Note for *Quantum Optics*: Quantum Theory

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[Reference:]

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[Questions:]

- What is the *essence* of quantum mechanics (QM)?
  1. The Axiom of QM.
  2. Superposition.
  3. Purity of a quantum state.
  4. Entanglement.
  5. Measurement.
- Test of Quantum Mechanics by Optics.
  - Are we satisfied with the axioms of quantum mechanics (QM)?
  - Why QM can not be seen in daily life?
  - Do we need to extend and/or modify QM?
  - What is the link between QM and Gravity?

[Paradoxes of Quantum Theory:] In quantum theory, there are many interesting paradoxes, such as

- Geometric (Berry) phase
- Schrödinger's Cat paradox
- Einstein-Podolosky-Rosen paradox
- Local Hidden Variables theory
- Bell's inequality
- Quantum Zeno effect
- Alternative Quantum Mechanics
- Weak Measurement
- Two-vector formalism
- Entangled-History theory
- Arrow of Time
- . . .

I. AXIOMS OF QUANTUM MECHANICS

Every physical theory is formulated in terms of mathematical objects. It is thus necessary to establish a set of rules to map physical concepts and objects into mathematical objects that we use to represent them. Quantum mechanics is also based on some fundamental laws, which are called the *postulates* or *axioms* of quantum mechanics. The axioms we are going to see apply to the dynamics of closed quantum systems. We want to develop a mathematical model for the dynamics of closed systems: therefore we are interested in defining states, observables, measurements and evolution. Some subtleties will arise since we are trying to define measurement in a closed system, when the measuring person is instead outside the system itself.

1. **State:** The properties of a quantum system are completely defined by specification of its state vector $|\Psi\rangle$. The state vector is an element of a complex Hilbert space $\mathcal{H}$ called the space of states.

2. **Observable:** With every physical property $\hat{A}$ (energy, position, momentum, angular momentum, ...) there exists an associated linear, *Hermitian operator* $\hat{A}$ (usually called observable), which acts in the space of states $\mathcal{H}$. The eigenvalues of the operator are the possible values of the physical properties.

3. **Probability:**

   (a) If $|\Psi\rangle$ is the vector representing the state of a system and if $|\Phi\rangle$represents another physical state, there exists a probability $p(|\Psi\rangle, |\Phi\rangle)$ of finding $|\Psi\rangle$ in state $|\Phi\rangle$, which is given by the squared modulus of the scalar product on $\mathcal{H}$: : $p(|\Psi\rangle, |\Phi\rangle) = |\langle\Psi|\Phi\rangle|^2$ (Born Rule).

   (b) If $\mathcal{A}$ is an observable with eigenvalues a_k and eigenvectors $|k\rangle$, $\hat{A}|k\rangle = a_k|k\rangle$, given a system in the state $|\Psi\rangle$, the probability of obtaining a_k as the outcome of the measurement of $\hat{A}$ is $p(a_k) = |\langle k|\Psi\rangle|^2$. After the measurement the system is left in the state projected on the subspace of the eigenvalue a_k (Wave function collapse).

4. **Time evolution:** The evolution of a closed system is *unitary*. The state vector $|\Psi(t)\rangle$ at time t is derived from the state vector $|\Psi(t_0)\rangle$ at time t_0 by applying a unitary operator $\hat{U}(t, t_0)$, called the evolution operator: $|\Psi(t)\rangle = \hat{U}(t, t_0)|\Psi(t_0)\rangle$.

[References:]

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A. Notations:

- State properties:
  1. quantum state: $|\Psi\rangle = \sum_i \alpha_i |\psi_i\rangle$,
  2. completeness: $\sum_i |\psi_i\rangle\langle\psi_i| = I$, or $\int dx|x\rangle\langle x|$.
  3. probability interpretation (projection): $\Psi(x) = \langle x|\Psi\rangle$,
- Operators:
  1. operator: $\hat{A}|\Psi\rangle = |\Phi\rangle$,
  2. representation: $\langle\phi|\hat{A}|\psi\rangle$,
  3. adjoint of $\hat{A}$: $\langle\phi|\hat{A}|\psi\rangle = \langle\psi|\hat{A}^\dagger|\phi\rangle^*$,
  4. Hermitian operator: $\hat{H} = \hat{H}^\dagger$, *self-adjoint.*
  5. unitary operator: $\hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = I$.
  6. $\hat{U}$ can be represented as $\hat{U} = \exp(i\hat{H})$ if $\hat{H}$ is Hermitian.
  7. normal operator: $[\hat{A}, \hat{A}^\dagger] = 0$, the eigenstates of only a normal operator are *orthonormal.*
  8. hermitian and unitary operators are normal operators.
  9. The sum of the diagonal elements $\langle\phi|\hat{A}|\psi\rangle$ is call the *trace* of $\hat{A}$,

