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1 Overview

In the last lecture, we defined separable Hilbert spaces, bounded operators, operator norms, C^* -algebra, the spectrum of bounded operators, and self-adjoint and positive operators.

In this lecture, we discuss continuous functional calculus, polar decomposition of compact bounded operators, unitary operators, exponential maps, trace-class operators, trace norm, Hilbert–Schmidt operators. We point readers to [HZ11, Att] for background on topics covered in this lecture.

2 Properties of bounded linear operators

In this section, we continue our discussion on the properties of bounded linear operators. We begin by showing that in a limiting sense, the square root of any bounded positive semi-definite (PSD) operator can be defined.

2.1 Square root of a bounded positive semi-definite operator

Unlike the case of finite-dimensional Hilbert spaces, a bounded self-adjoint operator acting on an infinite-dimensional separable Hilbert space need not have a spectral decomposition. We will discuss later that the spectral decomposition only holds for a subclass of bounded linear operators that are called *compact* bounded operators. We recall from the previous lecture that a bounded operator may not necessarily have eigenvalues, but it has a spectrum.

Let \mathcal{H} denote a separable Hilbert space, let $\mathcal{L}(\mathcal{H})$ denote the set of bounded operators, and let $\mathcal{L}_S(\mathcal{H})$ denote the set of bounded self-adjoint operators. An operator $T \in \mathcal{L}(\mathcal{H})$ is positive semi-definite (PSD) if $\langle \psi | T \psi \rangle \geq 0, \forall \psi \in \mathcal{H}$. Moreover, PSD operators are also self-adjoint operators.

Lemma 1. *Let $T \in \mathcal{L}_S(\mathcal{H})$ be a bounded PSD operator. Then there is a unique bounded PSD operator \sqrt{T} satisfying $(\sqrt{T})^2 = T$.*

Proof. Instead of giving a complete proof, we just provide a sketch of the proof here. We point readers to [Att] for a detailed review of the proof.

As discussed in the previous lecture, if T is a self-adjoint operator, then the spectrum of T exists. Let $\sigma(T)$ denote the spectrum of T . In particular, if T is a PSD operator, then $\sigma(T) \subset \mathbb{R}_{\geq 0}$.

For an operator A acting on a finite-dimensional Hilbert space, one can find \sqrt{A} by applying the square-root function on eigenvalues. Although the same notion of functional calculus may not hold for bounded operators acting on a separable Hilbert space, we can approximate the square root of an operator by using polynomial functions. For the proof sketch, we recall the key properties of bounded operators. The operator norm of a bounded operator is finite. Moreover, from the homogeneity and triangle inequality of the operator norm, any linear combination of bounded operators is bounded. Furthermore, from the submultiplicativity of the operator norm, the multiplication of two bounded operators is also bounded.

The continuous functional calculus can be applied to any bounded operator. Let p denote a polynomial function. Then a polynomial function of a bounded operator T is defined as $p(T)$. For example, $p(T) = T + 2T^2 + 4T^3$ is a well defined polynomial function of T .

We now state an important theorem concerning the uniform convergence of polynomial functions to an arbitrary continuous function on a bounded interval.

Stone-Weierstrass theorem: Suppose f is a continuous real-valued function defined on the real interval $x \in [a, b]$. Then for every $\varepsilon > 0$, $\exists N_\varepsilon \in \mathbb{Z}^+$, such that $\forall n > N_\varepsilon$, the following holds

$$|p_n(x) - f(x)| \leq \varepsilon, \forall x \in [a, b], \quad (1)$$

where p_n denotes a polynomial function with degree n .

The basic idea is that there exists a sequence of polynomials $\{p_n\}_n$, such that a continuous function f can be defined as a limit of this sequence.

We now argue that there exists an explicit construction of the sequence of polynomials approximating a continuous function f . Let f denote a continuous function on the interval $x \in [0, 1]$. Consider the following Bernstein polynomial:

$$B_n(f)(x) = \sum_{k=0}^n f\left(\frac{k}{n}\right) \binom{n}{k} x^k (1-x)^{n-k}. \quad (2)$$

By using the law of large numbers and Chebyshev's inequality, it can be shown that $B_n(f)$ converges uniformly to f , i.e.,

$$\lim_{n \rightarrow \infty} \sup\{|B_n(f)(x) - f(x)| : x \in [0, 1]\} = 0. \quad (3)$$

As discussed earlier, for a PSD operator T , $\sigma(T) \in [0, \|T\|]$. Moreover, the function $f : x \rightarrow \sqrt{x}$ is continuous on $\sigma(T)$. Therefore, \sqrt{T} can be defined as a limit of the sequence of Bernstein polynomials. Moreover, it can be shown that \sqrt{T} is unique. \square

2.2 Compactness of bounded operators

Definition 2. A bounded operator $T \in \mathcal{L}(\mathcal{H})$ is compact if for all bounded sequences $\{\psi_n\}_n$, $\{\|T\psi_n\|\}_n$ has a convergent subsequence. Equivalently, $T \in \mathcal{L}(\mathcal{H})$ is compact if for all orthonormal bases $\{\psi_j\}_j$,

$$\lim_{j \rightarrow \infty} \|T\psi_j\| = 0. \quad (4)$$

2.3 Absolute value of a bounded operator

In Section 2.1, we showed that every bounded operator has a unique square root. By using the square root function, the absolute value of an operator can be defined.

