Introduction to the FRIB-TA Summer School: Quantum Computing and Nuclear Few- and Many-Body Problems with teaching plan and learning outcomes

Facility for Rare Isotope Beams, Michigan State University, USA

June 20

Introduction

Recent developments in quantum information systems and technologies offer the possibility to address some of the most challenging large-scale problems in science, whether they are represented by complicated interacting quantum mechanical systems or classical systems. The last years have seen a rapid and exciting development in algorithms and quantum hardware. The emphasis of this summer school is to highlight, through a series of lectures and hands-on exercises and practice sessions, how quantum computing algorithms can be used to study nuclear few- and many-body problems of relevance for low-energy nuclear physics. And how quantum computing algorithms can aid in studying systems with increasingly many more degrees of freedom compared with more classical few- and many-body methods. Several quantum algorithms for solving quantum-mechanical few- and many-particle problems with be discussed. The lectures will start with the basic ideas of quantum computing. Thereafter, through examples from nuclear physics, we will elucidate how different quantum algorithms can be used to study these systems. The results from various quantum computing algorithms will be compared to standard nuclear few- and many-body methods

Organizers: Alexei Bazavov (MSU), Scott Bogner (MSU), Heiko Hergert (MSU), Matthew Hirn (MSU), Morten Hjorth-Jensen (MSU), Dean Lee (MSU), Huey-Wen Lin (MSU), and Andrea Shindler (MSU)

Contact person: Morten Hjorth-Jensen, hjensen@msu.edu

Additional material in these slides. In addition to containing information about the school, we provide a reminder on **numpy** and a brief introduction to Qiskit. Please take a look at these notes before coming to the school. This material is provided at the end of the these introductory notes.

Aims and Learning Outcomes

The following topics will be covered.

1. Basic elements of quantum computing (first day) with introduction to relevant software, including

    (a) Introduction to quantum computing, qubits and systems of qubits
    (b) Measurements, Superposition and Entanglement
    (c) Gates, unitary transformations and quantum circuits
    (d) Quantum algorithms and implementation on a real quantum computer

2. Simulating quantum-mechanical few- and many-body systems

    (a) Quantum algorithms for quantum mechanical systems
    (b) Quantum simulation of the Schroedinger equation
    (c) Quantum computing and nuclear few- and many-body systems
    (d) Quantum state preparation and Quantum simulations
    (e) Quantum simulations on a real quantum computer

3. Quantum field theory and quantum computing

4. Noise, error correction and mitigation

All of the above topics will be supported by examples, hands-on exercises and project work.

Practicalities

1. Lectures Monday through Wednesday, starting at 830am, see schedule below

2. Hands-on sessions before lunch and in the afternoons till 6pm

3. For all lecture days we provide relevant jupyter-notebooks you can work on

Learning material and resources

1. Qiskit textbook, free online, see https://qiskit.org/textbook/preface.html

2. Scherer, The Mathematics of Quantum Computing, see https://link.springer.com/book/10.1007/978-3-030-12358-1

3. Chuang and Nielsen, Quantum Computation and Quantum Information, https://www.cambridge.org/highereducation/books/quantum-computation-and-quantum-informa01E10196D0A682A6AEFFEA52D53BE9AE#overview

4. Hundt, Quantum Computing for programmers, https://www.cambridge.org/core/books/quantum-computing-for-programmers/BA1C887BE4AC0D0D5653E71FFBEF61C6

Good resources. With the hands-on programming component we strongly recommend that you install Qiskit on your computer before the school starts.

1. For Qiskit, follow the instructions at https://qiskit.org/documentation/getting_started.html

2. We strongly recommend using the Jupyter notebook environment at https://quantum-computing.ibm.com/. This environment has Qiskit already set up and is free, just requires an email to register. It has built in support for Jupyter notebooks and should be sufficient for everything needed.