     $$\mathrm{Tr}(\hat{A}) = \sum_i \langle\phi_i|\hat{A}|\phi_i\rangle. \tag{1}$$

     The value of the trace of an operator is independent of the basis.
  10. The eigenvalues of a hermitian operator are real, $\hat{H}|\Psi\rangle = \lambda|\Psi\rangle$, where λ is real.
- Commutator:
  1. If $\hat{A}$ and $\hat{B}$ do not commute then they do not admit a common set of eigenvectors.
  2. If $\hat{A}$ and $\hat{B}$ are hermitian operators corresponding to classical dynamical variables a and b, then the commutator of $\hat{A}$ and $\hat{B}$ is given by

     $$[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A} = i\hbar\{a, b\}, \tag{2}$$

     where $\{a, b\}$ is the *classical Poisson bracket.*
- Measurement:
  1. Each act of measurement of an observable $\hat{A}$ of a system in state $|\Psi\rangle$ collapses the system to an eigenstate $|\psi_i\rangle$ of $\hat{A}$ with probability $|\langle\phi_i|\Psi\rangle|^2$.
  2. The average or the expectation value of $\hat{A}$ is given by

     $$\langle\hat{A}\rangle = \sum_i \lambda_i |\langle\phi_i|\Psi\rangle|^2 = \langle\Psi|\hat{A}|\Psi\rangle,$$

     where λ_i is the eigenvalue of $\hat{A}$ corresponding to the eigenstate $|\psi_i\rangle$.

II. DENSITY OPERATOR

For the quantum mechanical description, if we know that the system is in state $|\psi\rangle$, then an operator $\hat{O}$ has the expectation value,

$$\langle \hat{O} \rangle_{\rm qm} = \langle \psi | \hat{O} | \psi \rangle.$$

But, typically, we do not know that we are in state $|\psi\rangle$, then an *ensemble average* must be performed,

$$\langle \langle \hat{O} \rangle_{\rm qm} \rangle_{\rm ensemble} = \sum_n P_n \langle \psi_n | \hat{O} | \psi_n \rangle,$$

where the P_n is the probability of being in the state $|\psi_n\rangle$ and we introduce a density operator,

$$\hat{\rho} = \sum_n P_n |\psi_n\rangle\langle\psi_n|.$$

The expectation value of any operator $\hat{O}$ is given by,

$$\langle \hat{O} \rangle_{\rm qm} = {\rm Tr}[\hat{\rho}\,\hat{O}],$$

where Tr stands for trace.

A. Positive-semi-definite of Density Matrix:

The density operator is strictly *non-negative*, that is it has only non-negative eigenvalues, because for all $|\psi\rangle$,

$$\langle \psi | \hat{\rho} | \psi \rangle = \sum_n P_n |\langle \psi_n | \psi_n \rangle|^2 \geq 0.$$

Or equivalently, for A $n \times n$ Hermitian complex matrix $\mathcal{M}$ is said to be *positive-semi-definite* or or *non-negative definite* if

$$\vec{x}^* \, \mathcal{M} \, \vec{x} \geq 0, \qquad \text{for all} \quad \vec{x} \in \mathbb{C}^n,$$

where $\vec{x}^*$ is the conjugate transpose of $\vec{x}$.
Representing $\hat{\rho}$ in the eigenbasis, the eigenvalues of $\hat{\rho}$ can be interpreted as probabilities (because they must be normalized and non-negative) for the eigenstates.

However, for mixed states, there is no unique way of telling whether statistical fluctuations of observed quantities are caused

- by fluctuations in the state preparation (due to the lack of knowledge), or
- by fluctuations caused by the measurement process (due to the lack of complete control).

