VU Quantum Computing

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2.3 Postulates of Quantum Mechanics

Postulates

Postulate I:

- The state of an isolated physical system is completely described in terms of a unit vector in a complex Hilbert space.
- This unit vector is called *state vector* (or *wave function*) and the corresponding Hilbert space is the *state space* of the system.

Postulate II:

- The temporal development of a closed physical system is described by means of *unitary operators*.
- More specifically, for each time point t, there is a unitary operator $U(t)$ such that
$$|\Psi(s+t)\rangle = U(t)\,|\Psi(s)\rangle,$$
where $|\Psi(s)\rangle$ is the state of the system at time s and $|\Psi(s+t)\rangle$ the state of the system at time $s+t$.

Postulates (ctd.)

In particular:

Postulate II':
The temporal development of a closed quantum system is described in terms of the *Schrödinger equation*:

$$i\hbar \frac{\partial}{\partial t} |\Psi\rangle = H |\Psi\rangle \, .$$

- The constant $\hbar$ is given by

  $$\hbar = \frac{h}{2\pi} \quad (h = \text{Planck's constant})$$

  and H is a self-adjoined operator corresponding to the total energy of the system, called *Hamiltonian operator*.

Remarks

1. Since H is self adjoined, it has a spectral representation of the form

$$H = \sum_E E\,|E\rangle\,\langle E|,$$

where E are the eigenvalues of H and $|E\rangle$ the corresponding eigenvectors.

   - The vectors $|E\rangle$ are called the *energy eigenstates* and the values E represent the associated *energy value* of the state $|E\rangle$.

2. If H is time-independent, then a solution of the Schrödinger equation is given by

$$|\Psi(t_2)\rangle = U(t_2 - t_1)\,|\Psi(t_1)\rangle = e^{-\frac{i}{\hbar}(t_2-t_1)H}\,|\Psi(t_1)\rangle\,,$$

where $|\Psi(t_i)\rangle$ is the state of the system at time t_i ($i = 1, 2$).

3. The Schrödinger equation is a *linear* differential equation, i.e., if $|\psi_1\rangle$ and $|\psi_2\rangle$ are solutions, then so is $\lambda\,|\psi_1\rangle + \nu\,|\psi_2\rangle$ ($\lambda, \nu \in \mathbb{C}$).

$\Longrightarrow$ This is called the *superposition principle*.

Postulates (ctd.)

Postulate III:

- Measurements are described by self-adjoined operators, called *observables*.
  - These operators effect the state space of the considered system.
  - Each observable M has a spectral representation of form $M = \sum_m mP_m$, where $P_m = \sum_j |j\rangle \langle j|$ is the projection to the space of all eigenvectors $|j\rangle$ having eigenvalue m of M.
- Possible values of measurements are given by the eigenvalues of M.
  - If directly before the measurement the system is in state $|\Psi\rangle$, then $p(m) = \langle\Psi|P_m|\Psi\rangle$ gives the probability to measure the value m.
  - After the measurement of m, the system is in state

$$\frac{1}{\sqrt{p(m)}} P_m |\Psi\rangle ,$$

where the function $p(\cdot)$ satisfies the boundary condition $\sum_m p(m) = \sum_m \langle\Psi|P_m|\Psi\rangle = 1$.

Remarks

1. There is also a more general form of Postulate III and above version describes the postulate of *projective measurements* after John von Neumann.

2. For an observable M of a system in state $|\Psi\rangle$, the value $\langle M \rangle := \langle \Psi | M | \Psi \rangle$ is the so-called *expectation value*.

   - This number describes the theoretical mean of the measured values of the observable M providing the experiments are repeated infinitely often and the system is before each measurement in state $|\Psi\rangle$.
   - Furthermore, the value

     $$\Delta(M) := \sqrt{\langle (M - \langle M \rangle)^2 \rangle} = \sqrt{\langle M^2 \rangle - \langle M \rangle^2}$$

     is the *standard deviation* of M while $\Delta(M)^2$ is the *uncertainty* (or *variance*) of M.