3. See also Ryan Larose's (from 2019) Quantum computing bootcamp with Qiskit - https://github.com/rmlarose/qcbq.

4. See also https://www.ryanlarose.com/external-resources.html

Detailed lecture plan

The duration of each lecture is approximately 45-50 minutes and there is a small break of 10-15 minutes between each lecture. Longer breaks at 1030am-11am and 3pm-330pm, except for Monday where there is also the possibility fora guided FRIB tour. In-person attendance is the main teaching modus, but lectures and hands-on sessions will be broadcasted via zoom for those who cannot attend in person. The zoom link will be sent to those who have expressed that they cannot attend in person. The lectures will also be recorded.

Teachers.

- AB = Alexei Bazavov
- BH = Benjamin Hall
- DL = Dean Lee

- JW = Jacob Watkins

- JB = Joey Bonitati

- MHJ = Morten Hjorth-Jensen

- RL = Ryan Larose

- QZ - Zhenrong Qian

Monday June 20.

- 8am-830am: Welcome and registration

- 830am-930am: Introduction to quantum computing, qubits, systems of qubits, gates and quantum circuits (AB)

- 930am-1030am: Measurements, Superposition, Entanglement (AB)

- 1030am-11am: Break, coffee, tea etc

- 11am-12pm: Hands-on session with applications and introduction to software libraries (AB, JW, RL)

- 12pm-1pm: Lunch (shorter lunch, else 1h30m lunches)

- 1pm-2pm: Quantum algorithms (Time evolution) for solving quantum mechanical problems (DL, JB, JW, and ZQ), simple problems

- 2pm-3pm: Quantum algorithms (Phase estimation) for solving quantum mechanical problems (DL, JB, JW, and ZQ), simple problems

- 3pm-4pm: Break, coffee, tea or tour for FRIB for those interested. Please let us know if you are interested in a tour of FRIB.

- 4pm-6pm: Hands-on sessions and problem solving (AB+all)

Tuesday June 21.

- 830-930am: Time evolution, Suzuki-Trotter approximation and quantum simulations (DL and JW) (advanced topic)

- 930am-1030am: Introduction to VQE and simple model (BH)

- 1030am-11am: Break, coffee, tea etc

- 11am-12pm: Many-body theory and nuclear few- and many-body systems (BH and MHJ)

- 12pm-130pm: Lunch

- 130pm-230pm: Quantum algorithms (VQE) and nuclear physics with applications (BH and MHJ), part 1

- 230pm-330pm: Quantum algorithms (VQE) and nuclear physics with applications (BH and MHJ), part 2

- 330pm-4pm: Break, coffee, tea etc

- 4pm-6pm: Hands-on sessions and problem solving (BH and JW+all)

Wednesday June 22.

- 830am-930am: Noise, error correction and mitigation, part I (RL)

- 930am-1030am: Noise, error correction and mitigation, part II (RL)

- 1030am-11am: Break, coffee, tea etc

- 11am-12pm: Practicing error correction and mitigation, hands-on part (RL)

- 12pm-130pm: Lunch

- 130pm-230pm: Wrapping up and defining nuclear many-body system to study for hands-on session (All)

- 230pm-330pm: Start hands-on session (RL)

- 330pm-4pm: Break, coffee, tea etc

- 4pm-6pm: Hands-on sessions and problem solving (all)

Prerequisites

You are expected to have operating programming skills in programming languages like Python (preferred) and/or Fortran, C++, Julia or similar and knowledge of quantum mechanics at an intermediate level (senior undergraduate and/or beginning graduate). Knowledge of linear algebra is essential. Additional modules for self-teaching on Python and quantum mechanics are also provided.

Software and needed installations

We will make extensive use of Python as programming language and its myriad of available libraries. You will find Jupyter notebooks invaluable in your work.

If you have Python installed (we strongly recommend Python3) and you feel pretty familiar with installing different packages, we recommend that you install the following Python packages via **pip** as

1. pip install numpy scipy matplotlib ipython scikit-learn mglearn sympy pandas pillow

For Python3, replace **pip** with **pip3**.

