

Note for *Quantum Optics*: Density Matrix

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[Reference:]

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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 $\langle\phi|\hat{A}|\phi\rangle$ is call the *trace* of \hat{A} ,

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

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

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

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 $|\psi_i\rangle$.

I. 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,

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

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

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

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,

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

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 $|\psi\rangle$,

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

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

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

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.,

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

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

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

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 $\text{tr}(\rho) = 1$ and

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

D. Examples:

1. $|\Psi\rangle = c_1|\phi_1\rangle + c_2|\phi_2\rangle$, where $\langle\phi_i|\phi_j\rangle = \delta_{ij}$, orthonormal.
2. $\langle\Psi|\Psi\rangle = 1$, normalization condition: $|c_1|^2 + |c_2|^2 = 1$.
3. Pure states: let $|\Psi\rangle = \frac{1}{\sqrt{2}}|\phi_1\rangle + \frac{1}{\sqrt{2}}|\phi_2\rangle$, then we have

$$\hat{\rho}_1 = |\phi_1\rangle\langle\phi_1| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}^{-1}; \quad (3)$$

$$\hat{\rho}_2 = |\phi_2\rangle\langle\phi_2| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}^{-1}; \quad (4)$$

$$\hat{\rho}_\Psi = |\phi_1\rangle\langle\phi_1| = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} = \begin{pmatrix} \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}^{-1}; \quad (5)$$

4. Mixed states: let $\hat{\rho}_{mix} = \frac{1}{2}\hat{\rho}_1 + \frac{1}{2}\hat{\rho}_2$, then we have

$$\hat{\rho}_{mix} = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{d} \bar{I}_d; \quad (d=2) \quad (6)$$

$$= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}^{-1}; \quad (7)$$

5. Purity:

$$\text{tr}(\hat{\rho}_1^2) = 1; \quad (8)$$

$$\text{tr}(\hat{\rho}_2^2) = 1; \quad (9)$$

$$\text{tr}(\hat{\rho}_{\Psi}^2) = 1; \quad (10)$$

$$\text{tr}(\hat{\rho}_{mix}^2) = 1/2; \quad (11)$$

$$(12)$$

II. POISSON DISTRIBUTION

Coherent state $|\alpha\rangle$ has the Poisson distribution in the photon number,

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle. \quad (13)$$

A. i.i.d. limit:

For photons are *independent* of each other, the probability of occurrence of n photons, or photoelectrons in a time interval T is random. Divide the time period T into N intervals, the probability to find one photon per interval is, $p = \bar{n}/N$; while the probability to find no photon per interval is, $1 - p$. Then we have the probability to find n photons per interval is,

$$P(n) = \frac{N!}{n!(N-n)!} p^n (1-p)^{N-n}, \quad (14)$$

which is a *binomial distribution*.

By substituting $p = \bar{n}/N$, we have

$$P(n) = \frac{1}{n!} \frac{N!}{(N-n)! N^n} \bar{n}^n \left(1 - \frac{\bar{n}}{N}\right)^{N-n}. \quad (15)$$

Stirling's formula:

$$\ln(N!) = \ln 1 + \ln 2 + \dots + \ln N, \quad (16)$$

$$\approx \int_1^N \ln x dx, \quad i.e., \quad \int \ln x dx = x \ln x - x, \quad (17)$$

$$= N \ln N - N + 1, \quad (18)$$

$$\approx N \ln N - N. \quad (19)$$

When the number of photons is large enough, *i.e.*, $N \rightarrow \infty$, one has

$$\lim_{N \rightarrow \infty} \ln \left(\frac{N!}{(N-n)! N^n} \right) = N \ln N - N - N \ln(N-n) + n \ln(N-n) + N - n - n \ln N, \quad (20)$$

$$= 0, \quad \text{note: } N \gg n, \quad (21)$$

or

$$\lim_{N \rightarrow \infty} \left(\frac{N!}{(N-n)! N^n} \right) = 1. \quad (22)$$

In the same way,

$$\left(1 - \frac{\bar{n}}{N}\right)^{N-n} = 1 - (N-n)\frac{\bar{n}}{N} + \frac{1}{2!}(N-n)(N-n-1)\left(\frac{\bar{n}}{N}\right)^2 + \dots, \quad (23)$$

$$\approx 1 - \frac{\bar{n}}{1!} + \frac{\bar{n}^2}{2!} - \dots, \quad (24)$$

$$= e^{-\bar{n}}. \quad (25)$$

In the limit, $N \rightarrow \infty$, the probability for photon number becomes

$$P(n) = \frac{\bar{n}^n \exp(-\bar{n})}{n!}, \quad (26)$$

$$= \frac{|\alpha|^{2n} \exp(-|\alpha|^2)}{n!}, \quad (27)$$

where $\bar{n} \equiv |\alpha|^2$. This is the *Poisson distribution* and the characteristics of coherent light. Note that

$$\sum_{n=0}^{\infty} P(n) = 1. \quad (28)$$

B. Mean and Variance

The probability of finding the photon number n in the *Poisson distribution* is

$$P(n) \equiv |\langle n|\alpha\rangle|^2 = \frac{e^{-|\alpha|^2} |\alpha|^{2n}}{n!}, \quad (29)$$

for which the mean and variance of photon number are,

$$\langle \hat{n} \rangle = \sum_n n P(n) = |\alpha|^2 \equiv \bar{n}, \quad (30)$$

$$\langle \Delta \hat{n}^2 \rangle = \langle \hat{n}^2 \rangle - \langle \hat{n} \rangle^2 = |\alpha|^2 = \langle \hat{n} \rangle. \quad (31)$$

