

## **Indian Academy of Science**

## Summer Research Fellowship Programme 2023 Final-Week Report

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Objective: To implement the three flavour neutrino oscillations using PMNS theory for both vacuum and matter interaction as well as with and without CP violation (on a subspace of a two-qubit Hilbert space).

## Acknowledgement

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## 1 Introduction to Quantum Computing and NMR

#### 1.1 Quntum bit

In classical computer a bit is the basic unit of classical information. A bit can have two states either 0 or 1. A qubit on the other hand is the basic unit of quantum information. The two possible states of a qubit are  $|0\rangle$  and  $|1\rangle$  but unlike a bit a qubit can exist as a linear combination of states called a superposition.

$$|\phi\rangle = \alpha |0\rangle + \beta |1\rangle$$

where  $\alpha$  and  $\beta$  are complex numbers.

When we measure a qubit we get either the result 0, with probability  $\alpha^2$ , or the result 1, with probability  $\beta^2$ . Naturally,  $\alpha^2 + \beta^2 = 1$ , since the probabilities must sum to one. We can rewrite  $|\phi\rangle$  as:

$$|\phi\rangle = e^{i\gamma}(\cos(\theta/2)|0\rangle + e^{i\psi}\sin(\theta/2)|1\rangle$$

Now since  $e^{i\gamma}$  is a global phase and can be ignored. Therefore any qubit can be written in the format:

$$|\phi\rangle = (\cos(\theta/2)|0\rangle + e^{i\psi}\sin(\theta/2)|1\rangle$$

In case of a multi qubit system the state can be written as:

$$|\phi\rangle = \Sigma_j \alpha_j |\phi_j^1\rangle \otimes |\phi_j^2\rangle \dots \otimes |\phi_j^n\rangle$$
  
where  $|\phi_j^i\rangle \epsilon(|0\rangle, |1\rangle)$ 

### 1.2 Density Matrix Representation

The density matrix formulation is very useful in describing the state of an ensemble quantum system such as an ensemble of spins in NMR. For an ensemble with the probability  $p_i$  to be in  $|\psi_i\rangle$  state, the density operator is given as:

$$\rho = \Sigma_i p_i |\psi_i\rangle \langle \psi_i|$$

where  $\Sigma_i p_i = 1$ . If the system has only state  $|\psi\rangle$  then the desity operator is given by:

$$\rho = |\psi\rangle \langle \psi|$$

A density matrix has th following properties:

- 1)  $\rho$  is hermitian i.e.  $\rho = \rho^{\dagger}$
- 2)  $\rho$  is positive
- $3)Tr[\rho] = 1$
- 4) No global phase ambiguity

For a pure state ensemble the  $Tr[\rho^2] = 1$  but for a mixed ensemble the  $Tr[\rho^2] < 1$ . This can be used to distinguish between a pure and mixed state.

#### 1.3 Quantum Gates

Quantum Gates are the building blocks of quantum circuits. Basically any unitary matrix forms a quantum gate. Unlike the gates of a classical computer a quantum gate is reversible since it is a unitary matrix. It has been shown that a set of gates that consists of all one-qubit quantum gates and the two-qubit exclusive-OR gate is universal in the

sense that all unitary operations can be expressed as compositions of such gates. One set of such gates is the one dimensional rotation gates  $R_X$ ,  $R_Y$ ,  $R_Z$  and the CNOT gate. Some of the basic quantum gates in matrix form are:

1) Hadamard gate

$$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

2)Pauli X gate

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

3)Pauli Y gate

$$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

4)Pauli Z gate

$$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

5)CNOT gate

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

#### 1.4 Nuclear Magnetic Resonance

Nuclear magnetic resonance (NMR) describes a phenomenon wherein, an ensemble of nuclear spins precessing in a static magnetic field, absorb and emit radiation in the radiofrequency range in resonance with their Larmor frequencies. The total spin of the nuclei is described by the operator I and the component of the spin along the z-axis is described by the operator  $I_Z$ .

$$I |I, m\rangle = I(I+1) |I, m\rangle$$
  
 $I_Z |I, m\rangle = m |I, m\rangle$ 

Atomic nuclei with non-zero spin also possess a magnetic dipole moment  $\mu$  which is given as :

 $\mu = \gamma_n \hbar I$  where  $\gamma_n$  is the gyromagnetic ratio

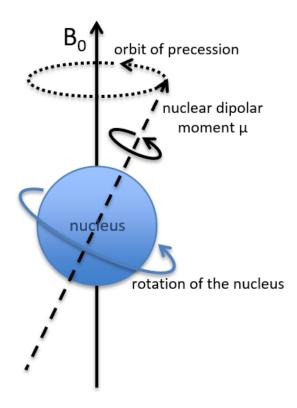
When an atomic nuclei with magnetic dipole moment  $\mu$  is placed in an external static magnetic field  $B_0$ , the nuclear state  $|I,m\rangle$  assume energy state from m=-I,-I+1,...+I. This splitting of the energy is called Zeeman effect and is described by the hamiltonian:

$$H_Z = -\mu B_0 = -\mu_z B_0 = -\gamma_n \hbar B_0 I_Z = -\hbar \omega_L I_Z$$

here  $\omega_L$  is the magnitude of lamor frequency which is the frequency with which the nuclei precess about the axis of the magnetic field.

$$\omega_L = \gamma_n B_0$$

From the above equation we see that the lamor frequency depends on the gyro magnetic ratio  $\gamma_n$ . This quantity is different for different nuclei and hence the lamor frequency.