Remarks (ctd.)

3. Two observable C, D always satisfy the *Heisenberg uncertainty relation*:

$$\Delta(C)\Delta(D) \geq \frac{1}{2}|\langle[C,D]\rangle| = \frac{1}{2}|\langle\Psi|[C,D]|\Psi\rangle|,$$

where $[C, D] := CD - DC$ is the *commutator* of C and D.

4. Two states $|\Psi_1\rangle$ and $|\Psi_2\rangle$ such that $|\Psi_2\rangle = e^{i\Theta}|\Psi_1\rangle$ $(\Theta \in \mathbb{R})$, i.e., which differ only by a global phase factor $e^{i\Theta}$, are indistinguishable from an experimental point of view, since for each operator A the following holds:

$$\begin{aligned}\langle\Psi_2|A|\Psi_2\rangle &= \langle e^{i\Theta}\Psi_1|A|e^{i\Theta}\Psi_1\rangle \\ &= \overline{e^{i\Theta}}e^{i\Theta}\langle\Psi_1|A|\Psi_1\rangle \\ &= e^{-i\Theta}e^{i\Theta}\langle\Psi_1|A|\Psi_1\rangle \\ &= \langle\Psi_1|A|\Psi_1\rangle .\end{aligned}$$

Postulates (ctd.)

Postulate IV:
The state space of a composite system S is given by the tensor product of its parts.

- That is, if S consists of n subsystems $S_1, \ldots, S_n$ and each S_i is in state $|\Psi_i\rangle$ ($i = 1, \ldots, n$), then the state vector $|\Psi\rangle$ of the overall system S is given by

$$|\Psi_1\rangle \otimes \cdots \otimes |\Psi_n\rangle \, .$$

2.4 Selected (Standard) Literature

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§3 Quantum Gates

3.1 Quantum Registers

Qubits

Definition:

- A *qubit* is a state vector of a quantum mechanical system whose state space V is two-dimensional, i.e., where V has a basis with two elements.
- We write the elements of the basis of V usually in the form $|0\rangle, |1\rangle$.

A qubit has therefore the following form:

$$|\Psi\rangle = \alpha |0\rangle + \beta |1\rangle \qquad \alpha, \beta \in \mathbb{C}$$

Since state vectors are unit vectors, i.e., $\langle \Psi \mid \Psi \rangle = 1$, for each state vector Ψ, it must hold that

$$|\alpha|^2 + |\beta|^2 = 1.$$

Remarks

- If the elements $|0\rangle$ and $|1\rangle$ of the basis are fixed, then we can write the state vectors also in *coordinate form*:
  - for $|\Psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle$ we write then $|\Psi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$.
  - Hence:
  $$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$
- Examples of quantum mechanical systems with two-dimensional state space are *spin-$\frac{1}{2}$ particles*, whose spin ("spin angular momentum") can have only two values, viz. $+\frac{1}{2}$ ("spin-up") or $-\frac{1}{2}$ ("spin-down").

Quantum Registers

- Systems with a 2-dimensional state space realise *1-qubit-quantum registers*.
- By joining several such systems one obtains more complex registers.
  - Postultate IV implies that the state space of composite systems are given by the tensor product of the state spaces of the respective constituent systems.

Quantum Registers (ctd.)

The state vector of a *2-qubit quantum register* can therefore be represented as follows:

- Let V_1, V_2 be 2-dimensional state spaces, where $\left|\Psi_0^i\right\rangle, \left|\Psi_1^i\right\rangle$ are the elements of the basis of V_i $(i = 1, 2)$ and let $\left|\Psi^i\right\rangle$ be arbitrary qubits from V_i:

$$\left|\Psi^1\right\rangle = \alpha_0^1 \left|\Psi_0^1\right\rangle + \alpha_1^1 \left|\Psi_1^1\right\rangle = \begin{pmatrix} \alpha_0^1 \\ \alpha_1^1 \end{pmatrix},$$

$$\left|\Psi^2\right\rangle = \alpha_0^2 \left|\Psi_0^2\right\rangle + \alpha_1^2 \left|\Psi_1^2\right\rangle = \begin{pmatrix} \alpha_0^2 \\ \alpha_1^2 \end{pmatrix},$$

where

$$\left|\Psi_0^1\right\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \left|\Psi_1^1\right\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \left|\Psi_0^2\right\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \left|\Psi_1^2\right\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Quantum Registers (ctd.)

