Title: Summer Undergrad 2020 - Numerical Methods (A) - Lecture 1

Speakers: Aaron Szasz

Collection: Summer Undergrad 2020 - Numerical Methods

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Abstract: Introduction to Ising model; review spin-1/2 and matrix representation of states  and operators; programming basics

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# Numerical Methods for Condensed Matter Physics

Goals: 1) Learn some numerical methods
2) Learn some important models from condensed matt.

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Goals: 1) Learn some numerical methods

2) Learn some important models from condensed matter

In particular,

"Quantum Ising model"

or

"Transverse-field Ising model"

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2) Learn some important models from condensed matter

In particular,

"Quantum Ising model"

or

"Transverse-field Ising model"

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

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or

"Transverse-field Ising model"

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

Day 1: background

Day 2: Introduce "Exact Diagonalization"

Use it to solve Ising model

Day 3: Continue Exact Diagonalization


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

<u>Day 1:</u> background

<u>Day 2:</u> Introduce "Exact Diagonalization"
Use it to solve Ising model

<u>Day 3:</u> Continue Exact Diagonalization,
XXZ model

<u>Day 4:</u> Matrix Product States (MPS)

<u>Day 5:</u> Use MPS to solve Ising, XXZ
more efficiently

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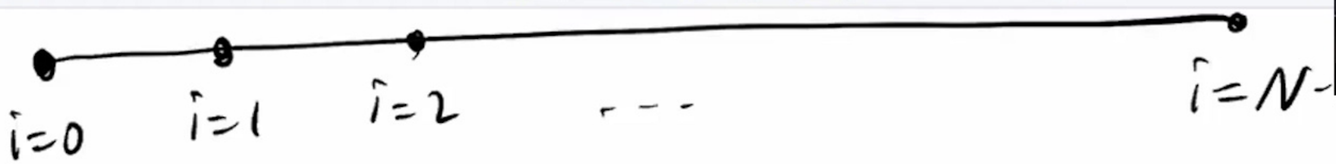


- $N$ atoms in a chain
- $1\ e^-$ per atom
- $e^-$ cannot move! Coulomb repulsion $\Rightarrow$ $1\ e^-$ per site is fixed
- For each atom, solve local Schrodinger eq. $\frac{p^2}{2m} + V(r) = H_i$
  $\Rightarrow$ orbitals: $s, p^x, p$

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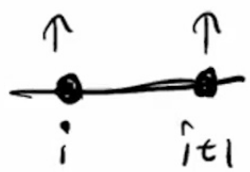
- For each atom, solve local Schrodinger eq. $\frac{p^2}{2m} + V(r) = H_i$
  $\Rightarrow$ orbitals: $s, p^x, p^y, p^z, d, \ldots$
- 1 degree of freedom still:
  **spin**
-  configurations
  $\uparrow\uparrow$, $\uparrow\downarrow$, $\downarrow\uparrow$, $\downarrow\downarrow$

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

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spin

- configurations
  $\uparrow\uparrow$, $\uparrow\downarrow$, $\downarrow\uparrow$, $\downarrow\downarrow$
  $i$, $i+1$

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

$J > 0$

1 for $\uparrow\uparrow$, $\downarrow\downarrow$

$-1$ for $\uparrow\downarrow$, $\downarrow\uparrow$

- $-h \sum_i S_i^x$

$\vec{B} = B\hat{x}$

lowest E: $\rightarrow$

highest E: $\leftarrow$

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## Spin-$\frac{1}{2}$

A state of a spin-$\frac{1}{2}$ system

$$|\psi\rangle = a|\uparrow\rangle + b|\downarrow\rangle, \quad |a|^2 + |b|^2 = 1$$

$\{|\uparrow\rangle, |\downarrow\rangle\}$ forms an orthonormal basis for the space of states

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orthonormal basis for the space of states

