

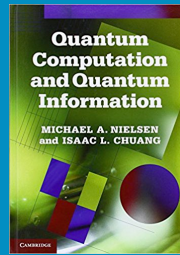


Quantum Computing Modeling in Scala

Constantin Gonciulea
Distinguished Engineer, JPMorgan Chase

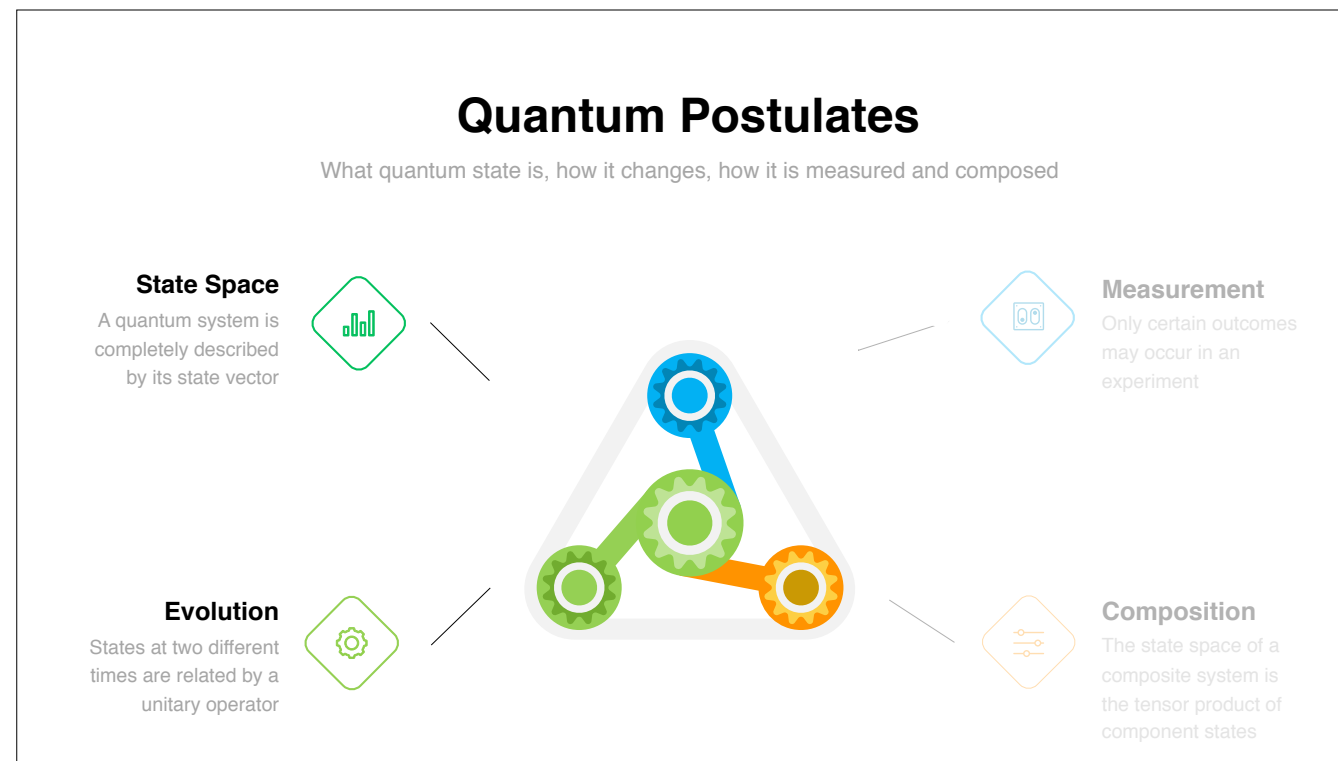
Earlier this year I started looking at Quantum Computing in more detail. Even though I took Quantum Mechanics classes in college and graduate school, I found out that Quantum Computing is better understood separately from Physics.

In fact, quantum state is not very different from classical or probabilistic state. I find having a common treatment of stateful computations in various contexts quite fascinating, and I have presented on this subject in a few Scala meetups over the years. It turns out that quantum state can be simulated with the same common approach that we, in the Scala world, are familiar with.