Definition 3. Let $T \in \mathcal{L}(\mathcal{H})$. The absolute value of the operator T is defined as

$$|T| \equiv \sqrt{T^\dagger T}. \quad (5)$$

2.4 Polar decomposition of bounded operators

The absolute value of a bounded operator as defined in Section 2.3 can be used to define the polar decomposition of bounded operators.

Lemma 4. Let $T \in \mathcal{L}(\mathcal{H})$. Then there exists a bounded operator $V \in \mathcal{L}(\mathcal{H})$ such that $T = V|T|$, where $\|V\psi\| = \|\psi\|, \forall \psi \in \text{supp}(V)$.

Proof. Consider the following chain of equalities for all $\psi, \phi \in \mathcal{H}$.

$$\langle |T|\psi ||T|\phi \rangle = \langle \psi ||T|^2 \phi \rangle \quad (6)$$

$$= \langle \psi | T^\dagger T \phi \rangle \quad (7)$$

$$= \langle T\psi | T\phi \rangle. \quad (8)$$

The first equality follows from the definition of the adjoint of $|T|$ and from the fact that $|T|^\dagger = |T|$. The second equality follows from the definition of the absolute value of T as defined in (5). The last equality follows from the definition of the adjoint of T^\dagger .

Therefore, the mapping is such that all inner products are preserved, i.e., the mapping is an isometry. This completes the proof. \square

We note that the isometry V in Lemma 4 is from $\text{ran}(|T|)$ to $\text{ran}(T)$. Moreover, it is a partial isometry in the sense that it is 0 for all the vectors in $\text{ran}^\perp(|T|)$.

2.4.1 Polar decomposition of compact bounded operators

In Lemma 4, we showed that for a bounded operator T , there exists an isometry V , such that $T = V|T|$. In this section, we argue that for a compact bounded operator, an explicit form of V can be defined in terms of orthonormal basis vectors.

Let $T \in \mathcal{L}(\mathcal{H})$ be a compact bounded operator. Then

$$T = \sum_{n=0}^{\infty} \lambda_n |\phi_n\rangle \langle \psi_n|, \quad (9)$$

where the sequence $\{\lambda_n\}_n \subset R^+ \setminus \{0\}$ is either finite or converges to zero, and $\{|\phi_n\rangle\}_n$ and $\{|\psi_n\rangle\}_n$ are orthonormal basis elements.

Then $|T|$ is given by

$$|T| = \sum_{n=0}^{\infty} \lambda_n |\psi_n\rangle\langle\psi_n|. \quad (10)$$

Moreover, an isometry V such that $T = V|T|$, is defined as

$$V = \sum_{n=0}^{\infty} |\phi_n\rangle\langle\psi_n|. \quad (11)$$

2.5 Unitary operators

We recall the definition of isomorphism from previous lectures. U is an isomorphism if the following holds for all $\phi, \psi \in \mathcal{H}$:

$$\langle U\phi | U\psi \rangle = \langle \phi | \psi \rangle. \quad (12)$$

Moreover, the operator norm of U is defined as

$$\|U\| = \sup_{\psi: \|\psi\|=1} \|U\psi\| = 1. \quad (13)$$

The first equality follows from the definition of the operator norm. The second equality follows from (12) by setting $\phi = \psi$.

Definition 5 (Unitary operators). A bounded operator $U \in \mathcal{L}(\mathcal{H})$ is unitary if $UU^\dagger = U^\dagger U = I$.

Theorem 6. *Let U be a linear map on \mathcal{H} . Then following assertions are equivalent:*

1. U is an isomorphism.
2. U is an onto isometry.
3. U is bounded and $UU^\dagger = U^\dagger U = I$.

Proof. 1. \Rightarrow 2.: It follows from (12) by picking $\phi = \psi$, so that $\|U\psi\| = \|\psi\|, \forall \psi \in \mathcal{H}$. Therefore, U is an onto isometry.

2. \Rightarrow 3.: Since U is an isometry, then for all $\psi, \phi \in \mathcal{H}$, the following holds

$$\|U\psi - U\phi\| = \|\psi - \phi\|. \quad (14)$$

Therefore, $U\phi = U\psi$ if and only if $\psi = \phi$, which implies that U is a bijective map.

Let $\phi \in \mathcal{H}$. Consider the following chain of equalities:

$$\langle \phi | \phi \rangle = \langle U\phi | U\phi \rangle \quad (15)$$

$$= \langle \phi | U^\dagger U \phi \rangle. \quad (16)$$

The first equality follows since U is an isometry. The last equality follows from the definition of the adjoint of U . From (16), it follows that $U^\dagger U = I$. Therefore, $U^{-1} = U^\dagger$, which further implies that $UU^\dagger = I$.