Under the hamiltonian  $\langle I_X \rangle$  and  $\langle I_Y \rangle$  oscillates with frequency  $\omega_L$ , whereas  $I_Z$  remains stationary. The eigenvalue of the Hamiltonian is given by:

$$E_m = -m\hbar\omega_L$$

#### 1.4.1 Resonance Phenomenon

The Larmor frequencies of the nuclear spins in a static magnetic field of a few Tesla are of the order of MHz. The transition between the spin states can be realized by means of selective RF(radio frequency) pulses applied perpendicular to the quantization axis.

$$B_1(t) = 2B_1 cos(\Omega t + \Phi)i$$

where  $\Omega$  is the frequency of the magnetic field. The Hamiltonian is given by :

$$H_{RF} = -\mu B_1(t) = -\gamma_n \hbar I_x [2B_1 cos(\Omega t + \Phi)]$$

The RF Hamiltonian can be treated as a perturbation to the main Zeeman Hamiltonian, considering that the magnitude of  $B_1(t)$ , is much smaller than that of  $B_0$ . Therefore, the dominating role is still played by  $H_Z$  and the effect of  $H_{RF}$  can be determined using standard time-dependent perturbation theory. Briefly, the result is that, when the frequency of the RF field is close to the Larmor frequency ( $\Omega \approx \omega_L$ ), i.e., on resonance, there is transitions between the eigenstates of  $H_Z$  given by probability:

$$P_{m \longrightarrow n} \propto \gamma_n^2 \hbar^2 B_1^2 |\langle m| I_X |n\rangle|^2$$

### 1.5 NMR Quantum Computing

Nuclear magnetic resonance quantum computing is one of the several proposed approaches for constructing a quantum computer, that uses the spin states of nuclei within molecules

as qubits. In 1997, D. G. Cory and I. L. Chuang independently proposed a NMR quantum computer that can be programmed much like a quantum computer. Their computational model uses an ensemble quantum computer wherein the results of a measurement are the expectation values of the observable. This computational model can be realized by NMR spectroscopy on macroscopic ensembles of nuclear spins. NMR Quantum computing using liquid sample was introduced known as the liquid state NMR. This uses molecules having non zero spin like  $CHCl_3$  (with  $C^{13}$  and  $H^1$ ),  $Si(CH_3)_4$  (with one  $Si^{29}$ ,  $C^{13}$  and one  $H^1$ )..etc.

#### 1.5.1 NMR Qubit

In case of an NMR quantum computer a qubit is realised by a spin  $\frac{1}{2}$  nuclei. The hamiltonian is given by:

$$H_Z = -\hbar\omega_L I_z$$

Now in case of N qubit sytem we have two nuclei of non zero spin  $\frac{1}{2}$  and also a J coupling interaction between them. The J-coupling (also called indirect or scalar coupling) is also an interaction between the nuclear magnetic dipole moments of neighbor nuclei, but in this case the interaction is not direct, being mediated by the electron cloud involved in the chemical bonds between the corresponding atoms.

The Hamiltonian is given by:

$$H = -\sum_{i=1}^{n} \hbar \omega_1 I_Z^i + 2\pi \sum_{i < j} \hbar J I_Z^i I_Z^j$$

#### 1.5.2 Initialisation

In NMR quantum computing the initialisation begins with setting the system to a pure state. For an ensemble of identical nuclei in thermal equilibrium, the population of each energy level is given by the Boltzmann distribution. For a two-level system

 $I = \frac{1}{2}$ , with the population  $n_-$  and  $n_+$  of the  $m = \frac{1}{2}$  and  $m = \frac{-1}{2}$  levels, respectively the ratio

$$\frac{n_{-}}{n_{+}} = e^{-\hbar\omega_L/k_BT}$$

where  $k_B$  is the Boltzmann constant and T is the absolute temperature of the ensemble. All the energy levels are almost equally populated and the initial state is mixed. Under the high temperature approximation the initial state of the system is given by:

$$\rho \approx \frac{1}{2^N} (I + \epsilon \Delta \rho_{eq})$$

where I is identity  $\epsilon$  is the purity factor and  $\rho_{eq}$  is the deviation density matrix. The problem of pure states in NMR can be overcome by preparing a pseudopure state which is isomorphic to a pure state. An ensemble of a pure state is given by  $\rho_{pure} = |psi\rangle \langle \psi|$  and the corresponding pseudopure state is given by:

$$\rho_{eq} = \frac{1 - \epsilon}{2^N} I + \epsilon |psi\rangle \langle \psi|$$

A pseudopure state in NMR can be prepared by several methods such as spatial averaging, temporal averaging and logical labelling.