**The postulates of quantum mechanics
were derived after a long process of trial
and (mostly) error, which involved a
considerable amount of guessing and
fumbling by the originators of the theory.**

This is a quote from the de facto textbook on Quantum Computing, pointing out that after many years of trial and error, Quantum experts arrived at 4 postulates that capture the essence of Quantum Mechanics. These postulates are also a self-contained foundation for Quantum Computing.



We will first address the first two postulates, which specify how quantum state is represented and how it evolves in time. More precisely, the state of a quantum system is modeled as a vector (collection of numbers), and state transformations have to keep the state valid, essentially by preserving an invariant.

Modeling state evolution is not specific to Quantum Computing, it is a core problem in any kind of computing. Functional programming in particular provides a clean, standard approach to manage state: **changes are flatMapped into the state.**

We are going to use this approach to model state changes in classical, probabilistic and quantum systems in a unified way.

Monadic State Evolution

The system state is defined by labeled values (allocations)



Examples: resource allocation, accounting systems, probabilistic systems, quantum systems

We are going to look at a class of systems whose state is represented by a **collection of labeled values**, which we can call **allocations**. The labels are fixed, and we can think of them as buckets or bins.

Examples of such systems are common:

- accounting systems, where the buckets are accounts, and the corresponding values are balances
- investment portfolios, where buckets are investment instruments like stocks or bonds, and the corresponding values are the allocation percentages for those instruments
- probabilistic systems, where the buckets are possible outcomes (called hypotheses), and the corresponding values are the probabilities of those outcomes
- quantum systems are similar to probabilistic systems, where the buckets are possible outcomes, and the corresponding values are called amplitudes (we will talk about them later)

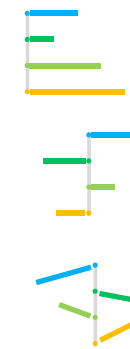
The state can be represented as a List of tuples for simplicity, but the MapLike data structure in the Scala language is a nice alternative. A state change is represented by a list of entries, one per bucket, and such an entry looks like the state itself. These entries are independent of the values in the buckets. They represent relative changes, like percentages, or transactions.

As an example, let's look at the portfolio allocation scenario. A change specifies how each instrument is reallocated. In the case of an accounting system, a change specifies what payments are made from each account into other accounts.

State Representation and Evolution

Unified monadic approach to classical, probabilistic and quantum state

```
trait UState[+This <: UState[This, B, V], B, V] {  
  protected val bins: List[(B, V)]  
  protected val m: Monoid[V]  
  
  protected val normalizeStateRule: List[(B, V)] => List[(B, V)] = identity  
  
  protected val combineBinsRule: List[(B, V)] => List[(B, V)] = { bs =>  
    bs.groupBy(_._1).toList.map {  
      case (b, vs) => (b, vs.map(_._2).foldLeft(m.empty)(m.combine))  
    }  
  }  
  protected val updateStateRule: ((B, V), B => List[(B, V)]) => List[(B, V)]  
  
  def create(bins: List[(B, V)]): This  
  
  def normalize(): This = create(normalizeStateRule(bins))  
  
  def flatMap(f: B => List[(B, V)]): This = {  
    val updates: List[(B, V)] = bins.flatMap({ case bv => updateStateRule(bv, f) })  
    create(normalizeStateRule(combineBinsRule(updates)))  
  }  
  
  def >>=(f: B => List[(B, V)]): This = flatMap(f)  
}
```



State: `List[(B, V)]`

Change: `B => List[(B, V)]`

We can abstract out a system's state **representation** and **transformation** in a way that applies to all the scenarios we mentioned. The state is captured in a collection of bin-value pairs. Typically the state is valid only if an invariant is maintained during evolution (e.g. the sum of values across bins is 1, or 0; for quantum state the values are vectors whose squared magnitudes have to add up to 1).

The flatMap method processes state changes and returns a new state. The state changes are relative, i.e. they are independent of the current bin values. Its implementation can be standardized if we have a specification of how to go from relative to absolute changes. This specification or rule is called updateStateRule here. In the portfolio allocation case, that means going from percentages to balances that need to be combined.