3. \Rightarrow 1.: Let $U \in \mathcal{L}(\mathcal{H})$, such that $U^\dagger U = UU^\dagger = I$. Then for all $\psi, \phi \in \mathcal{H}$, the following holds:

$$\langle \phi | \psi \rangle = \langle \phi | U^\dagger U \psi \rangle \quad (17)$$

$$= \langle U \phi | U \psi \rangle, \quad (18)$$

which implies that U is an isomorphism. \square

2.5.1 Eigenvalues of a unitary operator

Suppose that $U\psi = \lambda\psi$ for some non-zero $\psi \in \mathcal{H}$. Then

$$\langle \psi | \psi \rangle = \langle \psi | U^\dagger U \psi \rangle \quad (19)$$

$$= \langle \psi | \lambda^* \lambda \psi \rangle \quad (20)$$

$$= |\lambda|^2 \langle \psi | \psi \rangle, \quad (21)$$

which implies that $|\lambda| = 1$.

2.6 Connection between unitary and self-adjoint operators

In this section, we define the notion of exponential maps on $\mathcal{L}(\mathcal{H})$. Let $T \in \mathcal{L}(\mathcal{H})$ be a bounded operator. For $k \in \mathbb{N}$, define

$$F_k(T) \equiv \sum_{n=0}^k \frac{T^n}{n!}. \quad (22)$$

We note that $F_k(T)$ is a legitimate bounded operator for a finite k , which follows from the triangle inequality and the sub-multiplicativity of the operator norm.

Consider the following positive-valued function:

$$f_k(T) \equiv \sum_{n=0}^k \frac{\|T^n\|}{n!}, \quad (23)$$

where $T^0 = I$.

Consider the following chain of inequalities:

$$f_k(T) \leq \sum_{n=0}^k \frac{\|T\|^n}{n!} \quad (24)$$

$$\leq \sum_{n=0}^{\infty} \frac{\|T\|^n}{n!} \quad (25)$$

$$= e^{\|T\|} \quad (26)$$

$$< \infty. \quad (27)$$

The first inequality follows from the sub-multiplicativity of the operator norm. The second inequality follows as a sum of positive numbers is greater than 0. The first equality follows from the Taylor series expansion of the function e^x . The last strict inequality follows from the fact that the operator norm of a bounded operator is finite.

Form the aforementioned series of arguments, along with the triangle inequality for the operator norm, it follows that the series $\sum_{n=0}^{\infty} \frac{T^n}{n!}$ is absolutely convergent. Therefore, the exponential map of a bounded operator can be defined as

$$e^T \equiv \lim_{k \rightarrow \infty} F_k(T) . \quad (28)$$

For $T \in \mathcal{L}(\mathcal{H})$, and for all $a, b \in \mathbb{C}$, the following properties hold

$$e^{aT} e^{bT} = e^{(a+b)T} , \quad (29)$$

$$(e^{aT})^\dagger = e^{\bar{a}T^\dagger} . \quad (30)$$

For $T \in \mathcal{L}_S(\mathcal{H})$, $(e^{iT})^\dagger = e^{-iT}$, and $e^{iT} e^{-iT} = e^0 = I$, which implies that e^{iT} is a unitary operator.

2.7 Normal Operators

Definition 7 (Normal Operators). Let $T \in \mathcal{L}(\mathcal{H})$ be a bounded operator. Then T is normal if

$$TT^\dagger = T^\dagger T. \quad (31)$$

It is easy to check that both self-adjoint and unitary operators are normal operators.

For normal operators that are also compact, there is a spectral decomposition, i.e., there exists a sequence $\{\lambda_j\}_j$ of complex numbers and an orthonormal basis $\{\phi_j\}_j$ such that

$$T = \sum_{j=1}^{\infty} \lambda_j |\phi_j\rangle \langle \phi_j|. \quad (32)$$

Moreover, the action of T on a vector $|\psi\rangle \in \mathcal{H}$ is given by

$$T|\psi\rangle = \sum_{j=1}^{\infty} \lambda_j \langle \phi_j | \psi \rangle |\phi_j\rangle. \quad (33)$$

2.8 Trace-class operators

The trace is meaningful only for a subset of bounded operators.

Definition 8 (Trace of PSD operators). Let \mathcal{H} be a separable Hilbert space and $\{\phi_j\}_{j=1}^{\infty}$ be an orthonormal basis. Then for a PSD operator $T \in \mathcal{L}(\mathcal{H})$,

$$\text{Tr}\{T\} = \sum_{j=1}^{\infty} \langle \phi_j | T \phi_j \rangle. \quad (34)$$

Due to $T \geq 0$, the trace of T is a sum of non-negative numbers. Therefore, if the sum does not converge, $\text{Tr}\{T\} = \infty$.