B. Von Neumann entropy:

How can we discriminate pure from mixed states, or more generally, characterize the purity of a state? One option is the *von Neumann entropy*, i.e.,

$$S = -k_B \, \mathrm{tr}[\hat{\rho} \, \ln \hat{\rho}],$$

where k_B denotes the Boltzmann constant.

- $S(\rho)$ is zero if and only if ρ represents a pure state.
- $S(\rho)$ is maximal and equal to $\ln N$ for a maximally mixed state, N being the dimension of the Hilbert space.
- $S(\rho)$ is invariant under changes in the basis of ρ, that is, $S(\rho) = S(\hat{U}\rho\hat{U}^\dagger)$, with $\hat{U}$ a unitary transformation.
- $S(\rho)$ is additive for independent systems. Given two density matrices ρ_A, ρ_B describing independent systems A and B, we have

$$S(\rho_A \otimes \rho_B) = S(\rho_A) + S(\rho_B).$$

C. Purity of quantum states:

In quantum mechanics, and especially quantum information theory, the purity of a normalized quantum state is a scalar defined as

$$\gamma \equiv \mathrm{tr}[\hat{\rho}^2],$$

where $\hat{\rho}$ is the density matrix of the state. The purity defines a measure on quantum states, giving information on how much a state is mixed.

- The purity of a normalized quantum state satisfies

$$\frac{1}{d} \leq \gamma \leq 1,$$

  where d is the dimension of the Hilbert space upon which the state is defined.
- The upper bound is obtained by $\mathrm{tr}(\rho) = 1$ and

$$\mathrm{tr}(\hat{\rho}^2) \leq tr(\hat{\rho}) = 1.$$

D. Purity and entanglement in 2-qubits

A 2-qubits pure state $|\psi\rangle_{AB} \in H_A \otimes H_B$ can be written (using Schmidt decomposition) as $|\psi\rangle_{AB} = \sum_j \lambda_j |j\rangle_A |j\rangle_B$, where $\{|j\rangle_A\}, \{|j\rangle_B\}$ are the bases of H_A, H_B respectively, and $\sum_j \lambda_j^2 = 1, \lambda_j \geq 0$. Its density matrix is

$$\rho^{AB} = \sum_{i,j} \lambda_i \lambda_j |i\rangle_A \langle j|_A \otimes |i\rangle_B \langle j|_B.$$

- The degree in which it is entangled is related to the purity of the states of its subsystems,

  $$\rho_A = tr_B(\rho_{AB}) = \sum_j \lambda_j^2 |j\rangle_A \langle j|_A,$$

  and similarly for ρ_B.
- If this initial state is separable (i.e. there's only a single $\lambda_j \neq 0$, then ρ_A and ρ_B are both pure.
- Otherwise, this state is entangled and ρ_A, ρ_B are both mixed.
- For 2-qubits (pure or mixed) states, the Schmidt number (number of Schmidt coefficients) is at most 2.
- Using this and Peres–Horodecki criterion (for 2-qubits), a state is entangled if its *partial transpose* has at least one negative eigenvalue.
- The Peres–Horodecki criterion is a necessary condition, for the joint density matrix ρ of two quantum mechanical systems A and B, to be separable.
- It is also called the PPT criterion, for positive partial transpose.
- In the $2x2$ and $2x3$ dimensional cases the condition is also sufficient. It is used to decide the separability of mixed states, where the Schmidt decomposition does not apply.
- In higher dimensions, the test is inconclusive, and one should supplement it with more advanced tests, such as those based on *entanglement witnesses*
- In the context of localization, a quantity closely related to the purity, the so-called inverse participation ratio (IPR) turns out to be useful. It is defined as the inverse of the integral (or sum for finite system size) over the square of the density in some space, e.g., real space, momentum space, or even phase space, where the densities would be the square of the real space wave function $|\psi(x)|^2$, the square of the momentum space wave function

  $$|\tilde{\psi}(k)|^2,$$

  or some phase space density like the Husimi distribution, respectively.

