle = 2$

$|\psi\rangle = |\uparrow\downarrow\rangle \qquad \langle \sigma_0^z + \sigma_1^z \rangle = 0$

- $\langle \sigma_0^z \otimes \sigma_1^z \rangle$: measures tendency of the two spins to point // along z

$$|\uparrow\uparrow\rangle \to 1 \qquad |\downarrow\downarrow\rangle \to 1 \qquad \left.\begin{matrix} |\uparrow\downarrow\rangle \\ |\downarrow\uparrow\rangle \end{matrix}\right\} \longrightarrow -1$$

$\langle \mathcal{O}_A \, \mathcal{O}_B \rangle \to$ "Correlation function"

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$\langle O_A \; O_B \rangle \to$ "Correlation function"

- $\langle \sigma_0^x \otimes Id_1 + Id_0 \otimes \sigma_1^x \rangle / 2$
- $\langle \sigma_0^x \otimes \sigma_1^x \rangle$

One more comment

H has two parameters: J, h

But M

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One more comment

H has two parameters: J, h

But M, eig vals λ_i, vects v_i

aM, eig vals $a \cdot \lambda_i$, vects v_i

something

So H really only has one parameter: $\frac{h}{J}$

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So H really only has one parameter: $\frac{h}{J} \equiv g$

Important: if you have to numerically solve for every parameter pt, one parameter is much better than two!!

$$\frac{H}{J} = -\left(\sigma_0^z \otimes \sigma_1^z\right) - g\left(\sigma_0^x \otimes Id_1 + Id_0 \otimes \sigma_1^x\right)$$

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Comments on results

$$\langle \sigma_0^z \otimes Id_1 + Id_0 \otimes \sigma_1^z \rangle$$

- Why is it 0?
- Why does it jump?

$\underline{g=0}$: eigstates:

$\vert\uparrow\uparrow\rangle$	-1
$\vert\downarrow\downarrow\rangle$	-1
$\vert\uparrow\downarrow\rangle$	1
$\vert\downarrow\uparrow$	

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· Why does it jump?

$g=0$: eigstates:

$$\boxed{\begin{array}{ll} |\uparrow\uparrow\rangle & -1 \\ |\downarrow\downarrow\rangle & -1 \end{array}}$$

$$\begin{array}{ll} |\uparrow\downarrow\rangle & 1 \\ |\downarrow\uparrow\rangle & 1 \end{array}$$

GS: $|\varphi\rangle = a|\uparrow\uparrow\rangle + b|\downarrow\downarrow\rangle$

Calculate expec. val:

$$(\sigma_0^z + \sigma_1^z)|\varphi\rangle =$$

$$(a|\uparrow\uparrow\rangle - b|\downarrow\downarrow\rangle) +$$

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$$\frac{(\sigma_0^z + \sigma_1^z)}{2}|\psi\rangle =$$

$$\big(a|\uparrow\uparrow\rangle - b|\downarrow\downarrow\rangle\big) + \big(a|\uparrow\uparrow\rangle - b|\downarrow\downarrow\rangle\big)$$

$$\langle\psi|\frac{(\sigma_0^z + \sigma_1^z)}{2}|\psi\rangle = \cancel{2}\left(|a|^2 - |b|^2\right)$$

Python semi-randomly picks a, b

g=0 value is kind-of meaningless

<u>$g \neq 0$</u> Eigenstates

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$\underline{g \neq 0}$ Eigenstates respect symmetries of H

All spins: $|\downarrow\rangle \longleftrightarrow |\uparrow\rangle$

matrix for H doesn't change

$\Rightarrow$ ground state has $|\uparrow\rangle$ and $|\downarrow\rangle$ parts, but they're equal

For c

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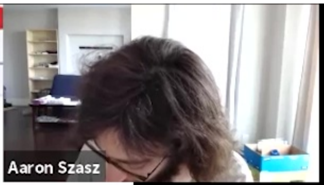

For comparison:

$\langle \sigma_0^z \otimes \sigma_1^z \rangle$:

Cancellation doesn't happen:

$$\langle \uparrow\uparrow | \sigma_0^z \otimes \sigma_1^z | \uparrow\uparrow \rangle$$
$$= \langle \downarrow\downarrow | \sigma_0^z \otimes \sigma_1^z | \downarrow\downarrow \rangle = 1$$