Theorem 9. *Let $T \in \mathcal{L}(\mathcal{H})$ be a PSD operator. Then $\text{Tr}\{T\}$ does not depend on the choice of orthonormal basis.*

Proof. Let $\{\phi_j\}_{j=1}^\infty$ and $\{\psi_j\}_{j=1}^\infty$ denote two different orthonormal basis. Consider the following chain of equalities:

$$\sum_j \langle \psi_j | T \psi_j \rangle = \sum_j \|T^{1/2} \psi_j\|^2 \quad (35)$$

$$= \sum_j \sum_k |\langle \phi_k | T^{1/2} \psi_j \rangle|^2 \quad (36)$$

$$= \sum_k \sum_j |\langle \psi_j | T^{1/2} \phi_k \rangle|^2 \quad (37)$$

$$= \sum_k \|T^{1/2} \phi_k\|^2 \quad (38)$$

$$= \sum_k \langle \phi_k | T \phi_k \rangle. \quad (39)$$

The first equality follows from Lemma 1. The second equality follows from Parseval's formula for the norm of a vector. The third equality follows from Tonelli's theorem. The fourth equality follows again from Parseval's formula. \square

Definition 10 (Trace-class operators). A bounded operator $T \in \mathcal{L}(\mathcal{H})$ is trace-class if

$$\text{Tr}\{|T|\} < \infty. \quad (40)$$

We denote the trace class operators acting on a separable Hilbert space \mathcal{H} by $\mathcal{T}(\mathcal{H})$. We now provide two examples of bounded operators that are not trace-class operators.

Example 11. The identity operator I is bounded but is not a trace-class operator since $\text{Tr}\{|I|\} = \infty$.

Example 12. Let A denote a shift operator. Then $|A| = (A^\dagger A)^{1/2} = I^{1/2} = I$, which implies that

$$\sum_j \langle \delta_j | \sqrt{A^\dagger A} \delta_j \rangle = \sum_j \langle \delta_j | I \delta_j \rangle \quad (41)$$

$$= \infty. \quad (42)$$

Therefore, A is not a trace-class operator.

Theorem 13. *Let $T \in \mathcal{T}(\mathcal{H})$ and let $\{\phi_j\}_{j=1}^\infty$ be an orthonormal basis. Then $\text{Tr}\{T\} = \sum_{j=1}^\infty \langle \phi_j | T \phi_j \rangle$ is the trace of the operator T and is independent of the basis chosen.*

Proof. We begin by showing that every trace-class operator is compact. Let T be a positive trace-class operator. Let $\{\phi_j\}_{j=1}^\infty$ be an orthonormal basis. Consider the following chain of inequalities:

$$\sum_j \|\sqrt{T} \phi_j\|^2 = \sum_j \langle \phi_j | T \phi_j \rangle \quad (43)$$

$$= \text{Tr}\{T\} \quad (44)$$

$$< \infty. \quad (45)$$

The second equality follows from Definition 8. The strict inequality follows because T is a trace-class operator. Therefore, $\|\sqrt{T}\phi_j\| \rightarrow 0$ as $j \rightarrow \infty$, which implies that \sqrt{T} is compact, which further implies that T is compact.

Now for an arbitrary trace-class operator T , $|T|$ is also trace-class, and since $|T|$ is positive, from the aforementioned arguments it follows that $|T|$ is compact. Moreover, from the polar decomposition, $T = U|T|$, we get that T is compact.

Let $\{\psi_j\}_j$ denote an orthonormal basis. Then, from (9), a trace-class operator $T \in \mathcal{T}(\mathcal{H})$ can be written as

$$T = \sum_j \lambda_j |\psi_j\rangle\langle\phi_j|. \quad (46)$$

Consider the following chain of inequalities:

$$|\mathrm{Tr}\{T\}| = \left| \sum_k \langle\varphi_k|T\varphi_k\rangle \right| \quad (47)$$

$$\leq \sum_k |\langle\varphi_k|T\varphi_k\rangle| \quad (48)$$

$$= \sum_{k,j} \lambda_j |\langle\varphi_k|\psi_j\rangle| |\langle\phi_j|\varphi_k\rangle| \quad (49)$$

$$\leq \sum_j \lambda_j \left[\sum_k |\langle\varphi_k|\psi_j\rangle|^2 \right]^{1/2} \left[\sum_k |\langle\varphi_k|\phi_j\rangle|^2 \right]^{1/2} \quad (50)$$

$$= \sum_j \lambda_j \|\psi_j\| \|\phi_j\| \quad (51)$$

$$= \sum_j \lambda_j \quad (52)$$

$$= \mathrm{Tr}[|T|] < \infty. \quad (53)$$

The first inequality follows as the absolute value a sum is smaller than a sum of absolute values. The second equality follows from (46). The second inequality follows from the Cauchy-Schwarz inequality. The third equality follows from the Parseval's formula.

Therefore, the aforementioned arguments establish the absolute convergence of $\mathrm{Tr}\{T\}$. Then from Fubini's theorem, the following holds

$$\sum_k \langle\varphi_k|T\varphi_k\rangle = \sum_k \sum_j \lambda_j \langle\varphi_k|\psi_j\rangle \langle\phi_j|\varphi_k\rangle \quad (54)$$

$$= \sum_j \lambda_j \sum_k \langle\phi_j|\varphi_k\rangle \langle\varphi_k|\psi_j\rangle \quad (55)$$

$$= \sum_j \lambda_j \langle\phi_j|\psi_j\rangle. \quad (56)$$

Therefore, the trace does not depend on the choice of $\{|\varphi_k\rangle\}_k$.