III. UNCERTAINTY RELATION

1. Non-commuting observable do not admit common eigenvectors.
2. Non-commuting observables can not have definite values simultaneously.
3. Simultaneous measurement of non-commuting observables to an arbitrary degree of accuracy is thus *incompatible*.
4. Variance: one can define

$$\Delta\hat{A}^2 = \langle\Psi|(\hat{A} - \langle\hat{A}\rangle)^2|\Psi\rangle = \langle\Psi|\hat{A}^2|\Psi\rangle - \langle\Psi|\hat{A}|\Psi\rangle^2.$$

5. For any two non-commuting observables,

$$[\hat{A}, \hat{B}] = i\hat{C},$$

we have the *uncertainty relation*:

$$\Delta A^2 \Delta B^2 \geq \frac{1}{4}[\langle\hat{F}\rangle^2 + \langle\hat{C}\rangle^2],$$

where

$$\hat{F} = \hat{A}\hat{B} + \hat{B}\hat{A} - 2\langle\hat{A}\rangle\langle\hat{B}\rangle,$$

where the operator $\hat{F}$ is a measure of correlations between $\hat{A}$ and$\hat{B}$.

For example, take the operators $\hat{A} = \hat{q}$ (position) and $\hat{B} = \hat{p}$ (momentum) for a free particle, one have

$$[\hat{q}, \hat{p}] = i\hbar \rightarrow \langle\Delta\hat{q}^2\rangle\langle\Delta\hat{p}^2\rangle \geq \frac{\hbar^2}{4}.$$

IV. SCHRÖDINGER EQUATION

The time evolution of a state $|\Psi\rangle$ is governed by the Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \hat{H}(t)|\Psi(t)\rangle, \tag{3}$$

where $\hat{H}(t)$ is the Hamiltonian, which is a hermitian operator associated with the total energy of the system. The solution of the Schrödinger equation is,

$$\begin{aligned} |\Psi(t)\rangle &= \overleftarrow{T}\exp[-\frac{i}{\hbar}\int_{t_0}^{t} \mathrm{d}\tau \hat{H}(\tau)]|\Psi(0)\rangle & (4) \\ &\equiv \hat{U}_S(t,t_0)|\Psi(t_0), & (5) \end{aligned}$$

where $(\overleftarrow{T})$ is the time-ordering operator. In the *Schrödinger picture*: the state is time-dependent, with the time-dependent coefficients; while the operators are time-independent. That is the time evolution of the states is described by

$$|\Psi(r,t)\rangle = \sum_i \alpha_i(t)|\psi_i(r)\rangle. \tag{6}$$

V. HEISENBERG EQUATION

Since the quantities of physical interest are the expectation values of operators, we can work in the *Heisenberg picture*, where

$$\langle\Psi(t)|\hat{A}|\Psi(t)\rangle = \langle\Psi(t_0)|\hat{A}(t)|\Psi(t_0)\rangle, \tag{7}$$

with the time evolution of operator.

$$\hat{A}(t) = \hat{U}_S^{\dagger}(t,t_0)\hat{A}\hat{U}_S(t,t_0). \tag{8}$$

evolves according to the Heisenberg equation,

$$i\hbar\frac{d}{dt}\hat{A}(t) = [\hat{A}, \hat{H}(t)]. \tag{9}$$

VI. INTERACTION PICTURE

Consider a system described by $|\Psi(t)\rangle$ evolving under the action of a hamiltonian $\hat{H}(t)$ decomposable as,

$$\hat{H}(t) = \hat{H}_0 + \hat{H}_1(t), \tag{10}$$

where $\hat{H}_0$ is time-independent. If we define

$$|\Psi_I(t)\rangle = \exp(i\hat{H}_0 t/\hbar)|\Psi(t)\rangle, \tag{11}$$

where $|\Psi_I(t)\rangle$ evolves accords to

$$i\hbar\frac{\partial}{\partial t}|\Psi_I(t)\rangle = \hat{H}_I(t)|\Psi_I(t)\rangle, \tag{12}$$

with the new Hamiltonian contributed from the interaction,

$$\hat{H}_I(t) = \exp(i\hat{H}_0 t/\hbar)\hat{H}_1(t)\exp(-i\hat{H}_0 t/\hbar). \tag{13}$$

The evolution is in the **interaction picture** generated by $\hat{H}_0$.