#### 2 Neutrino Oscillations

#### 2.1 Introduction

Neutrinos are fermionic particles first theorized by Wolfgang Pauli and later discovered in the Cowan–Reines neutrino experiment. They belong to the neutral lepton family, which makes it incredibly difficult to detect (because they only interact via the weak force) even though they are the most abundant subatomic particle in the universe. Three flovors of neutrinos were predicted by the standard model, electron muon and tau neutrinos. The electron neutrino was discovered by Reines and Cowan by observing electron antineutrinos released from a nuclear reactor in South Carolina, 26 years after Pauli's hypothesis. The second kind of neutrino, muon neutrino, was discovered by Lederman, Schwartz and Steinberger in 1962 with the first accelerator neutrino beam at Brookhaven National Laboratory. The tau neutrino was only discovered in 2000 in the Fermi laboratory.

The idea of neutrino oscillation first put forward by Pontecorvo in 1957, proposed that neutrino-antineutrino transition may occur in analogy with the neutral kaon mixing. Later Pontecorvo, Maki, Nakagawa and Sakata speculated that neutrino could change flavor while in flight, called "neutrino oscillation", if neutrinos have mass and mixing exists between flavor and mass eigenstates. In 1960 Raymond Davis observed a deficit in the electron neutrino produced in the nuclear fusion in sun from the value predicted by the standard solar model. This could only have been possible if neutrinos changed flavors as the travel to the earth. Later other experiments showed that the deficit was 70% from the predicted value.

This shortfall of solar neutrinos was explained by experiments led by this year's laureates, Arthur McDonald of Queen's University in Kingston, Canada, and Takaaki Kajita of the University of Tokyo. The work revealed that the three flavors of neutrino can interconvert as the particles stream through space. Kajita headed a team working at the Super-Kamiokande detector in Japan. The detector consists of a tank of 50,000 tons of water buried underground to shield it from cosmic rays. It detects electron and muon neutrinos coming not from the Sun but from the Earth's atmosphere, where neutrinos are produced by collisions of cosmic rays with atmospheric atoms. Very rarely, these neutrinos will collide with atomic nuclei in the detector's water molecules and generate flashes of light.

Later in 2001 and 2002, McDonald confirmed the same result with the detector called the Sudbury Neutrino Observatory (SNO) in Sunbury, Canada. These developments shared the 2015 Nobel Prize in Physics for the discovery of neutrino oscillations, which shows that neutrinos have mass.

### 2.2 PMNS Theory

Pontecorvo-Maki- Nakagawa-Sakata speculated that if neutrinos have mass mixing exists between the flovor and mass eigenstates.PMNS(Pontecorvo-Maki- Nakagawa-Sakata) theory states that each of the neutrino flavor basis (electron, muon and tau neutrinos) can be written as a superposition of three mass eigenstates (m1,m2 and m3). The transformation from neutrino mass basis to flavor basis is achieved by the PMNS matrix.

 $|\psi_{\rm a}\rangle = U_{\rm PMNS} |\psi_{\rm mi}\rangle$ where  $\alpha = e, \eta, \tau$  labelling the neutrino flavors and i=1,2,3 for the neutrino mass states

The PMNS matrix is characterised by three "mixing angles"  $\theta$ 12,  $\theta$ 13,  $\theta$ 23 and one CP-violating phase  $\delta$ cp. The PMNS matrix is given by:

$$U_{PMNS} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & c_{23} & s_{23} \\ 0 & -s_{23} & c_{23} \end{bmatrix} \begin{bmatrix} c_{13} & 0 & 0 s_{13} e^{-i\delta_{cp}} \\ 0 & 1 & 0 \\ -s_{13} e^{\delta_{cp}} & 0 & c_{13} \end{bmatrix} \begin{bmatrix} c_{12} & s_{12} & 0 \\ -s_{12} & c_{12} & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

The dynamics of neutrino oscillation in vacuum is governed by the Hamiltonian written in the mass eigenbasis as:

$$H_0{=}egin{bmatrix} 0 & 0 & 0 \ 0 & \delta m_{12}^2/2E & 0 \ 0 & 0 & \delta m_{13}^2/2E \end{bmatrix}$$

where  $\delta m_{12}^2 = m_2^2 - m_1^2 (\approx 7.5 \times 10^- 5 eV^2)$ ,  $\delta m_{13}^2 = m_3^2 - m_1^2 (\approx 2.5 \times 10^- 3 eV^2)$  and E is the neutrino energy (E  $\approx$  p(momentum).

From an initial state  $|v(0)\rangle$  the neutrino evolves in time t in matrix form as  $|v(t)\rangle = e^{-iHt} |v(0)\rangle$ 

where H is the Hamiltonian in the flavor basis.