For OSX users we recommend, after having installed Xcode, to install **brew**. Brew allows for a seamless installation of additional software via for example

1. brew install python3

For Linux users, with its variety of distributions like for example the widely popular Ubuntu distribution, you can use **pip** as well and simply install Python as

1. sudo apt-get install python3 (or python for pyhton2.7)

etc etc.

Python installers

If you don't want to perform these operations separately and venture into the hassle of exploring how to set up dependencies and paths, we recommend two widely used distrubutions which set up all relevant dependencies for Python, namely

- Anaconda,

which is an open source distribution of the Python and R programming languages for large-scale data processing, predictive analytics, and scientific computing, that aims to simplify package management and deployment. Package versions are managed by the package management system **conda**.

- Enthought canopy

is a Python distribution for scientific and analytic computing distribution and analysis environment, available for free and under a commercial license.

Furthermore, Google's Colab is a free Jupyter notebook environment that requires no setup and runs entirely in the cloud. Try it out!

Useful Python libraries

Here we list several useful Python libraries we strongly recommend (if you use anaconda many of these are already there)

- NumPy is a highly popular library for large, multi-dimensional arrays and matrices, along with a large collection of high-level mathematical functions to operate on these arrays

- The pandas library provides high-performance, easy-to-use data structures and data analysis tools

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- Xarray is a Python package that makes working with labelled multi-dimensional arrays simple, efficient, and fun!

- Scipy (pronounced "Sigh Pie") is a Python-based ecosystem of open-source software for mathematics, science, and engineering.

- Matplotlib is a Python 2D plotting library which produces publication quality figures in a variety of hardcopy formats and interactive environments across platforms.

- Autograd can automatically differentiate native Python and Numpy code. It can handle a large subset of Python's features, including loops, ifs, recursion and closures, and it can even take derivatives of derivatives of derivatives

- SymPy is a Python library for symbolic mathematics.

- scikit-learn has simple and efficient tools for machine learning, data mining and data analysis

- TensorFlow is a Python library for fast numerical computing created and released by Google

- Keras is a high-level neural networks API, written in Python and capable of running on top of TensorFlow, CNTK, or Theano

- And many more such as pytorch, Theano etc

All learning material and teaching schedule pertinent to the course is avaliable at this GitHub address. A simple **git clone** of the material gives you access to all lecture notes and program examples. Similarly, running a **git pull** gives you immediately the latest updates.

Numpy examples and Important Matrix and vector handling packages

There are several central software libraries for linear algebra and eigenvalue problems. Several of the more popular ones have been wrapped into ofter software packages like those from the widely used text **Numerical Recipes**. The original source codes in many of the available packages are often taken from the widely used software package LAPACK, which follows two other popular packages developed in the 1970s, namely EISPACK and LINPACK. We describe them shortly here.

- LINPACK: package for linear equations and least square problems.

- LAPACK:package for solving symmetric, unsymmetric and generalized eigenvalue problems. From LAPACK's website http://www.netlib.org it is possible to download for free all source codes from this library. Both C/C++ and Fortran versions are available.

- BLAS (I, II and III): (Basic Linear Algebra Subprograms) are routines that provide standard building blocks for performing basic vector and matrix operations. Blas I is vector operations, II vector-matrix operations and III matrix-matrix operations. Highly parallelized and efficient codes, all available for download from http://www.netlib.org.

Basic Matrix Features

Matrix properties reminder.

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \qquad \mathbf{I} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

The inverse of a matrix is defined by

$$\mathbf{A}^{-1} \cdot \mathbf{A} = I$$

Relations	Name	matrix elements
$A = A^T$	symmetric	$a_{ij} = a_{ji}$
$A = \left(A^T\right)^{-1}$	real orthogonal	$\sum_k a_{ik}a_{jk} = \sum_k a_{ki}a_{kj} = \delta_{ij}$
$A = A^*$	real matrix	$a_{ij} = a_{ij}$
$A = A^\dagger$	hermitian	$a_{ij} = a_{ji}$
$A = \left(A^\dagger\right)^{-1}$	unitary	$\sum_k a_{ik}a_{jk}^{= \sum_k a_{ki}} a_{kj} = \delta_{ij}$

Some famous Matrices.

