Quantum Coin Toss

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Abstract

The coin toss game is a classical application of probability and randomness that can be used as a tool to study fundamental ideas of statistics and cryptography. The quantum version of this game uses quantum mechanical principles that go beyond the classical heads or tails interpretation. This project aims to use the quantum coin toss game as a mechanism for studying the fundamental concepts of quantum computing, such as elementary quantum gate implementation, quantum superposition, and Fermi-Dirac and Bose-Einstein statistics. Elementary quantum gates and coin states are presented in terms of matrices and a systematic approach to implementing a simple quantum coin toss simulation on a quantum device is provided. The worksheet assumes some exposure to Dirac notation, fundamental postulates of quantum mechanics, the concept of a wave function and measurement, reduced density matrices, and elementary understanding of probability theory.

Introduction

Around forty years ago, Richard Feynman made an intriguing suggestion that, "*Nature isn't classical, [...], and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy.*"[1] Since then, great progress has been made in terms of quantum simulation development, so much in fact that the first quantum computer, IBM Q System One, was developed in 2019.[2] The beginnings of quantum computing can be traced to early 1970s and are closely related to the articulation of the no-go (aka no-cloning) theorem, by James Park.[3] In 1990s, the first quantum algorithms were developed by David Deutsch, Richard Jozsa, and Peter Shor[4,5], leading to the first NMR quantum computers[6,7] in early 2000s, and an inflation of new areas of quantum computing research that has kept growing to this day. Quantum computing can be viewed as a mean of connecting quantum mechanics with information[8] and here we aim to explore its fundamentals through the quantum coin toss game and fundamental concepts of quantum statistics.

Theory

Bits of Classical Probability

Before diving into the quantum world, let us recall the basic principles of classical computing and classical probability. Classical computers use binary digits (bits) to represent information. A bit can be in one of the two states, 0 or 1, at any given time. For the purposes of our coin toss game, we will refer to the 0 state as the heads-up and the 1 state as the tails-up states. Once a fair coin is flipped, classical game theory predicts that there is a 50:50 chance of the coin landing heads-up or tails-up.

What if we were to flip two coins? In this case, since each coin could land heads-up or tails-up, there are four total outcomes to consider,

$$(0, 0), (0, 1), (1, 0), (1, 1).$$

Since each coin still has a 50:50 chance of landing heads-up or tails-up, to get the total probability of both coins landing heads-up or tails-up, we would simply multiply each coin's probabilities for each outcome. In this case, that would be,

$$\frac{1}{2} \cdot \frac{1}{2} = \frac{1}{4},$$

So, the probability of both coins landing heads-up or tails-up is now 25%. In a more general way, the total probability of an outcome from n number of coin flips is the product of probabilities of individual outcomes of each coin. Let us test this with a simple coin toss code below.

```
> restart;
  randomize():
  numFlips := 1:
  choices := ["Mileva","Einstein"]:
  r := rand(1..nops(choices)):
  Vector[row](numFlips, i->choices[r()]);
```

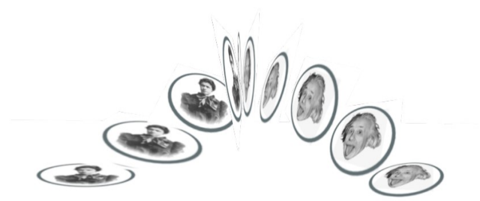

Figure 1. Imaginary classical coin as a visual representation of the flip. The middle portion depicts the 50:50 chance of the coin landing "heads-up" or "tails-up," where the heads-up state shows the Serbian physicist and mathematician and the first wife of Albert Einstein, Mileva Maric, and tails-up shows Albert Einstein. The graphic was created by the author, using GIMP.[9]

So far, we have only been dealing with fair coins. It is a simple exercise for the user to manipulate the above code and see how the outcomes change with respect to the 1/2 probability case.

Now, let us consider some fundamentals of quantum computing and quantum statistics.