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

Operators acting on spin-$\frac{1}{2}$:

$$\mathcal{O}: \quad \mathcal{O}|\uparrow\rangle = O_{11}|\uparrow\rangle + O_{21}|\downarrow\rangle$$
$$\mathcal{O}|\downarrow\rangle = O_{12}|\uparrow\rangle + O_{22}|\downarrow\rangle$$

Write in a matrix represent

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Write in a matrix representation:

① Assign vectors to $|\uparrow\rangle$, $|\downarrow\rangle$

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

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

② Find operators, other states in this basis

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$|\downarrow\rangle \to (\ 1\ )$

② Find operators, other states in this basis

$$\mathcal{O} = \begin{pmatrix} O_{11} & O_{12} \\ O_{21} & O_{22} \end{pmatrix}$$

$$\mathcal{O} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} O_{11} \\ O_{21} \end{pmatrix} = 1^{st} \text{ col of } \mathcal{O}$$

$$\mathcal{O} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} O_{12} \\ O_{22} \end{pmatrix} = 2^{nd} \text{ col}$$

$$\mathcal{O} = \begin{pmatrix} | & | \\ \mathcal{O}\begin{pmatrix} 1 \\ 0 \end{pmatrix} & \mathcal{O}\begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ | & | \end{pmatrix}$$

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$$O = \begin{pmatrix} | & | \\ O\begin{pmatrix}1\\0\end{pmatrix} & O\begin{pmatrix}0\\1\end{pmatrix} \\ | & | \end{pmatrix}$$

1st col of $O$:

$$O\begin{pmatrix}1\\0\end{pmatrix} \to O|\uparrow\rangle = O_{11}|\uparrow\rangle + O_{21}|\downarrow\rangle$$

$$\downarrow$$

$$O_{11}\begin{pmatrix}1\\0\end{pmatrix} + O_{21}\begin{pmatrix}0\\1\end{pmatrix}$$

$$= \begin{pmatrix}O_{11}\\O_{21}\end{pmatrix}$$

$$O\begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}O_{12}\\O_{22}\end{pmatrix}$$

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$$O_{11}\begin{pmatrix}1\\0\end{pmatrix} + O_{21}\begin{pmatrix}0\\1\end{pmatrix}$$

$$= \begin{pmatrix}O_{11}\\O_{21}\end{pmatrix}$$

$$\mathcal{O}\begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}O_{12}\\O_{22}\end{pmatrix}$$

$$\mathcal{O} = \begin{pmatrix}O_{11} & O_{12}\\O_{21} & O_{22}\end{pmatrix}$$

---

Some important operators

We care about Hermitian operators,

$$\mathcal{O} = \mathcal{O}^\dagger$$

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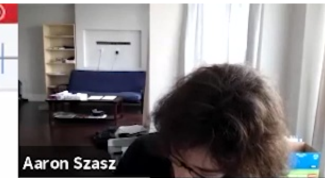


## Some important operators

We care about Hermitian operators,

$$\mathcal{O} = \mathcal{O}^\dagger \leftarrow \text{transpose, complex conjugate}$$

2x2 matrices, any Hermitian operator can be written as

$$\mathcal{O} = a\,\mathrm{Id} + b\sigma^z + c\sigma^x + d\sigma^y \quad \text{where}$$

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## Some important operators

We care about Hermitian operators,

$$\mathcal{O} = \mathcal{O}^\dagger \leftarrow \text{transpose, complex conjugate}$$

$2\times 2$ matrices, any Hermitian operator can be written as

$$\mathcal{O} = a\,\mathrm{Id} + b\sigma^z + c\sigma^x + d\sigma^y \quad \text{where}$$

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

$$\sigma^z\left(|\uparrow\rangle\right) = \sigma^z\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |\uparrow\rangle$$

