Lectures 1,2 : Postulates of Quantum Mechanics

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Outline

- Postulates of quantum mechanics, as applied to two-level quantum systems (qubits!).

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- Quantum states, operators and time-evolution.

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- Quantum states, operators and time-evolution.
- A brief glimpse into the mathematical framework of quantum theory ... and quantum computing!

Recap: The Qubit

- A quantum bit is described by a general superposition of the form,
$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle, \quad \alpha, \beta \in \mathbb{C},$$
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- The **bra-ket** notation: Qubit states are represented as ket-vectors ($|.\rangle$).
$|0\rangle$ is called "ket-0" and $|1\rangle$ is called "ket-1".

How does the quantum world work?

Three Questions

1. How does one specify the state of a quantum system at a given time?
2. Can we predict what its state will be at later time?
3. What can we say about the physical quantities that we obtain by making measurements on the system?

We will answer these questions in the form of three postulates, each of which addresses one of them.

Postulate 1 (The State of a Quantum System)

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- If $|v\rangle, |w\rangle \in \mathbb{V}$, then, $\alpha|v\rangle + \beta|w\rangle \in \mathbb{V}$, for all complex scalars $\alpha, \beta \in \mathbb{C}$.
- **Basis:** A d-dimensional linear vector space is spanned by d orthogonal vectors, say, $\{|e_1\rangle, |e_2\rangle, \ldots, |e_d\rangle\}$, so that every $|v\rangle \in \mathbb{V}$ can be written as $|v\rangle = \sum_{i=1}^{d} v_i|e_i\rangle$, where $v_i \in \mathbb{C}$ are complex numbers.

Matrix representation and inner-product

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- The **inner product** is defined as the matrix product of the bra and the ket:

$$\langle v|w\rangle = \begin{pmatrix} v_1^* \, v_2^* \ldots v_d^* \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_d \end{pmatrix} = \sum_{i=1}^{d} v_i^* w_i.$$

Two-level quantum systems

- How does one figure out the relevant Hilbert space for a system? We will illustrate some of the ideas through examples.
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- **Linearity** and the **superposition principle:** If $|\psi\rangle, |\phi\rangle \in \mathbb{C}^2$ represent two states of the qubit, then any complex linear combination $\alpha|\psi\rangle + \beta|\phi\rangle$ is also a valid state of the qubit ($\alpha, \beta \in \mathbb{C}$).

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- Two state vectors $|v\rangle$ and $|w\rangle$ represent the same state if they are related by

$$|v\rangle = \lambda\,|w\rangle \quad \text{for some non-zero complex number} \quad \lambda \in \mathbb{C}\,.$$

One uses this to normalize the vector to have unit norm, that is, $\langle v|v\rangle = 1$. Thus the quantum state is determined up to an overall phase.

Qubit state space

- The state space of a qubit is *spanned* by the pair of orthonormal states $\{|0\rangle, |1\rangle\}$. This is called the **standard** or **computational** basis.

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- Geometric visualization: Any arbitrary qubit state can be represented as,

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|1\rangle, \ \theta \in [0, \pi], \ \phi \in [0, 2\pi],$$

since the state is (a) normalized ($|\alpha|^2 + |\beta|^2 = 1$) and (b) overall phase is not fixed.

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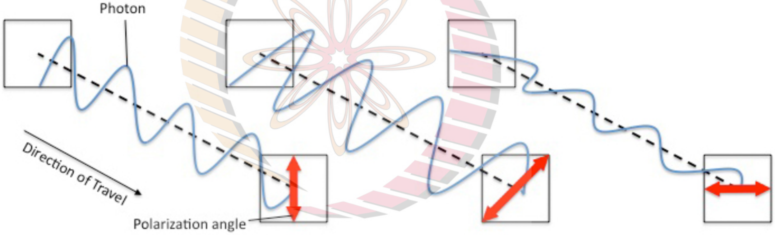
- This suggests a mapping to points of the surface of a unit sphere in real, 3-d space: **Bloch-Poincaré** sphere.