Now we know the hamiltonian in the mass basis and can be converted to the flavor basis using the PMNS matrix.

$$H = U_{PMNS} H_0 U_{PMNS}^{\dagger}$$

Thus  $|v(t)\rangle = e^{-iU_{PMNS}HU_{P}MNS^{\dagger}} |v(0)\rangle$ 

also written as 
$$|v(t)\rangle = U_{PMNS} \begin{bmatrix} 1 & 0 & 0 \\ 0 & e^{-i\delta m_{12}^2 t/2E} & 0 \\ 0 & 0 & e^{-i\delta m_{13}^2 t/2E} \end{bmatrix} U_{PMNS}^{\dagger} |v(0)\rangle$$

Now in case of matter interaction the Hamiltonian is given by:  $H_m = H + H_1$  where H is given by:  $H = U_{PMNS}H_0U_{PMNS}^{\dagger}$ 

and 
$$H_1 = \begin{bmatrix} V(x) & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Here V ( x ) is the neutrino weak interaction potential energy V =  $\sqrt{2}G_FN_e$  (where  $G_F$  is the Fermi constant,  $N_e$  is the electron number density in the medium,). Here we are only taking the case of constant matter interaction i.e.

$$V(x) = const$$

The hamiltonian 
$$H_m$$
 is given by; 
$$H_m = U_{PMNS} \begin{bmatrix} 0 & 0 & 0 \\ 0 & \delta m_{12}^2/2E & 0 \\ 0 & 0 & \delta m_{13}^2/2E \end{bmatrix} U_{PMNS}^{\dagger} + \begin{bmatrix} V(x) & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

#### 2.3 Why Quantum Simulation?

The idea of quantum simulations is the use of quantum systems to simulate other quantum systems in programmable fashion. It is impossible to truly simulate a quantum mechanical event using a classical universal device. According to the lecture by Feyman in 1981, the only way to simulate events in nature is by using a system that is quantum mechanical.

Oscillating neutrino beams exhibit quantum coherence over distances of thousands of kilometers. Precise measurements of parameters in the PMNS framework might lead to new physics beyond the Standard Model. However it is very difficult to determine this in neutrino oscillation experiments. Quantum simulation are the best alternatives to study this phenomenology. Thus if we could encode the state of neutrinos in some n qubit hilbert space and find unitary gates to evolve the quantum state, we could simulate neutrino oscillation on a quantum computer. However with the present level of technology quantum simulations are noisy. Thus noise reducing algorithms are also implemented to get accurate results.

At present many companies like IBM, Microsoft, Google etc... have made their quantum computers public. Also other quantum computers like NMR quantum computer, photonic quantum computer facilities are also available.

#### 3 Numerical Simulation

The first task of the project was to do the numerical simulation of of neutrino oscillation. The PMNS matrix has 4 parameters to be specified. The parameters that are reasonably well measured are the solar mixing angle  $\theta_{12} \approx 34^{\circ}$  the reactor mixing angle  $\theta_{13} \approx 8.5^{\circ}$  and the solar mass splitting  $\delta m_{12}^2 \approx 7.5 \times 10^{-5} eV^2$ . Parameters with well-determined partial information are the atmospheric mixing angle  $\theta_{23} \approx 45^{\circ}$  and the atmospheric mass splitting  $\delta m_{13}^2 \approx 2.5 \times 10^{-3} eV^2$ . However, the phase  $\delta$  in CP-violation still needs to be discovered with significant certainties. Thus numerical simulatons for  $\delta_{cp} = 0, \pi/2, \pi, -\pi/2$ was done. The numerical simulation are used to determine

- 1) The probability of finding the various neutrino flavors.
- 2) The distance over which the probability of finding the a neutrino flavor is maximum
- 3) Compare it with the experimental result
- 4) The period of neutrino oscillation for various energy E
- 5) The effect of matter interaction on neutrino oscillation

#### 3.1 Vacuum

Survival probability when the initial states were electron, muon and tau neutrinos with energy E=1GeV as a function of L/E (Where L is the distance given in kilometer and E is in GeV) were determined.

The initial state of the system was taken to be  $|v(0)\rangle_{\alpha}$  where  $\alpha=e,\eta,\tau$  labelling the neutrino flavors electron, muon and tau respectively. The system was evolved according to the hamiltonian

$$H = U_{PMNS} \begin{bmatrix} 0 & 0 & 0 \\ 0 & \delta m_{12}^2/2E & 0 \\ 0 & 0 & \delta m_{13}^2/2E \end{bmatrix} U_{PMNS}^\dagger$$
 Thus the state of the system at any particular time 't' is given by:

$$|v(t)\rangle = e^{-iHt} |v(0)\rangle$$

Now the probability of state being in various flavors is determined by:

$$|\langle v_{\alpha}||v_{t}\rangle|^{2}$$

The graph was plotted for probability vs L/E with  $\alpha = e, \eta, \tau$ . The following are the results for the three neutrino flavors as initial states.