In order to combine labeled values we need a combine operation with a neutral element, specified here by a monoid (e.g. addition or multiplication).

In some cases we need to normalize the state, in order to preserve an invariant, if the transformations do not enforce that invariant (that will be the case of probabilistic state, as we will see later).

Portfolio Balancing

Percentage based resource allocation

```
val bins: List[(String, Double)] = List("a" -> .2, "b" -> .1, "c" -> .3, "d" -> .4)

val m = MState[String](bins)
val changeA = List("a" -> .25, "b" -> .5, "c" -> .25)
val changeB = List("b" -> 1.0)
val changeC = List("c" -> 1.0)
val changeD = List("d" -> 1.0)

val state = m >=> Map("a" -> changeA, "b" -> changeB, "c" -> changeC, "d" -> changeD)

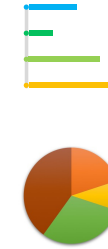
assert(state.bins.toSet == Set("a" -> .05, "b" -> .2, "c" -> .35, "d" -> .4))
```

Implementation

```
case class MState[B](bins: List[(B, Double)]) extends UState[MState[B], B, Double] {
  val m = new Monoid[Double] {
    override val empty: Double = 0.0
    override val combine: (Double, Double) => Double = _ + _
  }

  override val updateStateRule: ((B, Double), B => List[(B, Double)]) => List[(B, Double)] = {
    case ((b, v), f) => f(b).map { case (c, u) => (c, u * v) }
  }

  override def create(bins: List[(B, Double)]) = MState(bins)
}
```



Invariant: sum = 1

In the case of portfolio (re)balancing, the buckets are the investment instruments and the values are the corresponding allocation percentages. Of course, the percentages (in decimal form) have to add up to 1.

Consider the example of a portfolio with 4 instruments, with 20% of the total value in “a”, 10% in “b”, 30% in “c”, and 40% in “d”. And assume we want to reallocate “a” this way: 50% into “b”, and 25% into “c”. That means that 25% stays in “a”. The expected result is.

Now let’s look at the implementation. The combining operation is addition. The update rule takes an instrument “b” and distributes its value across all instruments: for each instrument “c” in “f(b)” we add the percentage of “b” specified in the change. This is equivalent to the linear algebra approach, where the change is interpreted as a matrix, and the values as a column vector.

Account Balances

State of a closed accounting system

```
val bins: List[(String, Double)] = List("a" -> 2, "b" -> 3, "c" -> 5, "d" -> -8, "e" -> -2)

val z = ZState[String](bins)
val changeA = List("a" -> -1.0, "b" -> 1.0)
val changeB = List("b" -> -2.0, "c" -> 1.0, "d" -> 1.0)

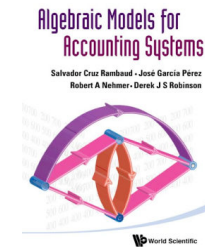
val state = z >>= Map("a" -> changeA, "b" -> changeB, "c" -> Nil, "d" -> Nil, "e" -> Nil)

assert(state.bins.toSet == Set("a" -> 1.0, "b" -> 2.0, "c" -> 6.0, "d" -> -7.0, "e" -> -2.0))
```

Implementation

```
case class ZState[B](bins: List[(B, Double)]) extends UState[ZState[B], B, Double] {
  val m = new Monoid[Double] {
    override val empty: Double = 0.0
    override val combine: (Double, Double) => Double = _ + _
  }
  override val updateStateRule: ((B, Double), B => List[(B, Double)]) => List[(B, Double)] = {
    case ((b, v), f) => List((b -> v)) ++ f(b)
  }

  override def create(bins: List[(B, Double)]) = ZState(bins)
}
```



Invariant: sum = 0

Let's quickly go through the example of an accounting system. The invariant for the state of such a system is that the sum of all account balances has to be zero. The book shown to the right presents an algebraic approach that is similar to what we are showing here, including this invariant.

A change specifies for each account what payments are made into other accounts.