□

Definition 14 (Trace norm). Let $T \in \mathcal{T}(\mathcal{H})$ be a trace-class operator. Then the trace norm is defined as

$$\|T\|_1 \equiv \text{Tr}\{|T|\} . \quad (57)$$

Lemma 15. Let $T \in \mathcal{T}(\mathcal{H})$. Then

$$\|T\|_1 \equiv \sup_{U \in \mathcal{U}(\mathcal{H})} |\text{Tr}[UT]|, \quad (58)$$

where $\mathcal{U}(\mathcal{H})$ denotes a set of bounded unitary operators.

The following relation holds between the operator norm and the trace norm for all $T \in \mathcal{T}(\mathcal{H})$:

$$\|T\| \leq \|T\|_1 . \quad (59)$$

Let $S \in \mathcal{L}(\mathcal{H})$ be a bounded operator. Even though $\text{Tr}\{S\}$ is not finite for all bounded operators, $\text{Tr}\{ST\}$ is finite whenever $T \in \mathcal{T}(\mathcal{H})$. It follows from the following inequality:

$$|\text{Tr}\{ST\}| \leq \|T\|_1 \|S\| , \quad (60)$$

which follows from Holder's inequality.

Definition 16 (Hilbert-Schmidt norm). Let $T \in \mathcal{L}(\mathcal{H})$. Then Hilbert-Schmidt norm of T is defined as

$$\|T\|_2 = \|T\|_{\text{HS}} \equiv \text{Tr}\{T^\dagger T\}^{1/2} . \quad (61)$$

Moreover, Hilbert-Schmidt operators are those for which

$$\|T\|_2 < \infty. \quad (62)$$

The following relation holds between different norms of operators acting on a separable Hilbert space.

$$\|T\| \leq \|T\|_2 \leq \|T\|_1 . \quad (63)$$

Moreover, from Cauchy-Schwarz inequality, we get

$$|\text{Tr}\{ST\}|^2 \leq \|S\|_2^2 \|T\|_2^2 . \quad (64)$$

References

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1 Overview

In the last lecture, we discuss continuous functional calculus, polar decomposition of compact bounded operators, unitary operators, exponential maps, trace-class operators, trace norm, Hilbert–Schmidt operators.

In this lecture, we discuss norm topology, weak operator topology, spectral and singular value decompositions for compact operators, duality of trace-class and bounded operators, effects, partial trace, quantum channels, Stinespring dilations, and operator-norm forms. We point readers to [HZ11, Att] for background on topics covered in this lecture.

2 Different notions of convergence

In this section, we discuss different notions of convergence for a sequence of bounded operators to another bounded operator.

Definition 1 (Convergence with respect to uniform topology). Let $\{T_n\}_n \subset \mathcal{L}(\mathcal{H})$ denote sequence of bounded operators and let $T \in \mathcal{L}(\mathcal{H})$ be a bounded operator. Then the sequence $\{T_n\}_n$ converges to T with respect to the uniform or norm topology if

$$\lim_{n \rightarrow \infty} \|T_n - T\| = 0. \quad (1)$$

Definition 2 (Convergence with respect to weak operator topology). Let $\{T_n\}_n \subset \mathcal{L}(\mathcal{H})$ denote sequence of bounded operators and let $T \in \mathcal{L}(\mathcal{H})$ be a bounded operator. Then the sequence $\{T_n\}_n$ converges to T with respect to the weak operator topology if for all $\psi, \phi \in \mathcal{H}$

$$\lim_{n \rightarrow \infty} |\langle \phi | T_n \psi \rangle - \langle \phi | T \psi \rangle| = 0 \quad (2)$$

Proposition 3. *If a sequence $\{T_j\}_j \subset \mathcal{L}(\mathcal{H})$ converges to $T \in \mathcal{L}(\mathcal{H})$ in norm topology, then it also converges to T weakly.*

Proof. For all $\psi, \phi \in \mathcal{H}$, we have that

$$|\langle \phi | T_j \psi \rangle - \langle \phi | T \psi \rangle| = |\langle \phi | (T_j - T) \psi \rangle| \quad (3)$$

$$\leq \|\phi\| \|\psi\| \|T_j - T\|. \quad (4)$$

The equality follows from the linearity of operators. The inequality follows from Cauchy-Schwarz inequality and from the definition of the operator norm.

Therefore, if $\lim_{j \rightarrow \infty} \|T_j - T\| = 0$, then it follows that $\lim_{j \rightarrow \infty} |\langle \phi | T_j \psi \rangle - \langle \phi | T \psi \rangle| = 0$. \square

We now show an example of a sequence of operators that converges to another operator weakly but does not converge in norm topology.