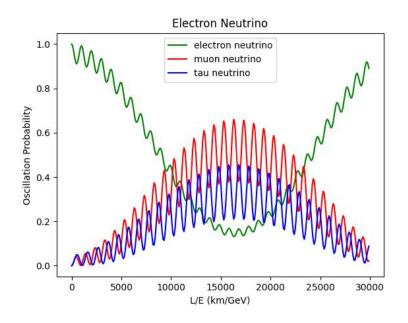


Figure 1:  $v(t=0) = v_e$  and  $\delta_{cp} = 0$ 

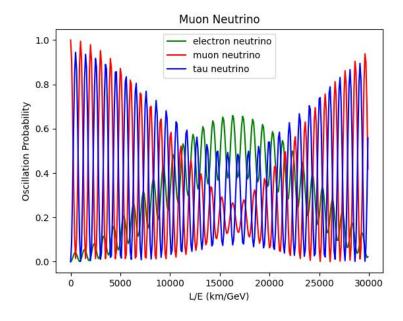


Figure 2:  $v(t=0) = v_{\eta}$  and  $\delta_{cp} = 0$ 

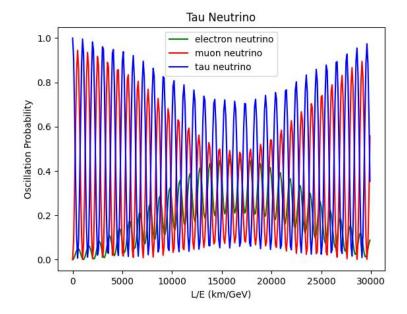


Figure 3:  $v(t=0) = v_{\tau}$  and  $\delta_{cp} = 0$ 

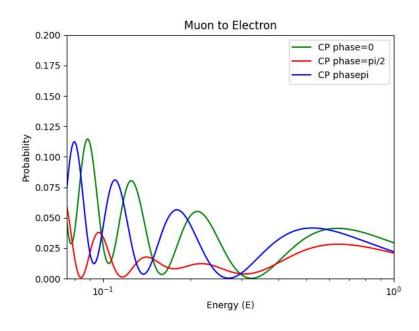


Figure 4: Probability of  $v_{\eta} \longrightarrow v_{e}$  for different E at L= 295 km

#### 3.2 Matter Interaction

In case of matter interaction the hamiltonian

$$H_m = U_{PMNS} \begin{bmatrix} 0 & 0 & 0 \\ 0 & \delta m_{12}^2 / 2E & 0 \\ 0 & 0 & \delta m_{13}^2 / 2E \end{bmatrix} U_{PMNS}^{\dagger} + \begin{bmatrix} V(x) & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

and the state of the system at any particular time 't' is given by:  $|v(t)\rangle = e^{-iH_mt}|v(0)\rangle$ . Here V(x) is taken to be a constant. The numerical simulation for  $V(x) = 0, 10^{-3}, 10^{-5}$  is done with the initial state being  $v_{\eta}$  (muon nutrino)

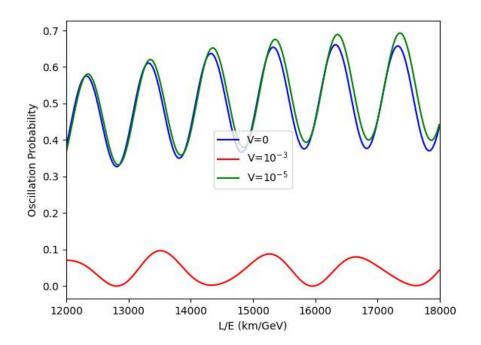


Figure 5:  $P_{\eta} \longrightarrow P_e$  for  $\delta_{cp} = 0$ 

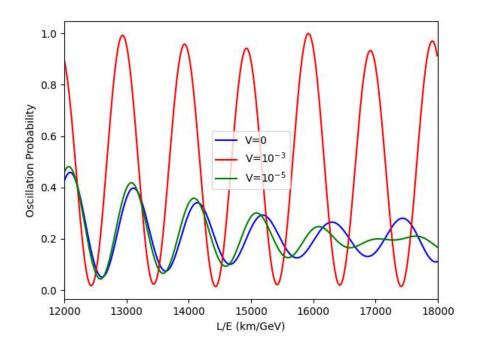


Figure 6:  $P_{\eta} \longrightarrow P_{\eta}$  for  $\delta_{cp} = 0$ 

### 4 Quantum Simulations

In order to do quantum simulations of neutrino oscillations, the system needs to be represented in a two-qubit hilbert space. Each of the orthogonal states  $|0,0\rangle$ ,  $|0,1\rangle$ ,  $|1,0\rangle$  represents the three neutrino flavors - electron, muon, tau respectively. The forth state  $|1,1\rangle$  is taken to be a sterile neutrino (Sterile neutrinos are hypothetical particles that are believed to interact only via gravity and not via any of the other fundamental interactions of the Standard Model) that is considered decoupled to the other three states.

The PMNS matrix in the two-qubit hilbert space can be represented as:

$$U_{PMNS} = R_{23}(\theta_{23}).R_{13}(\theta_{13}, \delta_{cp}).R_{12}(\theta_{12})$$

$$R_{23}(\theta_{23}) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & c_{23} & s_{23} & 0 \\ 0 & -s_{23} & c_{23} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$R_{13}(\theta_{13}, \delta_{cp}) = \begin{bmatrix} c_{13} & 0 & s_{13}e^{-i\delta_{cp}} & 0 \\ 0 & 1 & 0 & 0 \\ -s_{13}e^{\delta_{cp}} & 0 & c_{13} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$R_{12}(\theta_{12}) = \begin{bmatrix} c_{12} & s_{12} & 0 & 0 \\ -s_{12} & c_{12} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

where c and s stands for cos and sin respectively.