- Diagonal if $a_{ij} = 0$ for $i \neq j$

- Upper triangular if $a_{ij} = 0$ for $i > j$

- Lower triangular if $a_{ij} = 0$ for $i < j$

- Upper Hessenberg if $a_{ij} = 0$ for $i > j + 1$

- Lower Hessenberg if $a_{ij} = 0$ for $i < j + 1$

- Tridiagonal if $a_{ij} = 0$ for $|i - j| > 1$

- Lower banded with bandwidth p: $a_{ij} = 0$ for $i > j + p$

- Upper banded with bandwidth p: $a_{ij} = 0$ for $i < j + p$

- Banded, block upper triangular, block lower triangular....

More Basic Matrix Features.

Some Equivalent Statements. For an $N \times N$ matrix $\mathbf{A}$ the following properties are all equivalent

- If the inverse of $\mathbf{A}$ exists, $\mathbf{A}$ is nonsingular.

- The equation $\mathbf{Ax} = 0$ implies $\mathbf{x} = 0$.

- The rows of $\mathbf{A}$ form a basis of R^N.

- The columns of $\mathbf{A}$ form a basis of R^N.

- $\mathbf{A}$ is a product of elementary matrices.

- 0 is not eigenvalue of $\mathbf{A}$.

Numpy and arrays

Numpy provides an easy way to handle arrays in Python. The standard way to import this library is as

```
import numpy as np
```

Here follows a simple example where we set up an array of ten elements, all determined by random numbers drawn according to the normal distribution,

```
n = 10
x = np.random.normal(size=n)
print(x)
```

We defined a vector x with $n = 10$ elements with its values given by the Normal distribution $N(0, 1)$. Another alternative is to declare a vector as follows

```
import numpy as np
x = np.array([1, 2, 3])
print(x)
```

Here we have defined a vector with three elements, with $x_0 = 1$, $x_1 = 2$ and $x_2 = 3$. Note that both Python and C++ start numbering array elements from 0 and on. This means that a vector with n elements has a sequence of entities $x_0, x_1, x_2, \ldots, x_{n-1}$. We could also let (recommended) Numpy to compute the logarithms of a specific array as

```
import numpy as np
x = np.log(np.array([4, 7, 8]))
print(x)
```

In the last example we used Numpy's unary function *np.log*. This function is highly tuned to compute array elements since the code is vectorized and does not require looping. We normaly recommend that you use the Numpy intrinsic functions instead of the corresponding **log** function from Python's **math** module. The looping is done explicitly by the **np.log** function. The alternative, and slower way to compute the logarithms of a vector would be to write

```python
import numpy as np
from math import log
x = np.array([4, 7, 8])
for i in range(0, len(x)):
    x[i] = log(x[i])
print(x)
```

We note that our code is much longer already and we need to import the **log** function from the **math** module. The attentive reader will also notice that the output is $[1, 1, 2]$. Python interprets automagically our numbers as integers (like the **automatic** keyword in C++). To change this we could define our array elements to be double precision numbers as

```python
import numpy as np
x = np.log(np.array([4, 7, 8], dtype = np.float64))
print(x)
```

or simply write them as double precision numbers (Python uses 64 bits as default for floating point type variables), that is

```python
import numpy as np
x = np.log(np.array([4.0, 7.0, 8.0]))
print(x)
```

To check the number of bytes (remember that one byte contains eight bits for double precision variables), you can use simple use the **itemsize** functionality (the array x is actually an object which inherits the functionalities defined in Numpy) as

```python
import numpy as np
x = np.log(np.array([4.0, 7.0, 8.0]))
print(x.itemsize)
```