The combining operation is addition. The update rule says that we need to combine the current balance for each account with the relative changes specified by the payments into that account

Probabilistic State

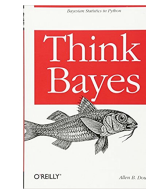
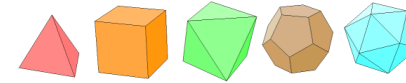
Each possible outcome is assigned a probability

Repeatedly rolling one of the 5 platonic solid dice yields the following sequence: 6, 6, 8, 7, 7, 5, 4.
Guess which die was used?

Priors:
4 0.2 #####
6 0.2 #####
8 0.2 #####
12 0.2 #####
20 0.2 #####

After a 6 is rolled:
4 0.0
6 0.3921 #####
8 0.2941 #####
12 0.1960 #####
20 0.1176 #####

After 6, 8, 7, 7, 5, 4 are rolled after the first 6:
4 0.0
6 0.0
8 0.9432 #####
12 0.0552 ##
20 0.0015



For the probabilistic state, let's go through an example first. Assume that we choose one of the 5 dice shaped as regular polyhedra, having 4, 6, 8, 12 and 20 faces, respectively. After rolling the chosen die a few times, we are trying to guess which die was chosen.

Before seeing the result of the first roll, we assign the same probability to each die. If the first roll is a 6, we know for sure that the die was not the tetrahedron (which has 4 faces). The probabilities of the other dice are updated, and intuitively the more faces a die has, the less likely it was to be the chosen one. The precise updated probabilities are obtained by multiplying the current probabilities by the corresponding likelihoods of the rolled number to be a face of the dice and then normalizing the state. We need to normalize because the likelihoods are not probabilities, so they do not add up to 1.

If we roll the chosen die more times we can improve our guess. For example, if we see the sequence shown here, we can rule out the die with 6 faces (the cube), because numbers higher than 6 are present in the sequence. The die with 8 faces is the most probable because a wider range of numbers would have been expected from having more faces.

Probabilistic State

Bayes Theorem

```
case class PState[B](bins: List[(B, Double)]) extends UState[PState[B], B, Double] {  
  val m = new Monoid[Double] {  
    override val empty: Double = 1.0  
    override val combine: (Double, Double) => Double = _ * _  
  }  
  
  override val updateStateRule: ((B, Double), B => List[(B, Double)]) => List[(B, Double)] = {  
    case ((b, v), f) => f(b).map { case (c, u) => (c, u * v) }  
    //case ((b, v), f) => List((b -> v)) ++ f(b) // both work  
  }  
  
  override val normalizeStateRule = { bs: List[(B, Double)] =>  
    val sum = bs.map(_._2).foldLeft(0.0)(_ + _)  
    if (sum == 1.0) bs else bs.map {  
      case (b, v) => (b, v / sum)  
    }  
  }  
  
  override def create(bins: List[(B, Double)]) = PState(bins)  
}
```



Invariant: normalized sum = 1

Change: data point likelihoods

```
val change = Map(  
  "a" -> List("a" -> 0.2),  
  "b" -> List("b" -> 0.7),  
  "c" -> List("c" -> 0.0))
```

Let's look at the implementation. The combining operation is multiplication. As mentioned before, we need a normalization procedure, which just scales all values so they add up to 1.

A change triggered by a new data point is represented by the likelihoods of that data point being compatible with the possible outcomes. For a given outcome there is only one “reallocation”, because outcomes are independent, only the likelihood corresponding to one outcome at a time is non-zero.

The update rule is the same as the one used in the portfolio balancing, and the same as a linear transformation. Each outcome probability is multiplied by the likelihood of the new data point assuming that particular outcome. Interestingly enough, the update rule used for an accounting system also works, because combining the current probability with the corresponding likelihood is done by multiplying them.