The hamiltonian in two-qubit hilbert space can be written as:

$$H_0 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & \delta m_{12}^2 / 2E & 0 & 0 \\ 0 & 0 & \delta m_{13}^2 / 2E & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

### 4.1 Building the Quantum Circuit

To make the quantum circuit, the PMNS matrix needs to be written in terms of the basic quantum gates such as the controlled-u rotation gates, C-NOT gate and the Pauli X gate.

The controlled-u rotation gate when the target qubit is the LSB(Least significant bit):

$$CU^{0}(\theta,\lambda,\phi) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\theta/2)e^{-i(\phi+\lambda)} & 0 & -\sin(\theta/2)e^{-i(\phi-\lambda)} \\ 0 & 0 & 1 & 0 \\ 0 & \sin(\theta/2)e^{i(\phi-\lambda)} & 0 & \cos(\theta/2)e^{i(\phi+\lambda)} \end{bmatrix}$$

The controlled-u rotation gate when the target qubit is the MSB (Most significant bit):

$$CU^{1}(\theta, \lambda, \phi) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \cos(\theta/2)e^{-i(\phi+\lambda)} & -\sin(\theta/2)e^{-i(\phi-\lambda)} \\ 0 & 0 & \sin(\theta/2)e^{i(\phi-\lambda)} & \cos(\theta/2)e^{i(\phi+\lambda)} \end{bmatrix}$$

The C-NOT gate when the target is the LSB:

$$C_X^0 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

The C-NOT gate when the target is the MSB:

$$C_X^1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

The Pauli X gate is:

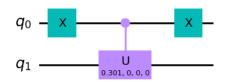
$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

Now each of the gates  $R_{23}(\theta_{23})$ ,  $R_{13}(\theta_{13}, \delta_{cp})$  and  $R_{12}(\theta_{12})$  is expressed in terms of  $CU^0(\theta, \lambda, \phi)$ ,  $CU^1(\theta, \lambda, \phi)$ ,  $C_X^0$ ,  $C_X^1$  and X gates as the follows (note that  $q_0$  is the MSB and  $q_1$  is the LSB):

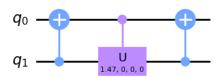
1) 
$$R_{12}(\theta 12) = (I \otimes X).CU^{1}(-2\theta_{12}, 0, 0).(I \otimes X)$$

$$q_0 = 0$$
 $q_1 = 0$ 
 $q_1 = 0$ 
 $q_1 = 0$ 
 $q_2 = 0$ 
 $q_3 = 0$ 
 $q_4 = 0$ 
 $q_5 = 0$ 
 $q_6 = 0$ 
 $q_6$ 

2) 
$$R_{13}(\theta 13, \delta_{cp}) = (X \otimes I).CU^{0}(-2\theta_{13}, \delta_{CP}, -\delta_{CP}).(X \otimes I)$$



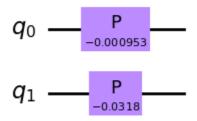
3) 
$$R_{23}(\theta 23) = CU_X^0 \cdot CU^1(-2\theta_{23}, 0, 0) \cdot CU_X^0$$



The matrix 
$$e^{-iH_0t} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & e^{-i\delta m_{12}^2 t/2E} & 0 & 0 \\ 0 & 0 & e^{-i\delta m_{13}^2 t/2E} & 0 \\ 0 & 0 & 0 & x \end{bmatrix}$$
 (x can be any value) can be

written in terms of the  $P(\lambda)$  (where  $P(\lambda) = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\lambda} \end{bmatrix}$ ) gate as follows:

$$e^{iH_0t} = P(-\delta m_{12}^2 t/2E) \otimes P(-\delta m_{13}^2 t/2E)$$



Therefore the circuit for the unitary matrix  $U = U_{PMNS}.e^{-iH_0t}.U_{PMNS}^{\dagger}$  is as follows:

$$U = R_{23}(\theta_{23}).R_{13}(\theta_{13}, \delta_{cp}).R_{12}(\theta_{12}).e^{-iH_0t}.R_{12}(-\theta_{12}).R_{13}(-\theta_{13}, \delta_{cp}).R_{23}(-\theta_{23})$$

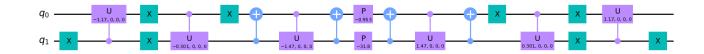


Figure 7: Unitary Matrix U

### 4.2 IBM Qiskit

IBM has developed some of the most advanced quantum computers in the world. Moreover they have given free cloud access to their quantum computers through Qiskit framework. Qiskit is an open-source software development kit for working with quantum computers at the level of circuits, pulses, and algorithms and running them on prototype quantum devices on IBM Quantum Experience or on simulators on a local computer. The primary version of Qiskit uses Python programming language and is well supported on the Jupyter Notebook environment.