The state vector of the composite system is given by:

$$\left|\Psi^{1,2}\right\rangle = \left|\Psi^{1}\right\rangle \otimes \left|\Psi^{2}\right\rangle = \begin{pmatrix} \alpha_0^1 \\ \alpha_1^1 \end{pmatrix} \otimes \begin{pmatrix} \alpha_0^2 \\ \alpha_1^2 \end{pmatrix} = \begin{pmatrix} \alpha_0^1\alpha_0^2 \\ \alpha_0^1\alpha_1^2 \\ \alpha_1^1\alpha_0^2 \\ \alpha_1^1\alpha_1^2 \end{pmatrix} = \begin{pmatrix} \alpha_{00} \\ \alpha_{01} \\ \alpha_{10} \\ \alpha_{11} \end{pmatrix}.$$

Quantum Registers (ctd.)

The elements of the basis of $V_1 \otimes V_2$ are given by:

$$|00\rangle = \left|\Psi_0^1\right\rangle \otimes \left|\Psi_0^2\right\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$|01\rangle = \left|\Psi_0^1\right\rangle \otimes \left|\Psi_1^2\right\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

$$|10\rangle = \left|\Psi_1^1\right\rangle \otimes \left|\Psi_0^2\right\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

$$|11\rangle = \left|\Psi_1^1\right\rangle \otimes \left|\Psi_1^2\right\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

Quantum Registers (ctd.)

- Consequently:

$$\left|\Psi^{1,2}\right\rangle = \alpha_{00}\left|00\right\rangle + \alpha_{01}\left|01\right\rangle + \alpha_{10}\left|10\right\rangle + \alpha_{11}\left|11\right\rangle$$

- The generalisation for *n-qubit quantum registers* is analogous.

Remarks

- An element $|\Psi\rangle$ of an n-qubit register which cannot be represented as a tensor product of single qubits is called *entangled*.
  - That is, if $|\Psi\rangle$ is entangled, then there are no 1-qubit states $\left|\Psi^1\right\rangle, \left|\Psi^2\right\rangle, \dots, |\Psi^n\rangle$ such that

$$|\Psi\rangle = \left|\Psi^1\right\rangle \otimes \left|\Psi^2\right\rangle \otimes \cdots \otimes |\Psi^n\rangle \,.$$

  - For instance, the 2-qubit register $|\Psi\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$ is entangled.
    - ☞ $|\Psi\rangle$ is called *Bell state* or *EPR pair* ("EPR" stands for "Einstein-Podolsky-Rosen" in view of their famous 1935 paper trying to show that quantum mechanics theory is incomplete).

☞ Entangled states play a central role in quantum computing.

- ➥ Such states have the property that one part of the register can be changed by measuring another part of it.

3.2 Quantum Computers

Quantum Computers

- From Postulate II we know that the temporal development of a state vector is determined in terms of a unitary operator.
  - The temporal development of an n-qubit quantum register is therefore also determined by a unitary operator.
  - Such operators over an n-qubit quantum register are called an *n-qubit quantum gate*.

- An n-qubit quantum gate is represented by a unitary $2^n \times 2^n$-matrix.
  - A *quantum computer* is a physical realisation of a combination of $k > 0$ quantum gates which operate over m-qubit quantum registers.
  - The *input* of a quantum computer is the initial state of the corresponding physical system, and the *output* is the result of a measurement after a run of the system.