Quantum State

Complex numbers (2 -dimensional vectors) as values

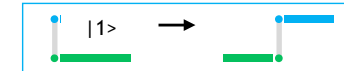
```
case class QState[B](bins: List[(B, Complex)]) extends UState[QState[B], B, Complex] {  
  val m = new Monoid[Complex] {  
    override val empty: Complex = Complex.zero  
    override val combine: (Complex, Complex) => Complex = Complex.plus  
  }  
  
  override val updateStateRule: ((B, Complex), B => List[(B, Complex)]) => List[(B, Complex)] = {  
    case ((b, v), f) => f(b).map { case (c, u) => (c, u * v) }  
  }  
  
  override def create(bins: List[(B, Complex)]) = QState(bins)  
}
```



Invariant:
sum of squared magnitudes
= 1

Example: the Hadamard transformation

```
val sq = toComplex(1 / math.sqrt(2))  
val H = Map(  
  "|0>" -> List("|0>" -> sq, "|1>" -> sq),  
  "|1>" -> List("|0>" -> sq, "|1>" -> -sq)  
)
```



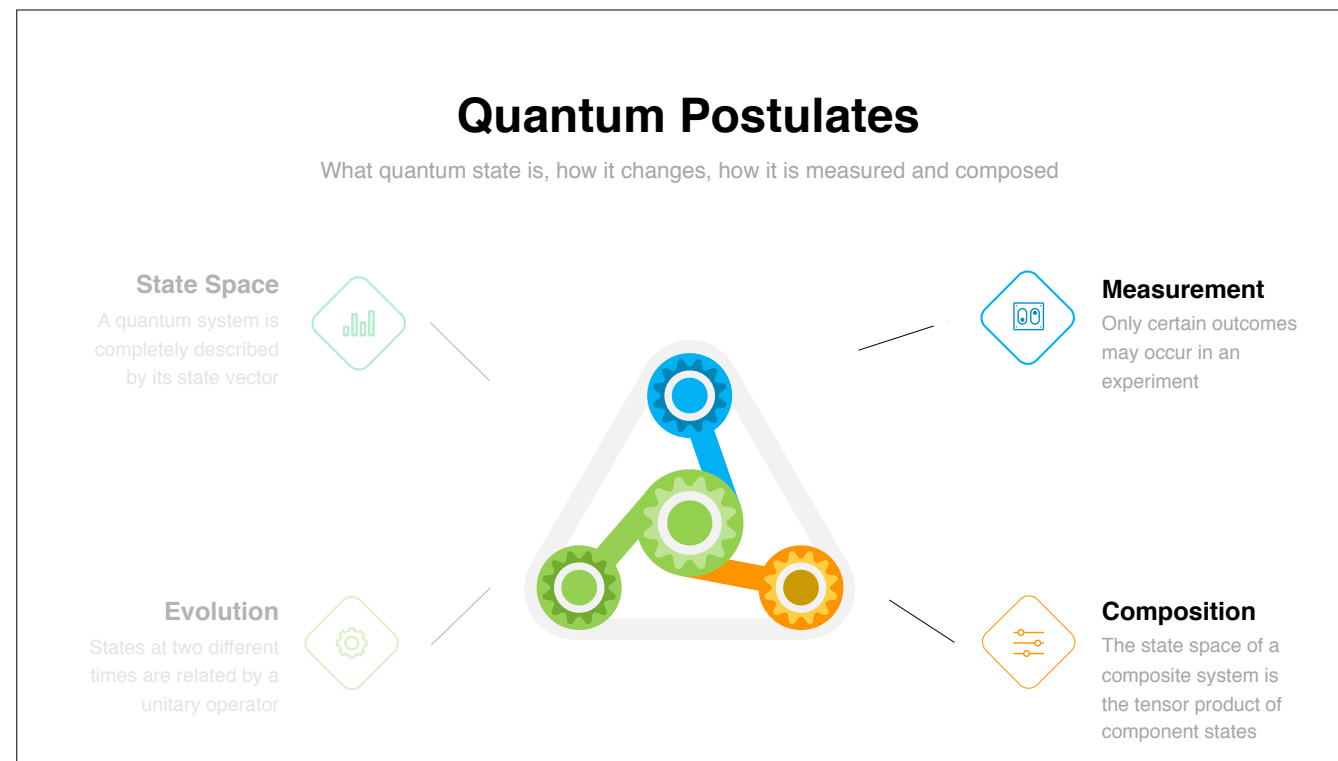
The buckets of a quantum system state are the possible outcomes that can be measured. We will discuss measurement on the next slide, but as far as representation and evolution, quantum state is very similar to portfolio allocation, except the “allocations” are complex numbers, called amplitudes, whose squared magnitudes add up to 1.