#### 4.2.1 QasmSimulator

The QasmSimulator backend is designed to mimic an actual IBM quantum computer. The quantum measurements in a real IBM quantum computer has a lot of noise in the result. But the QasmSimulator can simulate quantum circuits both ideally and subject to noise modeling. The circuit in figure 5 was run in the QasmSimulator to verify the circuit and compare it with the numerical simulations. The following results were obtained.

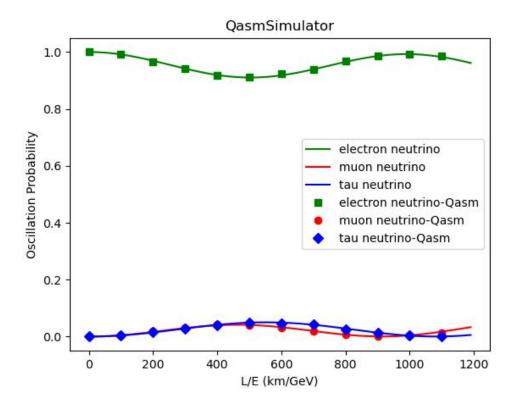


Figure 8:  $v(t=0) = v_e \text{ and } \delta_{cp} = 0$ 

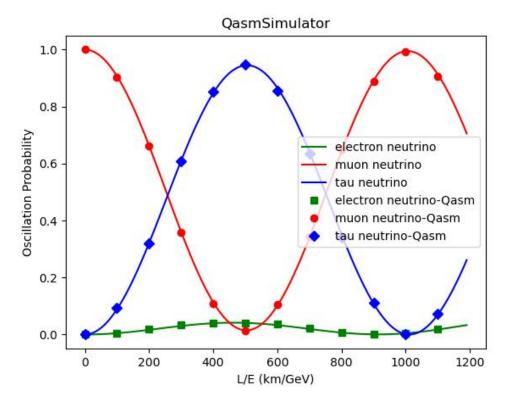


Figure 9:  $v(t=0) = v_{\eta}$  and  $\delta_{cp} = 0$ 

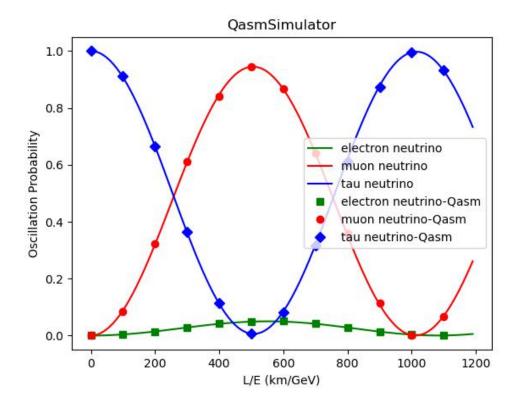


Figure 10:  $v(t=0) = v_{\tau} \text{ and } \delta_{cp} = 0$ 

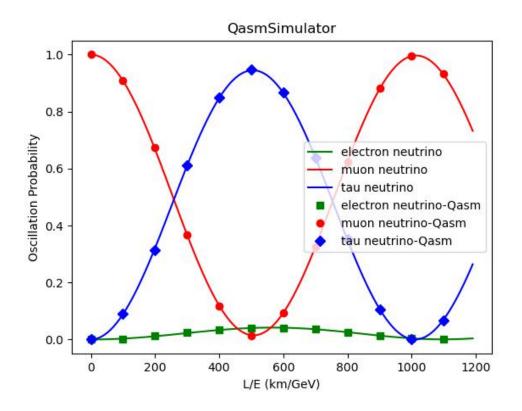


Figure 11:  $v(t=0) = v_{\eta} \text{ and } \delta_{cp} = \pi$ 

The QasmSimulator measurements matches exactly with the theoritical results. This proves that the quantum circuit built is accurate.

#### 4.2.2 Real Quantum Simulations

The quantum circuit was run on the "ibmq-manila" backend. The results obtained had a lot of noise which made the measurements deviate from thetheoritical results. Thus the "CompleteMeasFitter" and "complete-meas-cal" functions were imported from the qiskit.ignis.mitigation package. This reduced the error by significant amount. The following results were obtained from the real quantum computer simulations.