III. THERMAL STATES

By applying density matrix for the mixed states, we define the *thermal states* as

$$\rho_{th} = \sum_n P(n) |n\rangle\langle n|, \quad (32)$$

$$\text{with } P(n) = \frac{1}{\bar{n} + 1} \left(\frac{\bar{n}}{\bar{n} + 1}\right)^n, \quad \bar{n} = \frac{1}{\exp[\hbar\omega/k_B T] - 1}. \quad (33)$$

A. Boltzmann's law

In the quantized EM fields, the eigen-energies of photons are discrete,

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right).$$

Accordingly to the Boltzmann's law, the probability to find a state with the energy E_n is proportional to

$$P(n) \propto \exp[-E_n/k_B T],$$

where T denotes the temperature, and k_B is the Boltzmann's constant. Then, to find n photons in the mode with the energy E_n is

$$P(n) = \frac{\exp[-E_n/k_B T]}{\sum_{n=0}^{\infty} \exp[-E_n/k_B T]}, \quad (34)$$

$$= \exp[-E_n/k_B T] (1 - \exp[-\hbar\omega/k_B T]); \quad E_n = n \hbar\omega \quad (35)$$

The mean photon number following Boltzmann's law is

$$\bar{n} = \sum_{n=0}^{\infty} n P(n) = \frac{1}{\exp[\hbar\omega/k_B T] - 1}, \quad (36)$$

which gives the *Planck formula*. In terms of the mean photon number \bar{n} , the probability to find n photons is

$$P(n) = \frac{1}{\bar{n} + 1} \left(\frac{\bar{n}}{\bar{n} + 1} \right)^n, \quad (37)$$

which is called the *Bose-Einstein distribution*, and used as the distribution function for the *thermal light source* from the black-body radiations.

The variance of the Bose-Einstein distribution is

$$\Delta n^2 = \bar{n} + \bar{n}^2, \quad (38)$$

which is larger than that of a Poisson distribution.

B. Thermal light

The electromagnetic radiation emitted by a hot body is generally called *thermal light*, or *black-body radiance*. The energy density within the angular frequency range ω to $\omega + d\omega$ is given by the Planck's law:

$$\rho(\omega, T) = \text{DOS} \cdot \text{mean number of photons} \cdot \text{energy per photon } d\omega, \quad (39)$$

$$= \frac{\hbar\omega^2}{\pi^2 c^3} \hbar\omega \bar{n} d\omega, \quad (40)$$

$$= \frac{\hbar\omega^3}{\pi^2 c^3} \frac{1}{\exp[\hbar\omega/k_B T] - 1} d\omega. \quad (41)$$

C. Statistics

Follow the Boltzmann's law, the expectation value the energy is given by

$$\langle E \rangle = \sum_n E_n P(E_n) = \frac{\sum_n E_n \exp[-E_n/k_B T]}{\sum_n \exp[-E_n/k_B T]}. \quad (42)$$

Here the energy is quantized, $E_n = n\hbar\omega$. We can define the variable

$$\beta \equiv \frac{1}{k_B T},$$

and take the partial derivative of the mean energy with respect to β , that is,

$$\frac{\partial \langle E \rangle}{\partial \beta} = -\langle E^2 \rangle + \langle E \rangle^2. \quad (43)$$

Then, we can find the variance of energy

$$\langle \Delta E^2 \rangle = -\frac{\partial \langle E \rangle}{\partial \beta} = k_B T^2 \frac{\partial \langle E \rangle}{\partial T}. \quad (44)$$

D. Wave noise

If we replace the mean energy by the density of state, *i.e.*, $\langle E \rangle = V\rho(\omega, T) d\omega$, with the volume V , then

$$\langle \Delta E^2 \rangle d\omega = -\frac{\partial \langle E \rangle}{\partial \beta} d\omega = -V \frac{\partial \langle \rho \rangle}{\partial \beta} d\omega. \quad (45)$$

By substituting

$$\rho(\omega, T) = \frac{\hbar\omega^3}{\pi^2 c^3} \frac{1}{\exp[\hbar\omega/k_B T] - 1},$$

we have

$$\langle \Delta E^2 \rangle d\omega = V \left[\hbar\omega\rho + \frac{\pi^2 c^3}{\omega^2} \rho^2 \right] d\omega. \quad (46)$$

The energy fluctuations can be connected to the photon number fluctuations per mode through

$$\langle \Delta E^2 \rangle d\omega = \text{DOS} \cdot \text{variance of photon number} \cdot \text{energy per mode} \cdot \text{total volume}, \quad (47)$$

$$= g(\omega) d\omega \Delta n^2 (\hbar\omega)^2 V. \quad (48)$$

In comparison, we have

$$\Delta n^2 = \frac{\pi^2 c^3}{\hbar\omega^3} \rho + \left(\frac{\pi^2 c^3}{\hbar\omega^3} \rho \right)^2, \quad (49)$$

$$\equiv \bar{n} + \bar{n}^2, \quad (50)$$

with the assignment

$$\bar{n} = \frac{\pi^2 c^3}{\hbar\omega^3} \rho. \quad (51)$$

The second term in the number fluctuations has its origin from the classical radiation, which is call the *wave noises*.