Physical examples of qubit systems

(a) Polarization states of light



$|0\rangle \equiv |H\rangle$ (horizontally polarized state)
$|1\rangle \equiv |V\rangle$ (vertically polarized state).

Physical examples of qubit systems

(b) Spin-1/2 systems:
The spin (angular momentum) along any direction takes on one of two values : $\pm\frac{1}{2}$ in units of $\hbar$ ($= \frac{h}{2\pi}$, Planck's constant)

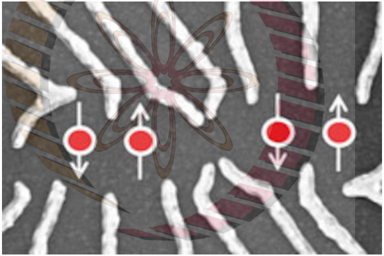
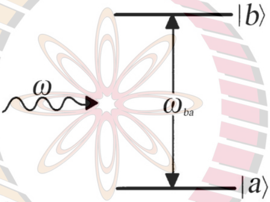


Figure: Spin qubits on Gallium-Arsenide semiconductors, Blühm Lab (RWTH Aachen)

$|0\rangle \equiv |+\frac{1}{2}\rangle \equiv |\uparrow\rangle$ (spin-up state)
$|1\rangle \equiv |-\frac{1}{2}\rangle \equiv |\downarrow\rangle$ (spin-down state).

Physical examples of qubit systems

(c) Two- level atoms



$|0\rangle \equiv |a\rangle$ (ground state)
$|1\rangle \equiv |b\rangle$ (excited state).

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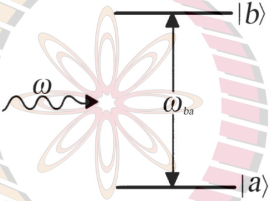

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- Superconducting qubits, which form the backbone of the IBM Q architecture are artificial two-level atoms!

Basis states

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- Physically, for a spin-$1/2$ system, $\{|0\rangle, |1\rangle\}$ correspond to the spin-up and spin-down states along the z-direction.
  Then,
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- **Exercise:** Check the orthogonality relations for all three qubit bases!

Basis transformation

- Transforming from one basis to another:

$$|+\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right); \qquad |-\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right)$$

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- This can be represented as the action of the linear operator U,

$$U|0\rangle = |+\rangle,\ U|1\rangle = |-\rangle,\ U|+\rangle = |0\rangle,\ U|-\rangle = |1\rangle,$$

where U can be represented as the matrix,

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

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- Note that U is a unitary matrix, $U^\dagger U = UU^\dagger = I$, where $U^\dagger = (U^*)^T$ is the conjugate-transpose (or adjoint).
- U is indeed the same as the Hadamard gate H, an important quantum gate!

Outer product

- For a d-dimensional vector space, the outer product $|v\rangle\langle w|$ represents a $d \times d$ matrix.

$$|v\rangle\langle w| = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_d \end{pmatrix} \begin{pmatrix} w_1^* w_2^* \dots w_d^* \end{pmatrix} = \begin{pmatrix} v_1 w_1^* & v_1 w_2^* & \dots & v_1 w_d^* \\ v_2 w_1^* & v_2 w_2^* & \dots & v_2 w_d^* \\ \vdots & \vdots & \dots & \vdots \\ v_d w_1^* & v_d w_2^* & \dots & v_d w_d^* \end{pmatrix}$$

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- The operator U that transforms $\{|0\rangle, |1\rangle\} \leftrightarrow \{|+\rangle, |-\rangle\}$ can be represented as,

$$U = |+\rangle\langle 0| + |-\rangle\langle 1| = |0\rangle\langle +| + |1\rangle\langle +|.$$

Physical Quantities (Observables)

- Classically, the state space is described by the position and momentum of the particle at the given time. Physical quantities or observables are functions of $(\mathbf{x}, \mathbf{p})$.