Qubits of Quantum Probability[10]

Quantum computers operate using quantum bits (qubits) that can exist in states $|0\rangle$ and $|1\rangle$, analogous to the classical 0 and 1 states, where

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \text{ and } |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

The main difference between qubits and bits is that qubits can also exist in a linear combination of states,

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle.$$

This property is often referred to as a superposition of states $|0\rangle$ and $|1\rangle$, where α and β are complex numbers. In contrast to the classical bit, a qubit can exist in a continuum of states between $|0\rangle$ and $|1\rangle$, until it is measured. Once we measure a qubit, there is a $|\alpha|^2$ probability of the result being 0 and a $|\beta|^2$ probability of the result being 1, where $|\alpha|^2 + |\beta|^2 = 1$. In other words, making a measurement of a qubit collapses it from being in a superposition of $|0\rangle$ and $|1\rangle$ states to a specific state. Since $|\alpha|^2 + |\beta|^2 = 1$, we can express the superposition of $|0\rangle$ and $|1\rangle$ as,

$$|\psi\rangle = \cos\frac{\theta}{2}\left|0\right\rangle + e^{i\varphi}\sin\frac{\theta}{2}\left|1\right\rangle,$$

where θ and ϕ represent values on a 3-D unit sphere, also known as the Bloch sphere.

Qubits are not only mathematical objects but are also physically realizable and their existence has been confirmed experimentally. Some examples include photon polarization, nuclear spin alignment in a uniform magnetic field, and two spin states of an electron. To accurately describe measurement probabilities of such qubits, it is necessary to account for their bosonic (integer value spin) or fermionic (half-integer value spin) nature.

Let us consider our coin toss model once again, only now the coin's quantum properties will also be considered. We will refer to $|0\rangle$ as the heads-up and $|1\rangle$ as the tails-up states. Two cases will be examined, one for a general bosonic system and the other for a general fermionic system. Note that bosons and fermions are indistinguishable particles.

<u>Case I</u>

Based on Bose-Einstein statistics[11, 12], which is used for particles with integer spins (e.g., photons, gluons, W and Z bosons, etc.), the following outcomes of a toss of two quantum coins are possible,[13]

$$|0\,0\rangle,\ \frac{|01\rangle + |10\rangle}{\sqrt{2}},\ |11\rangle$$

where $|0\,0\rangle$ and $|11\rangle$ are analogous to the classical (0, 0) and (1, 1) outcomes, respectively. Unlike in the previously discussed classical case, here the probability of both coins landing heads-up ($|0\,0\rangle$) or tails-up ($|11\rangle$) is $\frac{1}{3}$. Some physical examples of this property are discussed in Ref [12].

<u>Case II</u>

Fermi-Dirac statistics[14], used for half-integer spin particles (e.g., protons, electrons, neutrons, neutrinos, etc.), predicts only one outcome, precisely

$$\frac{|01\rangle - |10\rangle}{\sqrt{2}}.$$

This result may seem odd at first, but recalling the Pauli exclusion principle, it becomes clear why $|0\,0\rangle$ and $|11\rangle$ states are forbidden outcomes. Additionally, the antisymmetrization of a fermionic wavefunction leads to the "-" sign in the above expression.

At this point, it should be clear to the reader that classical and quantum statistics do not operate in the same way. Classical statistics predicts outcomes based on an assumption that the coins are statistically independent and distinguishable. In the quantum regime, it is necessary to consider spin as an additional degree of freedom of a particle that then determines what the possible outcomes of a system, such as the coin toss, may be.

Elementary Quantum Gates[10]

Classical computers use wires and logic gates to form electrical circuits that facilitate information flow. Quantum computers, analogously, use quantum circuits built of wires and elementary quantum gates that allow for information storage and processing. Here, we will present some elementary single qubit gates in their matrix forms to serve as a framework for the circuitry workflow that will be desribed in the following section.

Pauli Gates

X, Y, and Z Pauli matrices act as Pauli gates and rotate a qubit by π rad around the x- , y-, and z-axis of the Bloch sphere, respectively.

