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Applied Quantum Computing Workshop

Introduction to Quantum Computing

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Outline

- Mathematical Preliminary Remarks
- Superposition & Entanglement
- How to Program a Real Device
- Where Are We?

Mathematical Preliminary Remarks

Kets and Vector Spaces

Kets are column vectors in Braket (Dirac) notation $|\psi\rangle \equiv \vec{\psi}$

Definition

Vector Space $\mathcal{V}$:

- $|u\rangle + |v\rangle \in \mathcal{V}$
- $a|u\rangle \in \mathcal{V}$
- $|u\rangle + (|v\rangle + |w\rangle) = (|u\rangle + |v\rangle) + |w\rangle$
- $|u\rangle + |v\rangle = |v\rangle + |u\rangle$
- $|0\rangle$ (zero vector) $\in \mathcal{V}$
- $-|u\rangle \in \mathcal{V}$
- $a(b|u\rangle) = (ab)|u\rangle$
- $1|u\rangle = |u\rangle$
- $a(|u\rangle + |v\rangle) = a|u\rangle + a|v\rangle$
- $(a+b)|u\rangle = a|u\rangle + b|u\rangle$

$|\psi\rangle \in \mathcal{V}$:= Quantum State $\rightarrow$ Holds all information about the particle

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- For any physical quantity, $|\psi\rangle$ is in a superposition of all possible outcome kets with coefficients related to the probability of that outcome

  Example: Energy

  - Discret energy eigenstates $E_1, E_2, \ldots$
  - $|\psi\rangle = a_1 |E_1\rangle + a_2 |E_2\rangle + \ldots$ (could be infinite outcomes)

- For discret values $\Rightarrow$ Sums and coefficient values
- For continuous values $\Rightarrow$ Integrals and coefficient wavefunctions

! Outcome states form a basis for the vector space $\mathcal{V}$!

- Outcome states == eigenstates
- Possible outcome states can be infinite ↯
  - ↪ Infinite combination of basis states to form $|\psi\rangle \in \mathcal{V}$ may violate Definition 1
  - ⇒ Every convergent sum of vectors must converge to an element inside the vector space (*Cauchy Completeness*)

Definition

A Hilbert space $\mathcal{H}$ is a Cauchy complete, infinite-dimensional, complex vector space with an inner product.

For a Hilbert space $\mathcal{H}$ Definition 1 is extended by $\sum_i^\infty |e_i\rangle \in \mathcal{H}$

Usually: Quantum Vector Space = Hilbert Space

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Definition

Inner product on $\mathcal{H}$ is a mapping $\langle\cdot|\cdot\rangle : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$, satisfying:

- $\langle u|av + bw\rangle = a\langle u|v\rangle + b\langle u|w\rangle$
- $\langle u|v\rangle = \langle v|u\rangle^*$ (Complex Conjugate)
- $\langle u|u\rangle \geq 0 : \forall u \in \mathcal{H}$, with equality if and only if $u = \mathbf{0}$

Length of vector u in terms of inner product (*Norm*): $||u|| = \sqrt{\langle u|u\rangle} \in \mathbb{R}$, since $\langle u|u\rangle \in \mathbb{R}$

$\hookrightarrow$ Measures magnitude of u in $\mathcal{H}$

Orthogonality: $u \perp v \leftrightarrow \langle u|v\rangle = 0$

Definition

Bras are Hermitian conjugates of kets and therefore row vectors. A bra is a linear functional that acts on ket vectors to produce (complex) numbers.

- $\forall \, |u\rangle \in \mathcal{H} : \exists \, \langle u| \in \mathcal{H}^*$
- $|u\rangle^\dagger = \langle u|$

! Bra is an operator in $\mathcal{H}^*$ (Hilbert Dual Space) !

$\hookrightarrow$ **Dual Space** $:=$ Given a vector space $\mathcal{V}$ the corresponding dual space $\mathcal{V}^*$ is the vector space of all linear functionals in $\mathcal{V}$.

$\hookrightarrow$ **Linear Functional** $:=$ Any linear map $L : \mathcal{V} \to \mathbb{C}$

Bra & Braket

To extract a certain value of physical information from the state $|\psi\rangle$ we need a linear functional mapping $L\,|\psi\rangle \to c$

- Bra $\langle\cdot|$:= linear functional L
- $\langle\cdot|\,|\psi\rangle$ (*compare to inner product*)
  - ↪ **Riesz Representation Theorem:** For any linear functional L that operates linearly on vectors $v \in \mathcal{H}$, there exists a unique vector u such that the action of L on v can be represented as the inner product of u and v.
  - $\Rightarrow \langle\phi|\,|\psi\rangle \overset{!}{=} \langle\phi|\psi\rangle$

Bra and inner product are formally different mathematical entities!