Gets around

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Gets around symmetry problem:
better measure of tendency
of spins to point along $\hat{z}$

$\langle \sigma_i^z \otimes \sigma$

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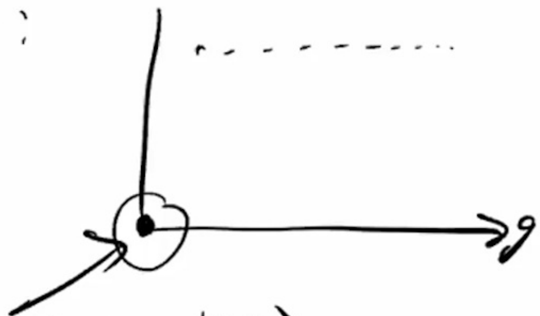
$\langle \sigma_0^x \otimes \sigma_1^x \rangle$:



picks $|\uparrow\uparrow\rangle$

$$(\sigma_0^x \otimes \sigma_1^x)|\uparrow\uparrow\rangle = |\downarrow\downarrow\rangle$$

$$\langle \downarrow\downarrow|\uparrow\uparrow\rangle = 0$$

but if GS is $|\uparrow\uparrow\rangle + |'$

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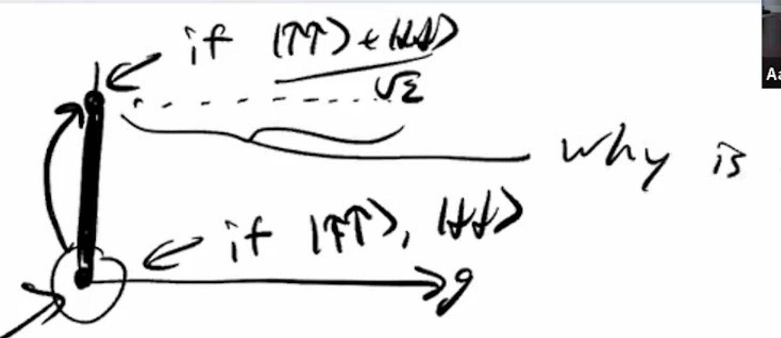
$\langle \sigma_0^x \otimes \sigma_1^x \rangle$:



picks $|\uparrow\uparrow\rangle$

$$(\sigma_0^x \otimes \sigma_1^x)|\uparrow\uparrow\rangle = |\downarrow\downarrow\rangle$$

$$\langle \downarrow\downarrow | \uparrow\uparrow \rangle = 0$$

but if GS is $\frac{|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle}{\sqrt{2}}$ equal

$$(\sigma_0^x \otimes \sigma_1^x)|\quad\rangle = \frac{|\downarrow\downarrow\rangle + |\uparrow\uparrow\rangle}{\sqrt{2}}$$

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$$(\sigma_0^x \otimes \sigma_1^x)|+\rangle = \frac{|\downarrow\downarrow\rangle + |\uparrow\uparrow\rangle}{\sqrt{2}}$$

Constant: because it's a conserved quantity:

$$\big[H, \underbrace{\sigma_0^x \otimes \sigma_1^x}_{\text{flips both spins}}\big] = 0$$

but

$$H = -J(\underbrace{\sigma_0^z \otimes \sigma_1^z}_{\begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & 1 \end{pmatrix}}) - h(\sigma_0^x + \sigma_1^x)$$

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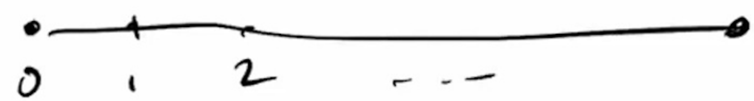
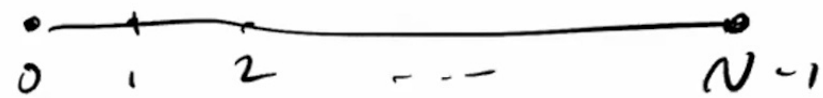
N-site Ising model

$$\frac{H}{J} = -\sum_i \sigma_i^z \sigma_{i+1}^z - g \sum_i \sigma_i^x$$



$$\frac{H}{J} = -\sum_i \sigma_i^z \sigma_{i+1}^z - g \sum_i \sigma_i^x$$



$\sigma_0^z \sigma_1^z$ means $\sigma_0^z \otimes \sigma_1^z \otimes Id_2 \otimes \cdots \otimes Id_{N-1}$