Example 4. Let $\{\Pi_j\}_j$ be a sequence of orthogonal projections. Let $\{\phi_j\}_{j=1}^\infty$ be an orthonormal basis. Then Π_j is projection onto $\text{span}\{\phi_k : k \in \{1, \dots, j\}\}$. Then consider that

$$|\langle \varphi | \Pi_j \psi \rangle - \langle \varphi | \psi \rangle| = |\langle \varphi | (I - \Pi_j) | \psi \rangle|. \quad (5)$$

We now write $|\psi\rangle$ as $|\psi\rangle = \sum_{j=1}^\infty \alpha_j |\phi_j\rangle$. Then $(I - \Pi_j)|\psi\rangle = \sum_{l=j+1}^\infty \alpha_l |\phi_l\rangle$, so that

$$|\langle \varphi | (I - \Pi_j) | \psi \rangle| = |\langle \phi | \sum_{l=j+1}^\infty \alpha_l |\phi_l\rangle| \quad (6)$$

$$\leq \|\phi\| \sum_{l=j+1}^\infty |\alpha_l|^2. \quad (7)$$

Since $\lim_{j \rightarrow \infty} \sum_{l=j+1}^\infty |\alpha_l|^2 = 0$, it implies that $\{\Pi_j\}_j$ converges to I in weak operator topology.

On the other hand, for a fixed j , $\|I - \Pi_j\| = 1$, by picking some unit vector in the space spanned by $I - \Pi_j$. Therefore,

$$\lim_{j \rightarrow \infty} \|I - \Pi_j\| = 1, \quad (8)$$

which implies that $\{\Pi_j\}_j$ does not converge to I in norm topology.

Definition 5 (Equivalence of two bounded operators). For operators $A, B \in \mathcal{L}(\mathcal{H})$, if $A = B$, then it should be understood in the weak sense, i.e., $\langle \phi | A \psi \rangle = \langle \phi | B \psi \rangle, \forall \phi, \psi \in \mathcal{H}$.

3 Duality of bounded operators and trace class operators

Definition 6 (Linear functional). A linear mapping f from a complex vector space V to \mathbb{C} is called a linear functional.

Definition 7 (Dual space of a vector space). Let V denote a normed vector space and let V^* denote the set of all continuous linear functionals. Then V^* is called the dual space of V .

A norm on V^* is defined as

$$\|f\| = \sup_{\|v\|=1} |f(v)|. \quad (9)$$

Theorem 8 (Riesz representation theorem). Let $f \in \mathcal{H}^*$. Then there exists a unique vector $\phi \in \mathcal{H}$ such that $f(\psi) = \langle \phi | \psi \rangle$. Moreover, $\|f\| = \|\phi\|$.

We now extend the discussion on the dual space of trace-class operators. Let $S \in \mathcal{L}(\mathcal{H})$ and let $T \in \mathcal{T}(\mathcal{H})$. Then a linear functional f_S on $\mathcal{T}(\mathcal{H})$ can be defined as

$$f_S(T) = \text{Tr}\{ST\}. \quad (10)$$

Theorem 9. *The mapping $S \rightarrow f_S$ is a linear bijection from $\mathcal{L}(\mathcal{H})$ to $\mathcal{T}(\mathcal{H})^*$, and $\|S\| = \|f_S\|, \forall S \in \mathcal{L}(\mathcal{H})$.*

Moreover, we can conclude the following:

1. $S \geq 0 \Leftrightarrow f_S(T) \geq 0, \forall T \geq 0$.
2. $S = S^\dagger \Leftrightarrow f_S(T) \in \mathbb{R}, \forall T = T^\dagger$.

4 Quantum Mechanics

4.1 Quantum states

A set $\mathcal{S}(\mathcal{H})$ of quantum states is defined as

$$\mathcal{S}(\mathcal{H}) = \{\rho \in \mathcal{T}(\mathcal{H}) : \rho \geq 0, \text{Tr}\{\rho\} = 1\}. \quad (11)$$

Theorem 10. *A quantum state $\rho \in \mathcal{S}(\mathcal{H})$ has a canonical convex decomposition of the form*

$$\rho = \sum_j \lambda_j P_j, \quad (12)$$

where $\{\lambda_j\}_j$ is a finite or an infinite sequence of positive numbers, such that $\sum_j \lambda_j = 1$, and $\{P_j\}_j$ is a set of orthogonal projections.

4.2 Effect

Effect is a mapping from the set of states $\mathcal{S}(\mathcal{H})$ to the interval $[0, 1]$, i.e., $\rho \rightarrow E(\rho) \in [0, 1]$. $E(\rho)$ is the probability of a “yes” answer to “the recorded measurement outcome belongs to a subset $X \subset \Omega$.”

