A crash course in quantum mechanics

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Ref: Nielsen, Chuang: "QI and QC"

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Have heard:
- Classical computers can be modelled as (reversible) Turing Machines
- Data can be encoded in binary numbers

Today: How is data stored and processed in a quantum computer (QC)

$\Rightarrow$ Need to understand the rules of quantum mechanics

Ingredients:

- Space of configurations: (Separable) Hilbert space over $\mathbb{C}$ with hermitean scalar product $(\cdot,\cdot)$
- Observables: Hermitian operators $A = A^+$ on $\mathcal{H}$ (measurable quantities)
- Time evolution: $\begin{cases} \text{Hamiltonian } H = H^+ \\ \text{Unitary operators } \mathcal{U}(t,t') \end{cases}$

1. States

Def: We call $|\psi\rangle \in \mathcal{H}$ a "state" if $\| \, |\psi\rangle \, \| = 1$
(non-standard) (norm = 1)

Def: For two states $|\psi\rangle, |\phi\rangle$ the scalar product $\langle \psi | \phi \rangle = (|\psi\rangle, |\phi\rangle)$ is called their "overlap"

2

Remarks: - The usage of "$|\cdot\rangle$" and "$\langle\cdot|\cdot\rangle$" is called "Dirac notation" or "bra/ket notation"
- $\langle\psi| \in \mathcal{H}^*$ is a (sesqui-linear) functional on $\mathcal{H}$
- A state satisfies $\langle\psi|\psi\rangle = 1$

Example: $\mathcal{H} = \mathbb{C}^2$ with basis $\begin{pmatrix}1\\0\end{pmatrix}, \begin{pmatrix}0\\1\end{pmatrix}$ represents a "qubit"

We frequently write $|0\rangle, |1\rangle$ or $\underbrace{|\uparrow\rangle, |\downarrow\rangle}_{\text{spin}}$.

The qubit can be measured with

$$\underbrace{\sigma^z}_{\text{Pauli matrix}} = \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}: \qquad \begin{aligned}\sigma^z|0\rangle &= +1\cdot|0\rangle = |0\rangle\\ \sigma^z|1\rangle &= \underbrace{-1}_{\text{eigenvalue}}\cdot|0\rangle = -|0\rangle\end{aligned}$$

For a general observable $A = A^+$ there exists an orthonormal basis $\{|\psi_i\rangle\}$ such that $A|\psi_i\rangle = \underbrace{\lambda_i}_{\substack{\text{(real) eigenvalues}\\ \text{(results of measurement)}}}|\psi_i\rangle$

Bits vs. qubits: Qubits can be in a <u>superposition</u>

(*) $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ (with $|\alpha|^2 + |\beta|^2 = 1$)

But now: $\sigma^z|\psi\rangle = \alpha|0\rangle - \beta|1\rangle \neq \lambda|\psi\rangle$ (generally)

So, what is the result of a measurement?

Probabilistic interpretation:

- Each measurement will return either $+1$ or -1
- $P(1) = |\alpha|^2$ and $P(-1) = |\beta|^2$ are the probabilities for ± 1 (if the measurement could be repeated many times)
- The state $|\psi\rangle$ "collapses" to either $|0\rangle$ or $|1\rangle$ (depending on the result of the measurement)

Note: $\langle A \rangle = \langle \psi | A | \psi \rangle$ is called the "expectation value" (of A in a state $|\psi\rangle$)

Example (*):
$$\langle \sigma^z \rangle = \underbrace{\left[\bar{\alpha}\langle 0| + \bar{\beta}\langle 1|\right]}_{\langle\psi|}\underbrace{\left[\alpha|0\rangle - \beta|1\rangle\right]}_{\sigma^z|\psi\rangle}$$
$$= |\alpha|^2 \underbrace{\langle 0|0\rangle}_{1} - |\beta|^2 \underbrace{\langle 1|1\rangle}_{1} - \bar{\alpha}\beta \underbrace{\langle 0|1\rangle}_{0} + \alpha\bar{\beta}\underbrace{\langle 1|0\rangle}_{0}$$
$$= |\alpha|^2 - |\beta|^2 = P(1)\cdot 1 + P(-1)\cdot(-1)$$

For N qubits we consider $\mathcal{H} = (\mathbb{C}^2)^{\otimes N}$ with "computational basis" $\{|i_1 i_2 \cdots i_N\rangle = |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_N\rangle\}$ where $i_k \in \{0,1\}$

Again, there are various types of entangled states...

$N=2$: Bell state $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ (+3 similar possibilities)

$N \geq 3$: GHZ state $\frac{1}{\sqrt{2}}(|0\cdots 0\rangle + |1 \cdots 1\rangle)$ (Greenberger, Horne, Zeilinger)

The Bell state is "maximally entangled". The measurement of the first qubit uniquely determines the outcome of a measurement of the second (due to the "collapse" of the state)

2. Time evolution

States evolve according to the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H |\psi(t)\rangle$$

This has the formal solution

$$|\psi(t)\rangle = \mathcal{U}(t,t_0)|\psi(t_0)\rangle$$

H time-independent

$$\text{with } \mathcal{U}(t,t_0) = \underbrace{\mathcal{T} e^{-\frac{i}{\hbar}\int_{t_0}^{t} H(\tau)\,d\tau}}_{\text{time-ordered exponential}} = e^{-\frac{i}{\hbar}(t-t_0)H}$$

__Remark:__ H hermitian $\leftrightarrow$ $\mathcal{U}(t,t_0)$ unitary
$(H = H^\dagger)$ $\qquad$ $(\mathcal{U}^\dagger = \mathcal{U}^{-1})$

Since unitary operators are always invertible, time evolution is __always reversible__!

__Important:__ – Unitary operators can create entanglement

– In QC one usually works with a preferred set of unitaries ("gates") but in practical applications one needs to find Hamiltonians H that realize them (for suitable choices of t, t_0)