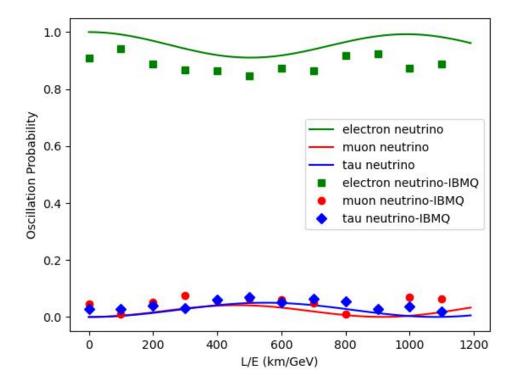


Figure 12:  $v(t=0) = v_e$  and  $\delta_{cp} = 0$ 

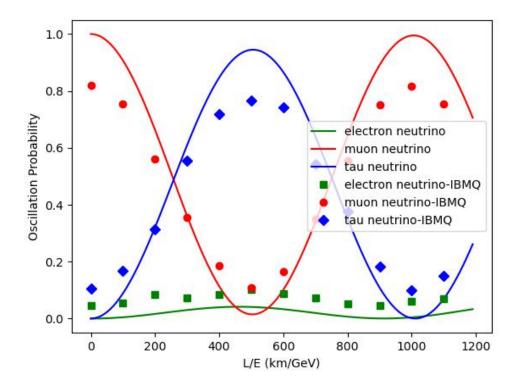


Figure 13:  $v(t=0)=v_{\eta} \ and \ \delta_{cp}=0$ 

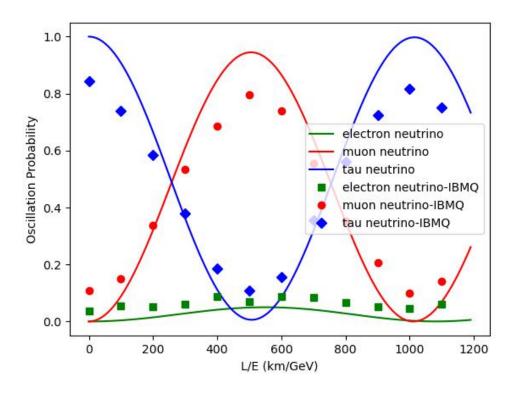


Figure 14:  $v(t=0) = v_{\tau} \text{ and } \delta_{cp} = 0$ 

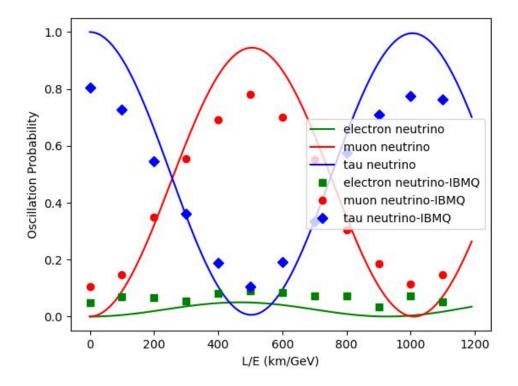


Figure 15:  $v(t=0) = v_{\tau}$  and  $\delta_{cp} = \pi$ 

### 5 Conclusion

During my 2-month internship, I gained valuable experience in the field of quantum simulation. Neutrino oscillation is a quantum phenomenon that has been studied for many decades. But the cost and time required to do neutrino oscillation experiments is substantial. Quantum computers offer a promising solution to this problem. Quantum computers are able to represent and manipulate quantum states with exponentially more precision than classical computers. This means that quantum computers could be used to simulate neutrino oscillations with much greater accuracy than classical computers.

I learned about the theoretical foundations of neutrino oscillations and the challenges involved in simulating them on a quantum computer. I was able to make quantum circuit to simulate the three flavor neutrino oscillation. The quantum circuit was based on the PMNS theory that explains neutrino oscillations. The simulations were first done on Qiskit, the framework to access the IBM quantum computer. This helped me in learn about building quantum circuits for any quantum system's. I was also able to learn Qiskit in detail and learnt the various packages in it, especially for error correction.

The most valuable part of my internship was to work in the NMR quantum computing facility available in the lab. I learnt the working principle NMR and about how a qubit can be realised in an NMR quantum computer. I was also able to help in making quantum circuits for the neutrino oscillation simulation in the NMR quantum computer. Working in the lab also helped me realise limitations in NMR quantum computer and the methods used to overcome the limitations in real-time.

### 6 References

- [1] Ioannisian, A. and Pokorski, S. (2018) 'Three neutrino oscillations in matter', Physics Letters B, 782, pp. 641–645. doi:10.1016/j.physletb.2018.06.001.
- [2] Freund, M. (2001) 'Analytic approximations for three neutrino oscillation parameters and probabilities in matter', Physical Review D, 64(5). doi:10.1103/physrevd.64.053003.
- [3] Giganti, C., Lavignac, S. and Zito, M. (2018) 'Neutrino oscillations: The rise of the pmns paradigm', Progress in Particle and Nuclear Physics, 98, pp. 1–54. doi:10.1016/j.ppnp.2017.10.001
- [4] Argüelles, C.A. and Jones, B.J. (2019) 'Neutrino oscillations in a quantum processor', Physical Review Research, 1(3). doi:10.1103/physrevresearch.1.033176.
- [5] Molewski, M.J. and Jones, B.J.P. (2022) 'Scalable qubit representations of neutrino mixing matrices', Physical Review D, 105(5). doi:10.1103/physrevd.105.056024.
- [6] Nguyen, H.C. et al. (2023) 'Simulating neutrino oscillations on a superconducting qutrit', Physical Review D, 108(2). doi:10.1103/physrevd.108.023013.
- [7] Nielsen, M.A. and Chuang, I.L. (2022) Quantum Computation and Quantum Information. Cambridge: Cambridge University Press.
- [8] Oliveira, I.S. (2007) NMR Quantum Information Processing. Amsterdam: Elsevier.