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Hadamard Gate

The Hadamard gate (H) is one of the most useful and most widely used quantum gates. It creates a superposition of $|0\rangle$ and $|1\rangle$ states.

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

Applications/Results

In this section, we will consider an example of a systematic approach to implementing a quantum coin toss experiment on a quantum device and provide a tool for identifying fermionic and bosonic qubits using the one-electron reduced density matrix formulation (1-RDM).

Workflow of a Quantum Coin Toss Experiment

1. State Preparation

First, let the user initialize the coin to state $|0\rangle$,

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}.$$

2. <u>State Time Evolution</u>

At this stage, let the coin interact with the quantum device. The quantum device applies the Hadamard gate to the initial coin state and transforms it into a superposition state as follows,

$$H|0\rangle = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}, \text{ where } H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}.$$

3. <u>The Coin Flip and Final Measurement</u>

Finally, let the user flip the coin, i.e., change its initial state. The coin flip is established by applying the X gate to the current coin state,

$$X(H|0\rangle) = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}, \text{ where } X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

We see that even though the user has flipped the coin, the state has not changed from that of the quantum device.

At this point, we go back to step 2 and the coin interacts with the quantum device once again before we obtain the final measurement. During this interaction, the Hadamard gate is applied on the current state so that the final state becomes,

$$H(X(H|0\rangle)) = \begin{bmatrix} 1 \\ 0 \end{bmatrix} = |0\rangle.$$

In the end, our measurement yields the initial state. It is easy to check that the outcome would be the same if the user had begun the game with the coin in state $|1\rangle$.Therefore, there is a 100% chance that the quantum device will win every game, no matter how the user initiates the state. This simple example of a quantum coin toss experiment that can be conducted on a real quantum device shows one way in which a fundamental principle of quantum mechanics, namely superposition, can be used to manipulate information in a way that classical probability theory does not allow.

However, it is important to note that we could have also designed a circuit where the state is measured after step 2, without the change of state in step 3. In this case, there would be a 50:50 chance of the outcome being $|0\rangle$ or $|1\rangle$. This version of the experiment would simply replicate a classical coin toss with an additional benefit that the coin tosses would be completely random.

Bose-Einstein and Fermi-Dirac Statistics on Quantum Devices

In the previous example, we saw how a simple quantum coin toss experiment can be conducted on a quantum device. More complicated coin toss experiments can be built based on similar ideas but more complex restrictions in terms of accessible theoretical and practical tools for the user and the device. In case the reader is interested in creating such experiments, we introduce a way of determining whether a particular qubit is bosonic or fermionic, using one-electron reduced density matrix (1-RDM) formulation [15], as this can be regarded as the starting point of the experimental design.

Fermionic Qubit

As the name implies, a fermionic qubit obeys Fermi-Dirac statistics. In other words, the following anticommutation relation must be satisfied,

$$\{\hat{a}_i, \hat{a}_j^\dagger\} = \hat{a}_i\hat{a}_j^\dagger + \hat{a}_j^\dagger\hat{a}_i = \delta_j^i,$$

where $\hat{a}_i$ and $\hat{a}_i^\dagger$ are creation and annihilation operators acting on orbital *i*.
For a qubit q, the 1-RDMs can be constructed as follows,

$$\text{1-RDM} = \begin{bmatrix} \hat{a}_{q,0}^\dagger\hat{a}_{q,0} & \hat{a}_{q,0}^\dagger\hat{a}_{q,1} \\ \hat{a}_{q,1}^\dagger\hat{a}_{q,0} & \hat{a}_{q,1}^\dagger\hat{a}_{q,1} \end{bmatrix}$$

$$\text{1-RDM} = \begin{bmatrix} \hat{a}_{q,0}\hat{a}_{q,0}^\dagger & \hat{a}_{q,0}\hat{a}_{q,1}^\dagger \\ \hat{a}_{q,1}\hat{a}_{q,0}^\dagger & \hat{a}_{q,1}\hat{a}_{q,1}^\dagger \end{bmatrix},$$

where the two-term expectation values are linear combinations of expectation values of Pauli matrices for the specified qubit.