→ Braket notation makes connection seamless

Observable Operators

Definition

Observables are any physical quantities one could measure and therefore "observe" from a particle. Observables are linear operators on $\mathcal{H}$, i.e. a map $\hat{M}$ on vector space that preserves linear structure of that space:

- $\hat{M}(|u\rangle + |v\rangle) = \hat{M}|u\rangle + \hat{M}|v\rangle$
- $\hat{M}(c|u\rangle) = c\hat{M}|u\rangle$

! Linear operator is an abstract map, while a matrix is a representation of a linear operator in a particular basis !

➥ Quantum mechanics has no standard basis

→ Work with abstract representations of operators

Observable Operators

- Possible outcomes of applying the linear operator corresponding to the observable (*measurement*) $\Rightarrow$ eigenvalues
- States corresponding to these outcomes $\Rightarrow$ eigenvectors ($:=$ eigenstates)
- Particle in superposition of all possible outcomes of measurement $\Rightarrow$ linear combination of observable's eigenvectors

Observable Operators

Observables satisfy the following conditions:

- Observables have real eigenvalues $e_i \in \mathbb{R}$
- Observable's eigenstates must span the entire vector space
  - $\hookrightarrow$ $span(|E_1\rangle, |E_2\rangle, \ldots) = \{\sum_i c_i |E_i\rangle : \forall c_i\}$
  - $\hookrightarrow$ Any quantum state can be written as linear combination of eigenstates
- Eigenstates must be mutually orthogonal

$\Rightarrow$ Oberservable's eigenstates form an orthonormal (eigen-)basis

Particles being in eigenstates have no uncertainty, repeated measurement yields the same eigenvalue every time.

Hermitian Operators

Definition

Each linear operator $\hat{A}$ defines a Hermitian adjoint operator $\hat{A}^\dagger$ that satisfies

- $\langle u|\hat{A}v\rangle = \langle\hat{A}^\dagger u|v\rangle$
- $\hat{A}^{\dagger\dagger} = \hat{A}$
- $(\hat{A}+\hat{B})^\dagger = \hat{A}^\dagger + \hat{B}^\dagger$
- $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger$

! The Hermitian adjoint of a scalar c is the complex conjugate: $c^\dagger = c^*$!

Definition

An operator $\hat{A}$ is hermitian, or self-adjoint, if and only if

- $\hat{A}^\dagger = \hat{A} \;\rightarrow\; \langle u|\hat{A}|v\rangle = \langle u|\hat{A}v\rangle = \langle\hat{A}u|v\rangle : \forall u, v \in \mathcal{H}$

! All observables are hermitian !

Definition

Operators that preserve the inner product structure, meaning the length of vectors and angles between them, i.e. $\langle u|v\rangle = \langle \hat{U}u|\hat{U}v\rangle$, are called unitary operators and satisfy the following property:

- $\hat{U}^{\dagger} = \hat{U}^{-1} \;\rightarrow\; \hat{U}^{\dagger}\hat{U} = \hat{U}\hat{U}^{\dagger} = \mathbf{I}$

! Following Definition 8, we can easily see that unitary operators conserve probability !

All eigenvalues of an unitary operator must have magnitude 1

- $|e_i|^2 = 1 : \forall\ eigenvalues(\hat{U})$
  - $\hookrightarrow$ Unit complex numbers
  - $\hookrightarrow$ All eigenvalues have unit length
- Eigenvalues tell us, how much the operator scales its eigenvector
  - $\hookrightarrow$ Unitary operators should not change the length of their (eigen-)vectors

    Example:

    Consider $\hat{U}$ on eigenvector $|v\rangle$

    $\hat{U}|v\rangle = \lambda|v\rangle$

    $||\hat{U}|v\rangle|| = ||\lambda|v\rangle||$

    $||\hat{U}|v\rangle|| = |\lambda|||v\rangle||$ (for $|v\rangle \neq \mathbf{0} : |||v\rangle|| > 0$

    $||\hat{U}|v\rangle|| = |||v\rangle|| \Rightarrow |\lambda| = 1$

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Quantum computing is (mathematically spoken) just linear algebra

- Quantum states are vectors represented as kets $|\cdot\rangle$
- Operators are matrices
- Eigenvalues are the ground states

Superposition & Entanglement

Superposition

Quantum Superposition is one of the fundamental principles of quantum mechanics / computing.