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$$\sigma^z(|\uparrow\rangle) = \sigma^z\begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}1\\0\end{pmatrix} = |\uparrow\rangle$$

$$\boxed{\begin{array}{llll} \text{Id}: \begin{array}{l}|\uparrow\rangle \mapsto |\uparrow\rangle \\ |\downarrow\rangle \mapsto |\downarrow\rangle\end{array}, & \sigma^z: \begin{array}{l}|\uparrow\rangle \mapsto |\uparrow\rangle \\ |\downarrow\rangle \mapsto -|\downarrow\rangle\end{array}, & \sigma^x: \begin{array}{l}|\uparrow\rangle \mapsto |\downarrow\rangle \\ |\downarrow\rangle \mapsto |\uparrow\rangle,\end{array} \\ & & \sigma^y: \begin{array}{l}|\uparrow\rangle \mapsto i|\downarrow\rangle \\ |\downarrow\rangle \mapsto -i|\uparrow\rangle\end{array} \end{array}}$$

Find matrices in a different basis.

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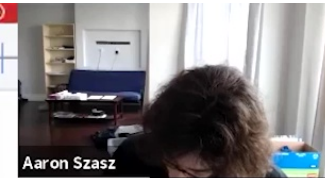


$|\downarrow\rangle \mapsto |\downarrow\rangle$, $\quad |\downarrow\rangle \mapsto -|\downarrow\rangle$, $\quad |\downarrow\rangle \mapsto |\uparrow\rangle$,

$\sigma^y: \ |\uparrow\rangle \mapsto i|\downarrow\rangle$

$|\downarrow\rangle \mapsto -i|\uparrow\rangle$

Find matrices in a different basis.

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

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

Step 1: check ON basis

$\langle\rightarrow|\rightarrow\rangle = 1$ ?

$= \frac{1}{\sqrt{2}}\langle\uparrow| + \langle$

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

Step 1: check ON basis

$$\langle\rightarrow|\rightarrow\rangle = 1 \; ?$$

$$= \left(\frac{1}{\sqrt{2}}\left(\langle\uparrow| + \langle\downarrow|\right)\right)\left(\frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right)\right)$$

$$= \frac{1}{2}\left(\langle\uparrow|\uparrow\rangle + \langle\uparrow|\downarrow\rangle + \langle\downarrow|\uparrow\rangle + \langle\downarrow|\downarrow\rangle\right)$$

$$= \frac{1}{2}\left(1 + 0 + 0 + 1\right) = 1$$

$$\langle\rightarrow|\leftarrow\rangle = 0$$

Step 2: Find matrices of $\sigma^z, \sigma^x, \sigma^y$ in

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$|\downarrow\rangle \mapsto -i|\uparrow\rangle$

Find matrices in a different basis.

eg $|\rightarrow\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right) = \begin{pmatrix}1\\0\end{pmatrix}$

$|\leftarrow\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle - |\downarrow\rangle\right) = \begin{pmatrix}0\\1\end{pmatrix}$ ← $\boxed{\text{definition of basis}}$

Step 1: check ON basis

$$\langle\rightarrow|\rightarrow\rangle = 1 \ ?$$

$$= \left(\frac{1}{\sqrt{2}}\left(\langle\uparrow| + \langle\downarrow|\right)\right)\left(\frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right)\right)$$

$$= \frac{1}{2}\left(\langle\uparrow|\uparrow\rangle + \langle\uparrow|\downarrow\rangle + \langle\downarrow|\uparrow\rangle + \langle\downarrow|\downarrow\rangle\right)$$

$$= \frac{1}{2}\left(1 + 0 + 0 + 1\right) = 1$$

$$\langle\rightarrow|\leftarrow\rangle = 0$$

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Step 2: Find matrices of $\sigma^z, \sigma^x, \sigma^y$ in this basis

$\sigma^z$: $1^{st}$ col is $\sigma^z \begin{pmatrix}1\\0\end{pmatrix}_{new}$

$$\sigma^z\left(\frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)\right) = \frac{1}{\sqrt{2}}\left(\underline{\sigma^z|\uparrow\rangle} + \underline{\sigma^z|\downarrow\rangle}\right)$$