σ_2^x means $Id_0 \otimes Id_1 \otimes \sigma_2^x \otimes Id_3 \otimes \cdots \otimes Id_{N-1}$

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σ_2^x means $Id_0 \otimes Id_1 \otimes \sigma_2^x \otimes Id_3 \otimes \cdots \otimes Id_{N-1}$

Steps:
1. Choose a basis
2. Find matrix for H
3. Find GS
4. Calculate stuff (eg $\langle \sigma_0^z \underset{Id_1 \cdots Id_{N-2}}{\otimes} \sigma_{N-1}^z \rangle$)

① N sites $\rightarrow$ 2^N basis st

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① N sites $\rightarrow 2^N$ basis states

$$\begin{array}{r} 0 \rightarrow \\ \\ \\ \\ 2^N-1 \rightarrow \end{array} \begin{pmatrix} 1 \\ 0 \\ \vdots \\ \vdots \\ 0 \end{pmatrix} = |\uparrow\uparrow \ldots \uparrow\rangle \qquad \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} = |\uparrow\uparrow \ldots \uparrow\downarrow\rangle$$

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index 2 : $|\uparrow\uparrow \ldots \uparrow\downarrow\uparrow\rangle$

index 3 : $|\uparrow\uparrow \ldots \uparrow\downarrow\downarrow\rangle$

index 4 : $|\uparrow\uparrow \ldots \downarrow\uparrow\uparrow\rangle$ ...

Need: function : index $\longmapsto$ spin list

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Need: function: index $\longmapsto$ spin list

$N = 3$

↑↑↑
↑↑↓
↑↓↑
↑↓↓
↓↑↑
↓↑↓
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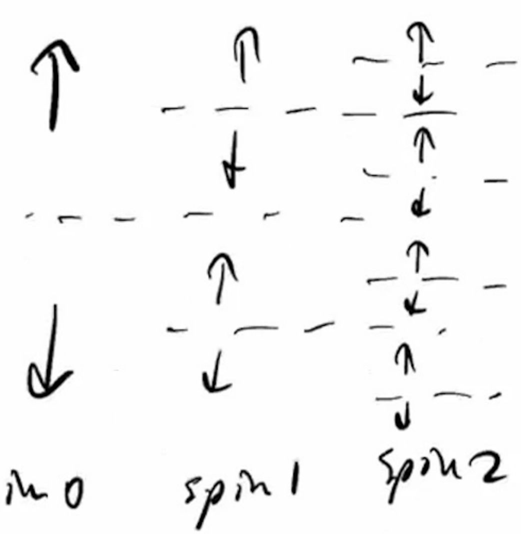
↓↓↓



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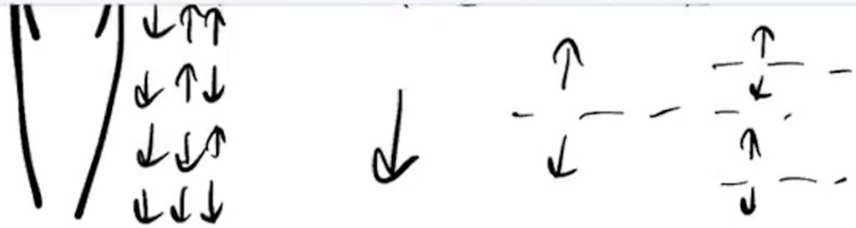