Basic assumption behind an effect is the following:

$$E(\lambda\rho_1 + (1 - \lambda)\rho_2) = \lambda E(\rho_1) + (1 - \lambda)E(\rho_2), \forall \rho_1, \rho_2 \in \mathcal{S}(\mathcal{H}), \lambda \in [0, 1], \quad (13)$$

Proposition 11. *Let E be an effect. Then there exists $\hat{E} \in \mathcal{L}_S(\mathcal{H})$ such that $E(\rho) = \text{Tr}[\hat{E}\rho], \forall \rho \in \mathcal{S}(\mathcal{H})$, where $0 \leq \hat{E} \leq I$.*

4.3 Partial trace

Definition 12 (Partial trace). $\text{Tr}_A : \mathcal{T}(\mathcal{H}_A \otimes \mathcal{H}_B) \rightarrow \mathcal{T}(\mathcal{H}_B)$ is a linear mapping satisfying

$$\text{Tr}\{\text{Tr}_A\{T_{AB}\}E_B\} = \text{Tr}\{T_{AB}(I_A \otimes E_B)\}, \quad (14)$$

$\forall T_{AB} \in \mathcal{T}(\mathcal{H}_A \otimes \mathcal{H}_B)$ and $E_B \in \mathcal{L}(\mathcal{H}_B)$.

The partial trace can be calculated as follows. Let $\{\psi_j\}_j$ and $\{\phi_k\}_k$ denote orthonormal bases for \mathcal{H}_A and \mathcal{H}_B , respectively. Then

$$\mathrm{Tr}_A\{T\} = \sum_{j,k,n} \left[\langle \psi_j |_A \otimes \langle \phi_k |_B T_{AB} |\psi_j\rangle_A \otimes |\phi_n\rangle_B \right] |\phi_k\rangle \langle \phi_n |_B. \quad (15)$$

4.4 State Purification

Let $\rho_A \in \mathcal{S}(\mathcal{H})$ denote a quantum state. Then a purification of ρ_A is a vector $|\psi\rangle_{RA} \in \mathcal{H}_R \otimes \mathcal{H}_A$ such that $\mathrm{Tr}_R\{|\psi\rangle\langle\psi|_{RA}\} = \rho_A$.

A purification of ρ_A can be constructed from the spectral decomposition of ρ_A .

$$\rho = \sum_j \lambda_j |\psi_j\rangle \langle \psi_j |_A, \quad (16)$$

where $\{|\psi_j\rangle\}_j$ is an orthonormal basis, as

$$|\psi\rangle_{RA} = \sum_j \sqrt{\lambda_j} |\psi_j\rangle_R |\psi_j\rangle_A. \quad (17)$$

4.5 Quantum channels

Definition 13 (Positivity of a linear map). A linear mapping $\mathcal{N}_{A \rightarrow B} : \mathcal{T}(\mathcal{H}_A) \rightarrow \mathcal{T}(\mathcal{H}_B)$ is positive if $\mathcal{N}(T) \geq 0, \forall T \geq 0, T \in \mathcal{T}(\mathcal{H})$.

Definition 14 (Complete positivity of a linear map). A linear map $\mathcal{N}_{A \rightarrow B} : \mathcal{T}(\mathcal{H}_A) \rightarrow \mathcal{T}(\mathcal{H}_B)$ is completely positive if $\mathrm{id}_R \otimes \mathcal{N}_{A \rightarrow B}$ is positive for all finite-dimensional \mathcal{H}_R .

Definition 15 (Quantum channel). A linear map $\mathcal{N}_{A \rightarrow B} : \mathcal{T}(\mathcal{H}_A) \rightarrow \mathcal{T}(\mathcal{H}_B)$ is a quantum channel if it is completely positive and trace preserving.

Definition 16 (Adjoint of a linear map). Let $\mathcal{N}_{A \rightarrow B} : \mathcal{T}(\mathcal{H}_A) \rightarrow \mathcal{T}(\mathcal{H}_B)$ be a linear map. The adjoint $\mathcal{N}^\dagger : \mathcal{L}(\mathcal{H}_B) \rightarrow \mathcal{L}(\mathcal{H}_A)$ of a linear map \mathcal{N} is a unique linear map satisfying the following set of equations:

$$\mathrm{Tr}\{\mathcal{N}(T)E\} = \mathrm{Tr}\{T\mathcal{N}^\dagger(E)\}, \quad (18)$$

$\forall T \in \mathcal{T}(\mathcal{H})$ and $E \in \mathcal{L}(\mathcal{H})$.

4.5.1 Stinespring dilation

Definition 17. Let $\mathcal{H}_A, \mathcal{H}_B$ and \mathcal{H}_E be Hilbert spaces, and let $\mathcal{N} : \mathcal{T}(\mathcal{H}_A) \rightarrow \mathcal{T}(\mathcal{H}_B)$ be a quantum channel. An isometric extension or Stinespring dilation $V \in \mathcal{L}(\mathcal{H}_A) \rightarrow \mathcal{L}(\mathcal{H}_B \otimes \mathcal{H}_E)$ of the channel \mathcal{N} is a linear isometry such that

$$\mathcal{N}(X_A) = \mathrm{Tr}_E[V X_A V^\dagger], \quad (19)$$

for all $X_A \in \mathcal{T}(\mathcal{H}_A)$.