Quantum Computers (ctd.)

- A *quantum algorithm*, then, is a particular circuit of quantum gates, specified by a unitary matrix U.
- If the circuit consists of k gates, then U is given by

$$U = A_k A_{k-1} \cdots A_1,$$

where each A_i is a unitary matrix describing the action of the i-th gate.

Quantum Turing Machines

- As shown by Yao (1993), quantum circuits are equivalent to the notion of a *quantum Turing machine* (QTM), as introduced by David Deutsch (1985).
  - Recall that a (classical) Turing machine M is a mathematical model of the notion of computation which manipulates symbols on a strip of a tape by means of a read/write head according to a given program.
  - The program specifies the operation of the machine depending on the state of M and the symbol read by the head of M.
  - ➥ In a QTM, the cells of the tape contain a *superposition* of states, i.e., qubits, which allows to encode the different inputs *simultanously* ("quantum parallelism").

☞ In the quantum computing literature, it is customary to specify quantum algorithms in terms of quantum circuits instead of QTMs.

3.3 Important Quantum Gates

1-bit Quantum Gates

- The *Pauli matrices* X, Y, Z:

$$X := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

- X is also referred to as the NOT *gate*, as

$$X\left|0\right\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \left|1\right\rangle$$

$$X\left|1\right\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \left|0\right\rangle$$

- It holds that $X^2 = Y^2 = Z^2 = I$, where I is the identity matrix

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

1-bit Quantum Gates (ctd.)

- The $\sqrt{\mathrm{NOT}}$ gate:

$$\sqrt{\mathrm{NOT}} := \frac{1}{2}\begin{pmatrix} 1+i & 1-i \\ 1-i & 1+i \end{pmatrix}.$$

- A repeated application of the $\sqrt{\mathrm{NOT}}$ gate coincides with the NOT operation, but a single application results in a quantum state that neither corresponds to the classical bit 0 nor the classical bit 1:

$$\sqrt{\mathrm{NOT}} \cdot \sqrt{\mathrm{NOT}} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = X = \mathrm{NOT} \quad \text{while}$$

$$\sqrt{\mathrm{NOT}}\,|0\rangle = \sqrt{\mathrm{NOT}}\begin{pmatrix}1\\0\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1+i\\1-i\end{pmatrix} = \frac{1+i}{2}\begin{pmatrix}1\\0\end{pmatrix} + \frac{1-i}{2}\begin{pmatrix}0\\1\end{pmatrix}$$

$$= \frac{1+i}{2}|0\rangle + \frac{1-i}{2}|1\rangle \quad \text{and likewise}$$

$$\sqrt{\mathrm{NOT}}\,|1\rangle = \frac{1-i}{2}|0\rangle + \frac{1+i}{2}|1\rangle.$$

1-bit Quantum Gates (ctd.)

- The *Hadamard gate* H:

$$H := \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

- It is one of the most useful gates in quantum computing.

- Like $\sqrt{\mathrm{NOT}}$, it maps a computational basis into a superposition of states:

$$H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle);$$

$$H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle).$$

1-bit Quantum Gates (ctd.)

Important property:

- If n qubits in state $|0\rangle$ are applied in parallel with the Hadamard gate, then the produced state is an equal superposition of all the integers in the range 0 to $2^n - 1$:

$$H|0\rangle \otimes H|0\rangle \otimes \cdots \otimes H|0\rangle = \frac{1}{\sqrt{2^n}} \sum_{j=0}^{2^n-1} |j\rangle,$$

  where $|j\rangle$ is the basis state indexed by the binary number that would correspond to the number j in base-10 notation.

- For example, in a 7-qubit register, the state $|19\rangle$ corresponds to the state $|0010011\rangle$ (the first two bits (00) are padding to make the binary number 7 bits in length).

1-bit Quantum Gates (ctd.)

- The utility of the Hadamard gate derives from that fact that by applying, in parallel, a separate Hadamard gate to each of n qubits in state $|0\rangle$, we can create an n-qubit superposition containing 2^n component eigenstates.