spin 0 spin 1 spin 2

spin 0: if index is in 1^{st} half, $\uparrow$

2^{nd} half, $\downarrow$

$\text{index} / \underbrace{2^{N-1}}_{4}$ throw away remainder

1st half: $\text{index} < 2^{N-1}$

$\Rightarrow 0$

2^{nd}

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2nd half, ↓

index $/2^{N-1}$ throw away remainder

$\underbrace{}_{4}$

1st half: index $< 2^{N-1}$

$\Rightarrow 0 \Rightarrow |\uparrow\rangle$

2nd half: $\Rightarrow 1 \Rightarrow |\downarrow\rangle$

spin = index $// 2^{N-1}$

↑ divide & throw away remainder

spin 1: index $// 2^{N-2}$; 1st $\frac{1}{4}$: 0

2^{n}

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3rd : 2 $\uparrow$

4th : 3 $\downarrow$

want: $0 \to 0$, $2 \to 0$

$1 \to 1$, $3 \to 1$

we can do this using **mod 2**

% 2

$(\text{index} // 2^{N-2})$ % 2 : $0 \Rightarrow |\uparrow\rangle$

$1 \Rightarrow |\downarrow\rangle$

⋮

spin 3 : $(\text{index} // 2^{N-3})$ % 2

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spin 3 : $(\text{index} // 2^{N-3}) \% 2$

etc

overall:

index

$\downarrow$

$$\left[\text{index}//2^{N-1},\ (\text{index}//2^{N-2})\%2,\ \ldots,\ \text{index}\%2\right]$$

function

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overall:

index

$$\downarrow$$

$$\left[\text{index}//2^{N-1}, (\text{index}//2^{N-2})\%2, \ldots, \text{index}\%2\right]$$

function: d2b → "decimal to binary"

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$$\left[\text{index}//2^{N-1},\ (\text{index}//2^{N-2})\%2,\ \ldots,\ \text{index}\%2\right]$$

function: d2b → "decimal to binary"

Reverse: b2d

$$[0, 1, 1, 0]$$

$$2^3 \cdot 0 + 2^2 \cdot 1 + 2 \cdot 1 + 0 = 6$$

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② **Find H**

$\boxed{\text{Method 1}}$ Kronecker product

$$\sigma_0^x \otimes Id_1 \qquad \begin{pmatrix} 0\begin{pmatrix}1&0\\0&1\end{pmatrix} & 1\begin{pmatrix}1&0\\0&1\end{pmatrix} \\ 1\begin{pmatrix}1&0\\0&1\end{pmatrix} & 0\begin{pmatrix}1&0\\0&1\end{pmatrix}\end{pmatrix} = \begin{pmatrix} & & 1 & \\ & & & 1 \\ 1 & & & \\ & 1 & & \end{pmatrix}$$

σ_0

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$$\underbrace{\sigma_0^x \otimes \sigma_1^z} \otimes \sigma_2^x$$

$$\boxed{(\sigma_0^x \otimes \sigma_1^z) \otimes \sigma_2^x = \sigma_0^x \otimes (\sigma_1^z \otimes \sigma_2^x)}$$

$$\begin{pmatrix} 0 & \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$$

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$$\underbrace{\sigma_0^x \otimes \sigma_1^z} \otimes \sigma_2^x$$

$$\boxed{(\sigma_0^x \otimes \sigma_1^z) \otimes \sigma_2^x = \sigma_0^x \otimes (\sigma_1^z \otimes \sigma_2^x)}$$

$$\begin{pmatrix} 0 & \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$$

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Ex from H:

$$\sigma_0^z \otimes \sigma_1^z \otimes Id_2 \otimes \cdots \otimes Id_{N-1}$$

- make a list of operators

$$[\sigma^z, \sigma^z, Id, Id \ldots Id]$$

$$[\sigma^z, \sigma^z] + [Id] * (N-2)$$

- repeated Kronecker

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$$\sigma_0^z \otimes \sigma_1^z \otimes Id_2 \otimes \dots \otimes Id_{N-1}$$

- make a list of operators

ops = [σz, σz, Id, Id ... Id]

[σz, σz] + [Id]*(N-2)

- repeated Kronecker product

```
mat = ops[0]
for op in ops[1:]:
    mat = np.kron(mat, op)
```

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Next time: method 2 → "column-by-column"

index of basis state ⟶ spin list

↓ apply term

vector representation = col of matrix ⟵ (spin list, coeff)

method 3: use the fact that the $\sum_i \sigma_i^z \sigma_{i+1}^z$ term is diagonal

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