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

$$= \begin{pmatrix}0\\1\end{pmatrix}_{new}$$

$2^{nd}$ col: $\sigma^z \begin{pmatrix}0\\1\end{pmatrix}_{new} \cdots = \begin{pmatrix}1\\0\end{pmatrix}_{new}$

$$\Rightarrow \sigma^z_{(new)} = \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}$$

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(new)

5 min exercise: $\sigma^x_{new}$, $\sigma^y_{new}$

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

$|\uparrow\rangle$, $|\downarrow\rangle$ $\leftarrow$ "z eigenstates"

$|\rightarrow\rangle$, $|\leftarrow\rangle$ $\leftarrow$ "x eigenstates"

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$|\rightarrow\rangle$, $|\leftarrow\rangle$ ← "x eigenstates"

Matrix version of change of basis:

| Given | Find |
| --- | --- |
| $\sigma^z_{old}$ | $\sigma^z_{new}$ |

~~col~~ col 1 of $\sigma^z_{new}$?

image of $\begin{pmatrix}1\\0\end{pmatrix}_{new}$

we know how to apply $\sigma^z$

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Matrix version of change of basis

Given $\sigma^z_{old}$ Find $\sigma^z_{new}$

~~col~~ col 1 of $\sigma^z_{new}$?

image of $\begin{pmatrix}1\\0\end{pmatrix}_{new}$

we know how to apply $\sigma^z$ to $\begin{pmatrix}1\\0\end{pmatrix}_{old}$ $\begin{pmatrix}0\\1\end{pmatrix}_{old}$

$$\begin{pmatrix}1\\0\end{pmatrix}_{new} \longrightarrow \begin{pmatrix}a\\b\end{pmatrix}_{old} \xrightarrow{\sigma^z_{old}} \begin{pmatrix}\tilde{a}\\\tilde{b}\end{pmatrix}_{old} \longrightarrow \begin{pmatrix}c\\d\end{pmatrix}_{new}$$

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~~col~~ col 1 of $\sigma^z_{new}$ ?

image of $\begin{pmatrix}1\\0\end{pmatrix}_{new}$

we know how to apply $\sigma^z$ to $\begin{pmatrix}1\\0\end{pmatrix}_{old}$ $\begin{pmatrix}0\\1\end{pmatrix}_{old}$

$$\begin{pmatrix}1\\0\end{pmatrix}_{new} \longrightarrow \begin{pmatrix}a\\b\end{pmatrix}_{old} \xrightarrow[old]{\sigma^z} \begin{pmatrix}\tilde{a}\\\hat{b}\end{pmatrix}_{old} \longrightarrow \begin{pmatrix}c\\d\end{pmatrix}_{new}$$

done by matrix mult.

want a matrix: $\underline{\begin{pmatrix}1\\0\end{pmatrix}_{new}} \to \begin{pmatrix}\ \end{pmatrix}_{old}$

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$\text{new}$ $\left(c\right)_{\text{old}}$ $\left(b\right)_{\text{old}} \to \left(d\right)_{\text{new}}$

done by matrix mult.

Want a matrix: $\begin{pmatrix}1\\0\end{pmatrix}_{\text{new}} \to \begin{pmatrix}\ \\ \ \end{pmatrix}_{\text{old}}$

1st col

$$\begin{pmatrix}1\\0\end{pmatrix}_{\text{new}} = |\rightarrow\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right) = \begin{pmatrix}1\\1\end{pmatrix}_{\text{old}} \Big/ \sqrt{2}$$

$$\begin{pmatrix}0\\1\end{pmatrix}_{\text{new}} = \begin{pmatrix}1\\-1\end{pmatrix}_{\text{old}} \Big/ \sqrt{2}$$