- These eigenstates represent all the possible bit strings one can write using n bits.

- This is one of the most important tricks of quantum computing as it gives the ability to load exponentially many indices into a quantum computer using only polynomially many operations.

1-bit Quantum Gates (ctd.)

Further 1-qubit gates:

- The *phase gate*: $S := \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$
- The *T-gate*: $T := \begin{pmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{pmatrix}$
- *Rotation gates*:
  - $R_X(\alpha) = e^{-i\alpha X/2} = \begin{pmatrix} \cos(\alpha/2) & -i\sin(\alpha/2) \\ -i\sin(\alpha/2) & \cos(\alpha/2) \end{pmatrix}$
  - $R_Y(\alpha) = e^{-i\alpha Y/2} = \begin{pmatrix} \cos(\alpha/2) & -\sin(\alpha/2) \\ \sin(\alpha/2) & \cos(\alpha/2) \end{pmatrix}$
  - $R_Z(\alpha) = e^{-i\alpha Z/2} = \begin{pmatrix} e^{-i\alpha/2} & 0 \\ 0 & e^{i\alpha/2} \end{pmatrix}$
  - $Ph(\delta) = e^{i\delta} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ ("global phase shift")

1-bit Quantum Gates (ctd.)

The NOT, $\sqrt{\mathrm{NOT}}$, and Hadamard gates can be obtained from sequences of rotation gates as follows:

$$
\begin{aligned}
\mathrm{NOT} &= R_X(\pi)Ph(\pi/2); \\
\mathrm{NOT} &= R_Y(\pi)R_Z(\pi)Ph(\pi/2); \\
\sqrt{\mathrm{NOT}} &= R_X(\pi/2)Ph(\pi/4); \\
\sqrt{\mathrm{NOT}} &= R_Z(-\pi/2)R_Y(\pi/2)R_Z(\pi/2)Ph(\pi/4); \\
H &= R_X(\pi)R_Y(\pi/2)Ph(\pi/2); \\
H &= R_Y(\pi/2)R_Z(\pi)Ph(\pi/2).
\end{aligned}
$$

2-bit Quantum Gates

- The CNOT-*gate* ("controlled NOT-gate"):

$$\mathrm{CNOT} := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

- CNOT has the following effect:

$$\mathrm{CNOT}\,|00\rangle = |00\rangle$$

$$\mathrm{CNOT}\,|01\rangle = |01\rangle$$

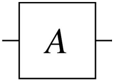
$$\mathrm{CNOT}\,|10\rangle = |11\rangle$$

$$\mathrm{CNOT}\,|11\rangle = |10\rangle$$

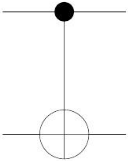
The first qubit is the *control bit*: if set, then the second qubit is inverted.

Graphical Representation

- Representation of a 1-qubit gate A:



- Representation of the CNOT gate:
  - the top line represents the control qubit and the bottom line the target qubit.



Universality

1. The Pauli matrices Z und Y are *universal* in the sense that each 1-qubit gate U can be represented as

$$U = e^{i\alpha} R_Z(\beta) R_Y(\gamma) R_Z(\delta)$$

   for suitable $\alpha, \beta, \gamma, \delta \in \mathbb{R}$.

2. Each n-qubit gate U ($n > 1$) can be represented in terms of $R_X(\cdot)$, $R_Y(\cdot)$, $R_Z(\cdot)$, $Ph(\cdot)$, and CNOT, i.e., these gates are universal for quantum computing.
   - N.B. In classical Boolean logic, e.g., $\{\mathrm{NOT}, \mathrm{AND}\}$ are universal.

3. It even holds:
   - For each $\varepsilon > 0$, each 1-qubit gate can be approximated to accuracy ε using $O(\log^c(1/\varepsilon))$ many H-, S-, CNOT- und T-gates, for some constant $c > 0$.