For a given qubit to be fermionic, the following conditions must be satisfied,

$$\hat{a}_{q,0}\hat{a}_{q,1}^\dagger = -\hat{a}_{q,1}^\dagger\hat{a}_{q,0} \text{ and } \hat{a}_{q,1}\hat{a}_{q,0}^\dagger = -\hat{a}_{q,0}^\dagger\hat{a}_{q,1}.$$

Let us consider an example of how a 1-RDM can be computed using the Quantum Chemistry package in Maple.

We begin by loading the commands of the Quantum Chemistry package using the Maple with command

```
> with(QuantumChemistry);
```

[*AOLabels*, *ActiveSpaceCI*, *ActiveSpaceSCF*, *AtomicData*, *BondAngles*, *BondDistances*, *Charges*, *ChargesPlot*, *ContractedSchrodinger*, *CorrelationEnergy*, *CoupledCluster*, *DensityFunctional*, *DensityPlot3D*, *Dipole*, *DipolePlot*, *Energy*, *ExcitationEnergies*, *ExcitationSpectra*, *ExcitationSpectraPlot*, *ExcitedStateEnergies*, *ExcitedStateSpins*, *FullCI*, *GeometryOptimization*, *HartreeFock*, *Interactive*, *Isotopes*, *MOCoefficients*, *MODiagram*, *MOEnergies*, *MOIntegrals*, *MOOccupations*, *MOOccupationsPlot*, *MOSymmetries*, *MP2*, *MolecularData*, *MolecularDictionary*, *MolecularGeometry*, *NuclearEnergy*, *NuclearGradient*, *OscillatorStrengths*, *Parametric2RDM*, *PlotMolecule*, *Populations*, *Purify2RDM*, *RDM1*, *RDM2*, *RTM1*, *ReadXYZ*, *Restore*, *Save*, *SaveXYZ*, *SearchBasisSets*, *SearchFunctionals*, *SkeletalStructure*, *Thermodynamics*, *TransitionDipolePlot*, *TransitionDipoles*, *TransitionOrbitalPlot*, *TransitionOrbitals*, *Variational2RDM*, *VibrationalModeAnimation*, *VibrationalModes*, *Video*] **(1.1)**

We recommend setting the global variable Digits to 15:

```
> Digits := 15;
```

$$Digits := 15 \quad \textbf{(1.2)}$$

Now, let us define the geometry of a hydrogen molecule, H_2, a suitable system for a single qubit representation where the two electrons may be used to represent the $|0\rangle$ and $|1\rangle$ states. The default unit of distance in the Quantum Chemistry package is Angstroms (1 Angstrom = 10^{-10} m), which we employ in this worksheet.

```
> h2 := [["H", 0, 0, -0.48], ["H", 0, 0, 0.48]];
```

$$h2 := [["H", 0, 0, -0.48000000], ["H", 0, 0, 0.48000000]] \quad \textbf{(1.3)}$$

The 1-electron reduced density matrix (1-RDM) can be calculated from the variational 2-RDM method with the command RDM1

```
> dm1 := RDM1(h2, method = Variational2RDM, active = [2, 4]);
```

$$dm1 := \begin{bmatrix} 1.94598674 & 0. \\ 0. & 0.05401326 \end{bmatrix} \quad \textbf{(1.4)}$$

Bosonic Qubit

A bosonic qubit obeys Bose-Einstein statistics. Unlike fermions, bosons must satisfy the commutation relation,

$$[\hat{b}_i, \hat{b}_j^\dagger] = \hat{b}_i\hat{b}_j^\dagger - \hat{b}_j^\dagger\hat{b}_i = \delta_j^i,$$

where $\hat{b}_i$ and $\hat{b}_i^\dagger$ are creation and annihilation operators acting on orbital *i*.