$\Rightarrow$ matrix is

$$\begin{pmatrix}1 & 1\\1 & -1\end{pmatrix} \Big/ \sqrt{2}$$

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$\begin{pmatrix} 1 & -1 \end{pmatrix}/\sqrt{2}$

reverse trans is <u>inverse</u>

Any matrix whose cols are ON vectors is unitary $\Rightarrow U^\dagger = U^{-1}$

$$\Rightarrow \left(\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}/\sqrt{2}\right)^{-1} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}/\sqrt{2}$$

$$\sigma^z_{new} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

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$(1\ -1)/\sqrt{2}$

reverse trans is <u>inverse</u>

Any matrix whose cols are ON vectors is unitary $\Rightarrow U^\dagger = U^{-1}$

$$\Rightarrow \left(\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}/\sqrt{2}\right)^{-1} = \begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}/\sqrt{2}$$

$$\sigma^z_{new} = \left[\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\right]\cdot \underline{\sigma^z_{old}} \cdot \underbrace{\left[\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\right]}$$

$$\underline{\qquad\qquad} \ (\ )_{new}$$

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$(1\ -1)/\sqrt{2}$

reverse trans is <u>inverse</u>

Any matrix whose cols are ON vectors is unitary $\Rightarrow U^{\dagger} = U^{-1}$

$$\Rightarrow \left(\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}/\sqrt{2}\right)^{-1} = \begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}/\sqrt{2}$$

$$\sigma^z_{new} = \left[\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\right] \cdot \sigma^z_{old} \cdot \underbrace{\left[\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\right]}$$

$$[\sigma^z(\,)]_{new} \longleftarrow [\sigma^z(\,)]_{old} \longleftarrow (\,)_{new}$$

$$[\sigma^z(\,)]_{old} \longleftarrow (\,)_{old}$$

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jupyter Numpy_basics Last Checkpoint: 5 hours ago (autosaved)


For our first task, we will practice using python to deal with a single spin-1/2 particle. The goal is to get used to python and iPython notebooks, as well as to exercise our linear algebra skills.

We consider a spin-1/2 system that has two basis states,

$$|\uparrow\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$
$$|\downarrow\rangle \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Here I use $\equiv$ to indicate a definition. The basis vectors on the right are defined to be equal to the kets on the left.

A general state will be of the form

$$|\psi\rangle = a|\uparrow\rangle + b|\downarrow\rangle,$$

where $|a|^2 + |b|^2 = 1$, ie it is a normalized pure quantum state of a spin-1/2 system. As a vector, this is represented as

$$|\psi\rangle = \begin{pmatrix} a \\ b \end{pmatrix}.$$

The important operators that act on these states are the identity operator and the spin operators. As usual in linear algebra, any operator is uniquely specified by how it acts on the basis states; using this approach, the operators are defined as follows:

$$\mathrm{Id}|\uparrow\rangle = |\uparrow\rangle$$
$$\mathrm{Id}|\downarrow\rangle = |\downarrow\rangle$$

$$\mathrm{Sx}|\uparrow\rangle = |\downarrow\rangle$$
$$\mathrm{Sx}|\downarrow\rangle = |\uparrow\rangle$$

$$\mathrm{Sx}|\uparrow\rangle = i|\downarrow\rangle$$
$$\mathrm{Sx}|\downarrow\rangle = -i|\uparrow\rangle$$

$$\mathrm{Sz}|\uparrow\rangle = |\uparrow\rangle$$
$$\mathrm{Sz}|\downarrow\rangle = -|\downarrow\rangle$$

These operators can then be represented as matrices, giving:

$$\mathrm{Id} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \mathrm{Sx} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \mathrm{Sy} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \mathrm{Sz} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

These are of course the usual Pauli matrices.

We will now practice writing these matrices using python. We first "import" the numerical python, or "numpy," package.

```
In [ ]: import numpy as np
```

Writing "as np" just lets us call the package whatever we want so we can type that instead of numpy when we use it later. "np" is the traditional abbreviation, so I highly recommended using it for all your programs.

Now I will demonstrate in the next line how to input a matrix.