Definition

Any state can be expanded as a sum of possibly infinite eigenstates of an Hermitian operator forming a complete basis. Such a superposition of eigenstates is called *quantum superposition*.

$\hookrightarrow$ Contrary to classical mechanics where properties are always well defined

On interaction with the external world, the superposition reduces to a single eigenstate (wave function collapse)

Born's Rule

Coefficients of eigenstates in the superposition of a particle are related to the probability of the outcome (collapsing into the eigenstate).

Definition

Born's rule states that the probability density of finding a system in a given state when measured is proportional to the square of the amplitude of the system's wavefunction at that state.

Definition

Qubit (Quantum Bit) is the basic unit of quantum information. A qubit is a 2-state quantum-mechanical system.

- Use spin property of the particle (spin-up, spin-down)
- Spin is an intrinsic property of all particles
- Spin-$\frac{1}{2}$ objects cannot be accurately described using classical physics
  - $\hookrightarrow$ Simple(st) system requiring quantum mechanics

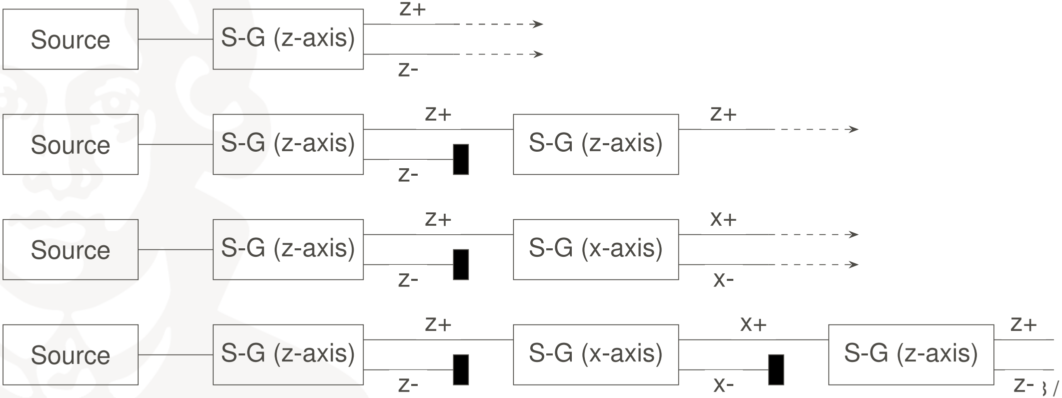
Stern-Gerlach Experiment

- Silver atoms send through spatially-varying magnetic field

Line 2 Repeated measurement in same basis yields same result (eigenstates)

Line 4 Changing measurement basis destroys all previous information

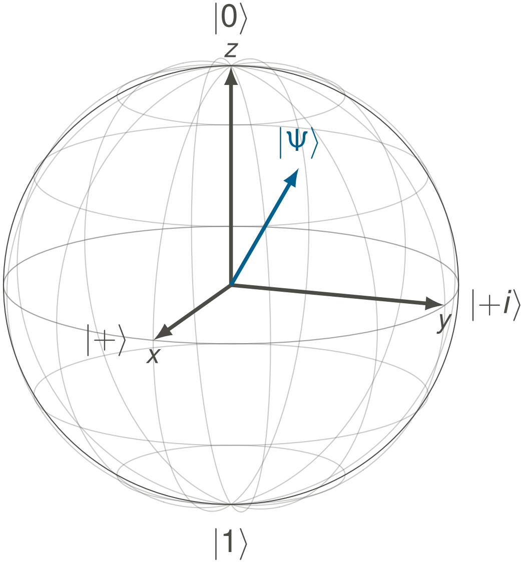
↪ Uncertainty Principle: spin cannot be measured on two perpendicular directions at the same time



Bloch Sphere

Abstract visualization of a qubit.

- North and south pole are *typically* chosen to correspond to the standard basis vectors $|0\rangle$ and $|1\rangle$
- Points on the surface correspond to pure states (any superposition of basis states)
- $|\Psi\rangle = \alpha |0\rangle + \beta |1\rangle$



Superposition

- Quantum state hold information about the two basis states at the same time
- Contrary to the classical information holding only single state information (0 *or* 1)
- QC can encode 2^n states simultaneously

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Definition

Quantum Entanglement is the phenomenon that occurs when a group of particles is generated in a way such that the quantum state of each particle of the group cannot be described independently of the state of the others.