The combining operation is addition for complex numbers or vectors. The update rule represents a linear transformation.

For the simple case of 2 buckets, we can think of a coin with an amplitude associated to each side. We can label the sides (possible outcomes) as $|0\rangle$ and $|1\rangle$. In general the coin is biased, as the magnitudes of the amplitudes of the two faces are not equal. Transforming the state changes the bias of the coin.

When such a quantum coin is tossed (the system state is measured), each side will materialize with a probability that is the squared magnitude of the amplitude corresponding to that face. Note that the sum of the probabilities is 1.

An example of state change is the Hadamard transformation, shown here. It can be applied to any valid state, but let's look at the case when we start with a biased quantum coin that always turns heads, so the amplitude of one side is 1. The new amplitude of each face is 1 over square root of 2, meaning that each side has a 50% probability of showing up. The quantum coin is in equal superposition.








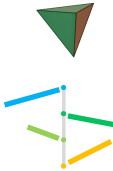








The last two postulates of quantum computing address state measurement and state composition.

In classical computing the state of a system can be read or measured any time, and the measurement reflects the current state of the system. In a quantum system, the state is not accessible, and a measurement yields one of the possible outcomes, with a probability that is equal to the squared magnitude of that outcome. In addition, the new state of the system after the measurement is a state that corresponds to the outcome that was measured. This is called state collapsing.

The buckets in a quantum system that is the composition of two quantum systems is a collection of pairs of buckets from the two systems. The value corresponding to such a pair is the product of the values corresponding to the component buckets. The Scala language's Tuple concept is all that is needed to represent composition of quantum states, but it is more practical to use indexed structures to simplify the representation.

Composition and Measurement

Qubits, superposition, entanglement

Qubits	Quantum State	Measurement Outcomes
	One amplitude for each possible outcome	The probability of an outcome is the squared magnitude of its associated amplitude
		<div><div> 0></div></div> <div><div> 1></div></div>
		<div><div> 00></div></div> <div><div> 01></div></div> <div><div> 10></div></div> <div><div> 11></div></div>

The buckets of a quantum system state are the possible outcomes that can be measured.

We can use quantum bits (essentially quantum coins previously described) as the units of composition, and binary words of possible outcomes as the buckets for the system composed of multiple quantum bits. In Quantum Computing the possible outputs for a quantum bit are 0 and 1, and the possible outputs of a system composed of n quantum bits are all binary words of length n.

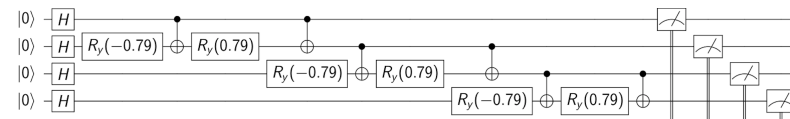
Calculating Fibonacci Numbers

Counting binary words with no consecutive ones

```
def fib(n: Int): QState[Word] = {  
  var state = pure(Word.fromInt(0, n))  
  for (i <- 0 until n) state = state >=> wire(i, H)  
  for (i <- 0 until n - 1) state = state >=> controlled(i, i + 1, ZERO)  
  state  
}
```

Circuit implementation:

```
for (i <- 0 until n - 1) state = state >=> wire(i + 1, Ry(-math.Pi/4)) >=>  
  controlled(i, i + 1, X) >=> wire(i + 1, Ry(math.Pi/4)) >=> controlled(i, i + 1, X)
```



F(1) = 2
F(2) = 3
F(3) = 5
F(4) = 8
F(5) = 13
F(6) = 21
F(7) = 34
F(8) = 55
F(9) = 89
F(10) = 144
F(11) = 233
F(12) = 377
F(13) = 610
F(14) = 987
F(15) = 1597

Controlled transformations are applied only to states whose labels are satisfying a predicate. The most important class of controlled transformations are the ones where the predicate checks that the outcome contains 1 in one of the positions.