Matrices in Python

Having defined vectors, we are now ready to try out matrices. We can define a 3×3 real matrix $\boldsymbol{A}$ as (recall that we user lowercase letters for vectors and uppercase letters for matrices)

```python
import numpy as np
A = np.log(np.array([ [4.0, 7.0, 8.0], [3.0, 10.0, 11.0], [4.0, 5.0, 7.0] ]))
print(A)
```

If we use the **shape** function we would get $(3, 3)$ as output, that is verifying that our matrix is a 3×3 matrix. We can slice the matrix and print for example the first column (Python organized matrix elements in a row-major order, see below) as

```python
import numpy as np
A = np.log(np.array([ [4.0, 7.0, 8.0], [3.0, 10.0, 11.0], [4.0, 5.0, 7.0] ]))
# print the first column, row-major order and elements start with 0
print(A[:,0])
```

We can continue this was by printing out other columns or rows. The example here prints out the second column

```python
import numpy as np
A = np.log(np.array([ [4.0, 7.0, 8.0], [3.0, 10.0, 11.0], [4.0, 5.0, 7.0] ]))
# print the first column, row-major order and elements start with 0
print(A[1,:])
```

Numpy contains many other functionalities that allow us to slice, subdivide etc etc arrays. We strongly recommend that you look up the Numpy website for more details. Useful functions when defining a matrix are the **np.zeros** function which declares a matrix of a given dimension and sets all elements to zero

```python
import numpy as np
n = 10
# define a matrix of dimension 10 x 10 and set all elements to zero
A = np.zeros( (n, n) )
print(A)
```

or initializing all elements to

```python
import numpy as np
n = 10
# define a matrix of dimension 10 x 10 and set all elements to one
A = np.ones( (n, n) )
print(A)
```

or as unitarily distributed random numbers (see the material on random number generators in the statistics part)

```python
import numpy as np
n = 10
# define a matrix of dimension 10 x 10 and set all elements to random numbers with x \in [0, 1]
A = np.random.rand(n, n)
print(A)
```

As we will see throughout these lectures, there are several extremely useful functionalities in Numpy. As an example, consider the discussion of the covariance matrix. Suppose we have defined three vectors $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z}$ with n elements each. The covariance matrix is defined as

$$
\boldsymbol{\Sigma} = \begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{bmatrix},
$$

where for example

$$
\sigma_{xy} = \frac{1}{n} \sum_{i=0}^{n-1} (x_i - \overline{x})(y_i - \overline{y}).
$$

The Numpy function **np.cov** calculates the covariance elements using the factor $1/(n-1)$ instead of $1/n$ since it assumes we do not have the exact mean values.

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The following simple function uses the **np.vstack** function which takes each vector of dimension $1 \times n$ and produces a $3 \times n$ matrix $\boldsymbol{W}$

$$\boldsymbol{W} = \begin{bmatrix} x_0 & x_1 & x_2 & \dots & x_{n-2} & x_{n-1} \\ y_0 & y_1 & y_2 & \dots & y_{n-2} & y_{n-1} \\ z_0 & z_1 & z_2 & \dots & z_{n-2} & z_{n-1} \end{bmatrix},$$

which in turn is converted into into the 3×3 covariance matrix $\boldsymbol{\Sigma}$ via the Numpy function **np.cov()**. We note that we can also calculate the mean value of each set of samples $\boldsymbol{x}$ etc using the Numpy function **np.mean(x)**. We can also extract the eigenvalues of the covariance matrix through the **np.linalg.eig()** function.

```
# Importing various packages
import numpy as np

n = 100
x = np.random.normal(size=n)
print(np.mean(x))
y = 4+3*x+np.random.normal(size=n)
print(np.mean(y))
z = x**3+np.random.normal(size=n)
print(np.mean(z))
W = np.vstack((x, y, z))
Sigma = np.cov(W)
print(Sigma)
Eigvals, Eigvecs = np.linalg.eig(Sigma)
print(Eigvals)

import numpy as np
import matplotlib.pyplot as plt
from scipy import sparse
eye = np.eye(4)
print(eye)
sparse_mtx = sparse.csr_matrix(eye)
print(sparse_mtx)
x = np.linspace(-10,10,100)
y = np.sin(x)
plt.plot(x,y,marker='x')
plt.show()
```