- Measurement of physical properties (e.g. momentum, position, ...) of entangled particles are correlated
- Entangled quantum state cannot be factored as a product of single-qubit states

Consider the Hadamard operator $H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$

and the controlled not operator (CNOT) $CX = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$

- Write the basis states in their vector form $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$; $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

Hadamard

What happens to the states when an Hadamard gate is applied?

$$H|0\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle := |+\rangle$$

$$H|1\rangle = \frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{2}}|1\rangle := |-\rangle$$

- The Hadamard transforms basis states into (uniform) superpositions
- Hadamard is reversible (applying two subsequent H results in the same state)
  - ↪ Hadamard operator is unitary and hermitian

- System consisting of multiple qubits can be written as tensor products of its qubit-states
- $$|0\rangle \otimes |0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = |00\rangle := |0\rangle_2$$

  $$|0\rangle \otimes |1\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = |01\rangle := |1\rangle_2$$

  $\dots$

CX

Apply CNOT on a system of 2 qubits

$$CX|00\rangle = |00\rangle$$
$$CX|01\rangle = |01\rangle$$
$$CX|10\rangle = |11\rangle$$
$$CX|11\rangle = |10\rangle$$

- The first qubit is called *Control Qubit*
- Second qubit is the *Target Qubit*
- The CNOT operator negates/flips the target if the control qubit is 1

Bell State

Perform a Hadamard on the first and a CNOT from first to second qubit of the system

$$CX\ H_1\ |00\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}} = |\Phi^+\rangle$$

- Performing this sequence of operators on all four basis states of the 2-qubit system yields the *Bell States*
  - ↪ Bell states are the maximally entangled states of the 2-qubit system
  - ↪ Measurement of first qubit guarantees measuring the second qubit yields the same value

Remember: Entangled states cannot be factored as a product of states

Consider $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ and $|\phi\rangle = \gamma|0\rangle + \delta|1\rangle$
Trying to factorize:

$$(\alpha|0\rangle + \beta|1\rangle) \otimes (\gamma|0\rangle + \delta|1\rangle) = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$$

$$\alpha\gamma|00\rangle + \alpha\delta|01\rangle + \beta\gamma|10\rangle + \beta\delta|11\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$$

$$\Rightarrow \alpha\gamma \stackrel{!}{=} \frac{1}{\sqrt{2}};\ \alpha\delta \stackrel{!}{=} 0;\ \beta\gamma \stackrel{!}{=} 0;\ \beta\delta \stackrel{!}{=} \frac{1}{\sqrt{2}}$$

$$\Rightarrow \alpha = 0 \lor \gamma = 0 \ \lightning$$

How to Program a Real Device

Coding

- Different Quantum Software Development Kits (QuantumSDKs) are available
  - ↪ One of them is Qiskit, provided and maintained by IBM
- Quantum code runs through multiple compilation and transpilation steps
  - Code on the most abstract level is compiled to an intermediate representation (IR), e.g. OpenQASM
  - IRs serve as a bridge to translate and optimize code-logic to quantum instructions
  - IR gets transpiled to the used hardware's specifics

Simulator vs. Emulator vs. Real Device

Simulator

- Simulates quantum operations using classical hardware
- Exact representation (no noise/error)
- Can be run on your personal computer

Emulator

- Mimics behavior of quantum algorithms using approximations
- Usually faster than exact simulation
- Can be run on personal computer

Real Device

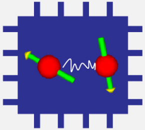
- Utilizes actual quantum hardware
- Provided through cloud access
- Subject to noise and decoherence
- Can require noise-mitigation (or better noise-correction)

Where Are We

Quantum Technology Readiness Level (QTRL)

QTRL

Quantum Technology Readiness Levels describing the maturity of Quantum Computing Technology



QTRL9	QCs (QAs) exceed power of classical computers
QTRL8	Scalable version of QC (QA) completed and qualified in test
QTRL7	Prototype QC (QA) built solving small but user-relevant problems
QTRL6	Components integrated in small quantum processor w/ error correction
QTRL5	Components integrated in small quantum processor w/o error correction
QTRL4	Multi-qubit system fabricated; classical devices for qubit manipulation developed
QTRL3	Imperfect physical qubits fabricated
QTRL2	Applications / technologically relevant algorithms formulated
QTRL1	Theoretical framework for quantum computation (annealing) formulated

Annealing

➥ QTRL 8

Gate-based

➥ QTRL 5