Postulate 2 (Observables of a Quantum System)

The observables of a quantum system (such as position, momentum, spin components) are described by (Hermitian operators) on the quantum state space.

- Recall that linear operators act on a ket vector from the left .
- **Example:** Spin observables of a spin-1/2 system.

Spin Observables

- Consider the operator S_z represented by the matrix,

$$S_z = \frac{\hbar}{2} Z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

- Then,

$$\begin{aligned} S_z|0\rangle &= \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2} |0\rangle \\ S_z|1\rangle &= \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\frac{\hbar}{2} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\frac{\hbar}{2} |1\rangle. \end{aligned}$$

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- Note that the action of S_z on $|0\rangle$ or $|1\rangle$ is simply a scalar $(\pm\frac{\hbar}{2})$ times $|0\rangle$ or $|1\rangle$.
- The spin-up ($|0\rangle$) and spin-down ($|1\rangle$) states corresponding to the Z-axis are eigenstates of the operator S_z.

Spin observables and eigenstates

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- Similarly, we can represent the observables corresponding to the X-component and Y-component of the spin as,

$$S_x = \frac{\hbar}{2} X = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \; S_y = \frac{\hbar}{2} Y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}.$$

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- **Exercise:** Verify the eigenvalue equations

$$\begin{aligned} S_x|+\rangle &= \frac{\hbar}{2}|+\rangle, S_x|-\rangle = -\frac{\hbar}{2}|-\rangle, \\ S_y|+i\rangle &= \frac{\hbar}{2}|+i\rangle, S_x|-i\rangle = -\frac{\hbar}{2}|-i\rangle. \end{aligned}$$

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- Note that the matrices X, Y and Z are Hermitian and unitary!

Hermitian Operators

- The operator S_z is Hermitian. It is equal to its conjugate-transpose: $\left((S_z)^T\right)^* = S_z$.

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- **Exercise:** Verify that S_x is also a Hermitian matrix.
- Hermitian operators have real eigenvalues. These eigenvalues represent the physical values of the corresponding observables.
- For a spin-$1/2$ system, the spin along the Z-axis can take one of two values $\pm\hbar/2$ corresponding to the states $|0\rangle$ and $|1\rangle$ respectively.
- The spin along the X-axis can take one of two values $\pm\hbar/2$ corresponding to the states $|+\rangle$ and $|-\rangle$ respectively.

Postulate 3 (Time Evolution in Quantum Mechanics)

Given a system in the state, $|\psi(t_0)\rangle \in \mathcal{H}$, at time t_0, the state at time $t > t_0$ is given by a unitary operator $U(t, t_0)$ i.e.,

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

The unitary operator satisfies
(i) $U(t_0, t_0) = I$,
(ii) For $t \geq t_1 \geq t_0$, one has $U(t, t_0) = U(t, t_1)U(t_1, t_0)$.
(iii) For $t < t_0$, $U(t_0, t) = U(t, t_0)^\dagger$.

- Unitary operators preserve the inner product and hence, preserve the norm.

$$\langle\psi(t)|\psi(t)\rangle = \langle\psi(t_0)U^\dagger U|\psi(t_0)\rangle = \langle\psi(t_0)|\psi(t_0)\rangle.$$

- All quantum gates are unitary matrices; they are all reversible transformations.

The Schrödinger equation

- We can rewrite the time-evolution as a differential equation called the Schrödinger equation

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

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- The Hamiltonian is in fact the Hermitian operator corresponding to the energy of the system.
- When H is independent of time, one can show that

$$U(t, t_0) = \exp\left(\frac{-iH\,(t-t_0)}{\hbar}\right) \ ,$$

where $e^A := \sum_{m=0}^{\infty} \frac{A^m}{m!}$ for any linear operator A.

References

- Modern Quantum Mechanics, J J Sakurai (Chapter 1)
- Feynman Lectures on Physics, Vol III
- Quantum Computing and Quantum Information, Nielsen and Chuang (Chapter 2)