Meet the Pandas

Another useful Python package is pandas, which is an open source library providing high-performance, easy-to-use data structures and data analysis tools for Python. **pandas** stands for panel data, a term borrowed from econometrics and is an efficient library for data analysis with an emphasis on tabular data. **pandas** has two major classes, the **DataFrame** class with two-dimensional data objects and tabular data organized in columns and the class **Series** with a focus on one-dimensional data objects. Both classes allow you to index data easily as we will see in the examples below. **pandas** allows you also to perform mathematical operations on the data, spanning from simple reshapings of vectors and matrices to statistical operations.

The following simple example shows how we can, in an easy way make tables of our data. Here we define a data set which includes names, place of birth and date of birth, and displays the data in an easy to read way. We will see repeated use of **pandas**, in particular in connection with classification of data.

```python
import pandas as pd
from IPython.display import display
data = {'First Name': ["Frodo", "Bilbo", "Aragorn II", "Samwise"],
        'Last Name': ["Baggins", "Baggins","Elessar","Gamgee"],
        'Place of birth': ["Shire", "Shire", "Eriador", "Shire"],
        'Date of Birth T.A.': [2968, 2890, 2931, 2980]
        }
data_pandas = pd.DataFrame(data)
display(data_pandas)
```

In the above we have imported **pandas** with the shorthand **pd**, the latter has become the standard way we import **pandas**. We make then a list of various variables and reorganize the aboves lists into a **DataFrame** and then print out a neat table with specific column labels as *Name*, *place of birth* and *date of birth*. Displaying these results, we see that the indices are given by the default numbers from zero to three. **pandas** is extremely flexible and we can easily change the above indices by defining a new type of indexing as

```python
data_pandas = pd.DataFrame(data,index=['Frodo','Bilbo','Aragorn','Sam'])
display(data_pandas)
```

Thereafter we display the content of the row which begins with the index **Aragorn**

```python
display(data_pandas.loc['Aragorn'])
```

We can easily append data to this, for example

```python
new_hobbit = {'First Name': ["Peregrin"],
              'Last Name': ["Took"],
              'Place of birth': ["Shire"],
              'Date of Birth T.A.': [2990]
              }
data_pandas=data_pandas.append(pd.DataFrame(new_hobbit, index=['Pippin']))
display(data_pandas)
```

Here are other examples where we use the **DataFrame** functionality to handle arrays, now with more interesting features for us, namely numbers. We set up a matrix of dimensionality 10×5 and compute the mean value and standard deviation of each column. Similarly, we can perform mathematial operations like squaring the matrix elements and many other operations.

```python
import numpy as np
import pandas as pd
from IPython.display import display
np.random.seed(100)
# setting up a 10 x 5 matrix
rows = 10
cols = 5
```

```
a = np.random.randn(rows,cols)
df = pd.DataFrame(a)
display(df)
print(df.mean())
print(df.std())
display(df**2)
```

Thereafter we can select specific columns only and plot final results

```
df.columns = ['First', 'Second', 'Third', 'Fourth', 'Fifth']
df.index = np.arange(10)

display(df)
print(df['Second'].mean() )
print(df.info())
print(df.describe())

from pylab import plt, mpl
plt.style.use('seaborn')
mpl.rcParams['font.family'] = 'serif'

df.cumsum().plot(lw=2.0, figsize=(10,6))
plt.show()


df.plot.bar(figsize=(10,6), rot=15)
plt.show()
```

We can produce a 4×4 matrix

```
b = np.arange(16).reshape((4,4))
print(b)
df1 = pd.DataFrame(b)
print(df1)
```

and many other operations.

The **Series** class is another important class included in **pandas**. You can view it as a specialization of **DataFrame** but where we have just a single column of data. It shares many of the same features as $_DataFrame. As with$ **DataFrame**, $most operations are vectorized, ach$