Let's build a quantum system that has only outcomes that are binary words of length n without consecutive ones. We first put every component quantum bit in equal superposition, so both 0 and 1 outcomes are possible and have equal probability of being measured. Then we add the constrain that if an outcome has 1 in a position, then it has to be followed by 0.

Running the system multiple times and counting the number of different possible outcomes allows to calculate the number of binary words of length n without consecutive ones. This is a Fibonacci number.

Thank You

Appendix

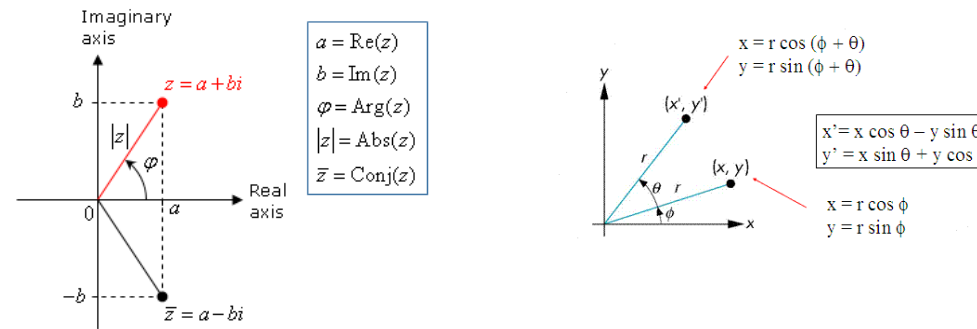
Credits

<https://github.com/jliszka/quantum-probability-monad>

<https://sigfpe.wordpress.com/2007/03/04/monads-vector-spaces-and-quantum-mechanics-pt-ii/>

Complex Numbers

Complex numbers (2 -dimensional vectors) as values



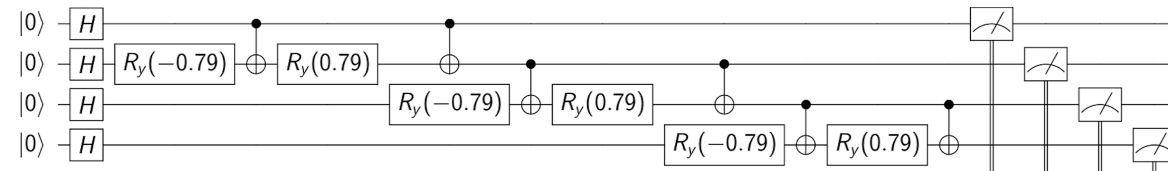
<http://www.thefouriertransform.com/math/complexmath.php>

I added this slide in order to have a quick refresher on complex numbers, the type of values used in quantum systems. I will not go into all the details, but we can refer back to this slide when needed. A complex number is a pair of real numbers, that can be viewed as a two dimensional vector, or as an arrow (Richard Feynman's favorite term). The magnitude or length of a complex number is derived from the Pythagorean Theorem as the square root of the sum of the squares of its components.

Vectors can be added, multiplied and rotated.

Circuits and Gates

Composing and measuring qbits



```
"Ry(pi/2)Z" should "equal H" in forAll { state: QState[Std] =>
  val y: QState[Std] = state >>= Z >>= Ry(math.Pi/2)
  val h: QState[Std] = state >>= H
  assert(y(S0).toString == h(S0).toString)
  assert(y(S1).toString == h(S1).toString)
}
```

```
"Ry(theta)" should "mix the amplitudes of |0> and |1> (like vector rotation)"
val theta = ts._1
val state = ts._2
val y: QState[Std] = Ry(theta)(state)
// same formula as 2-dimensional vector rotation (but with half angle)
val t0 = state(S0) * math.cos(theta/2) - state(S1) * math.sin(theta/2)
val t1 = state(S0) * math.sin(theta/2) + state(S1) * math.cos(theta/2)
assert(y(S0) == t0)
assert(y(S1) == t1)
```

The circuit computing model is a popular implementation of quantum computations, which happens to be used by IBM. In a real quantum computer, only a small number of transformations (called gates) is available, but any transformation can be build from them.

This is the equivalent of the system that outputs binary strings without consecutive ones. It uses a number of standard gates (H, Z, X, Ry).

Show and run code (Scala and Qiskit)