For a qubit q, the 1-RDMs look, essentially, the same as they did in the fermionic case,

$$\text{1-RDM} = \begin{bmatrix} \hat{b}^\dagger_{q,0}\hat{b}_{q,0} & \hat{b}^\dagger_{q,0}\hat{b}_{q,1} \\ \hat{b}^\dagger_{q,1}\hat{b}_{q,0} & \hat{b}^\dagger_{q,1}\hat{b}_{q,1} \end{bmatrix}$$

$$\text{1-RDM} = \begin{bmatrix} \hat{b}_{q,0}\hat{b}^\dagger_{q,0} & \hat{b}_{q,0}\hat{b}^\dagger_{q,1} \\ \hat{b}_{q,1}\hat{b}^\dagger_{q,0} & \hat{b}_{q,1}\hat{b}^\dagger_{q,1} \end{bmatrix}.$$

For a given qubit to be bosonic, the following conditions must be satisfied,

$$\hat{b}_{q,0}\hat{b}^\dagger_{q,1} = \hat{b}^\dagger_{q,1}\hat{b}_{q,0} \text{ and } \hat{b}_{q,1}\hat{b}^\dagger_{q,0} = \hat{b}^\dagger_{q,0}\hat{b}_{q,1}.$$

Conclusions

This worksheet explored the idea of a quantum coin toss and the way in which it can be implemented on a quantum device. Some fundamental ideas regarding quantum statistics, namely Fermi-Dirac and Bose-Einstein cases, are discussed in relation to the implementation of the quantum coin toss on a quantum device. Elementary quantum gates are introduced and the notion of a qubit is explained. A workflow of a sample quantum coin toss experiment is presented and used to portray the concept of superposition as the main difference between classical and quantum statistics. Finally, a general technique of classifying qubits as fermionic and bosonic is given in the one-electron reduced density matrix context.

Selected References

(1) International Journal of Theoretical Physics, **21**, 1982, p. 467-488, at p. 486 (final words)
(2) Aron, J. "IBM unveils its first commercial quantum computer". New Scientist. (2019) Retrieved February 13, 2021.
(3) Park, J.L. The concept of transition in quantum mechanics. Found Phys **1**, 23–33 (1970).
(4) Deutsch, D. & Jozsa, R. Rapid solutions of problems by quantum computation. Proceedings of the Royal Society of London A. **439**: 553–558 (1992).
(5) Shor, P.W. Algorithms for quantum computation: discrete logarithms and factoring. Proceedings 35th Annual Symposium on Foundations of Computer Science. IEEE Comput. Soc. Press: 124–134 (1994).
(6) Raussendorf, R & Briegel, H. J. A One-Way Quantum Computer. Physical Review Letters. **86** (22): 5188–91 (2001).
(7) "12-qubits Reached in Quantum Information Quest". ScienceDaily (2006) Retrieved February 15, 2021.
(8) Quantum Computing from the Ground Up. Riley Tipton Perry (University of New South Wales, Australia). Default Book Series. September 2012
(9) The GIMP Development Team. (2019). GIMP. Retrieved from https://www.gimp.org
(10) Nielsen, M. A. & Chuang, I. L. *Quantum Computation and Quantum Information*, Cambridge

University Press, 2000.
(11) Bose, S. N. Planck's law and light quanta hypothesis, Z. Phys. **26**, 178—181 (1924).
(12) Einstein, A. Quantentheorie des einatomigen idealen gases. Ber. Akad. Wiss. Berlin 261—267 (1924); 3—14, 18—25 (1925)
(13) Chow, C. & COhen, T. D. Quantum coins, dice, and children: Probability and quantum statistics. American Journal of Physics **68**, 829 (2000).
(14) Dirac, P.A.M. *The principle of quantum mechanics*, Clarendon Press (1967).
(15) Mazziotti, D. A. *Reduced-Density-Matrix Mechanics: With Application to Many-Electron Atoms and Molecules* (Wiley, New Jersey, 2007)