4.5.2 Operator-sum form

Proposition 18. *A map $\mathcal{N} : \mathcal{T}(\mathcal{H}_A) \rightarrow \mathcal{T}(\mathcal{H}_B)$ is a quantum channel if and only if there exists a sequence of bounded operators $\{A_k\}_k$ such that*

$$\mathcal{N}(T) = \sum_k A_k T A_k^\dagger, \quad (20)$$

$$\sum_k A_k^\dagger A_k = I, \forall T \in \mathcal{T}(\mathcal{H}_A).$$

References

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1 Overview

In this lecture, we work mostly with single-mode bosonic quantum systems. We first formally define photon-number states (also known as Fock states). We then introduce the annihilation and creation operators in Section 2.2 and the quadrature operators in Section 2.3. Then we study the existence of normalized eigenvectors for the introduced operators in Section 2.4. We end this lecture by developing the background for multiple-mode systems in Section 3.

2 Single-mode systems

A mode, informally, refers to a well defined degree of freedom of the system. An example of a single-mode bosonic quantum system is a photonic degree of freedom with a well defined polarization or frequency. Mathematically, a bosonic mode is described by a separable Hilbert space (that is, a Hilbert space that admits a countable orthonormal basis) equipped with canonical operators.

2.1 Photon-number states

Recall the Kronecker functions discussed earlier in Lecture 2 in the context of $l^2(\mathbb{N})$ space. Analogous to this, let us define the set $\{|n\rangle\}_{n=0}^{\infty}$ of photon-number states, which form a countable basis set for the separable Hilbert state. In second quantization, photon-number states correspond to the number of photons in a single mode of a bosonic system, that is, the number of photons in the system with particular frequency and a particular polarization. Since the photon-number states form a basis set for the separable Hilbert state, any state can be represented in terms of these states.

2.2 Annihilation and creation operators

Now, let us first define the **annihilation operator** by its action on the photon-number basis:

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle \quad \forall n \geq 1, \tag{1}$$

$$\hat{a}|0\rangle = 0. \tag{2}$$

From this, we deduce that matrix elements of the annihilation operator in the photon number basis are given as

$$\langle m | (\hat{a} |n\rangle) = \sqrt{n} \delta_{m,n-1} \quad \forall n \geq 1. \quad (3)$$

$$\langle m | (\hat{a} |n\rangle) = 0, \text{ for } n = 0. \quad (4)$$

Proposition 1. *The annihilation operator \hat{a} is an unbounded operator.*

Proof. The operator norm is defined as

$$\|\hat{a}\| = \sup_{\|\phi\|=\|\psi\|=1} |\langle \phi | \hat{a} | \psi \rangle| \quad (5)$$

Choose $|\phi\rangle = |n-1\rangle$, and $|\psi\rangle = |n\rangle$. Then,

$$|\langle \phi | \hat{a} | \psi \rangle| = \sqrt{n}. \quad (6)$$

By taking the limit $n \rightarrow \infty$, we find that

$$\sup_{\|\phi\|=\|\psi\|=1} |\langle \phi | \hat{a} | \psi \rangle| \geq \lim_{n \rightarrow \infty} \sqrt{n} = \infty. \quad (7)$$

So we conclude that $\sup_{\|\phi\|=\|\psi\|=1} |\langle \phi | \hat{a} | \psi \rangle| = \infty$. \square

Let us now define the **creation operator** \hat{a}^\dagger as the adjoint of the annihilation operator \hat{a} . We recover the action of the creation operator on $|n\rangle$, from the properties that we have established for the annihilation operator. Consider that

$$\langle m | (\hat{a}^\dagger |n\rangle) = (\hat{a} |m\rangle)^\dagger |n\rangle = \sqrt{m} \delta_{m-1,n}. \quad (8)$$

Set $m = n + 1$. Then, $\langle n + 1 | \hat{a}^\dagger |n\rangle = \sqrt{n + 1}$. Since $\langle m | \hat{a}^\dagger |n\rangle = 0$ for $m \neq n + 1$, this implies

$$\hat{a}^\dagger |n\rangle = \sqrt{n + 1} |n + 1\rangle \quad \forall n \geq 0. \quad (9)$$

We can prove that the creation operator is also unbounded by following an argument similar to the one for the annihilation operator.

Now, we obtain the canonical commutation relation (CCR) for the annihilation and creation operators:

$$[\hat{a}, \hat{a}^\dagger] = \hat{I}, \quad (10)$$

where the \hat{I} is the identity operator for the separable Hilbert space. Consider the action of $[\hat{a}, \hat{a}^\dagger]$ on an arbitrary number state $|n\rangle$:

$$[\hat{a}, \hat{a}^\dagger] |n\rangle = (\hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a}) |n\rangle = |n\rangle \quad \forall n \geq 0, \quad (11)$$

where we have skipped some algebraic steps. Since this holds for an orthonormal basis, we conclude that $[\hat{a}, \hat{a}^\dagger] = \hat{I}$. Similarly, we can obtain that $[\hat{a}^\dagger, \hat{a}] = -\hat{I}$, $[\hat{a}^\dagger, \hat{a}^\dagger] = 0$ and $[\hat{a}, \hat{a}] = 0$. We can then capture these CCR in a matrix as

$$\begin{bmatrix} [\hat{a}, \hat{a}^\dagger] & [\hat{a}, \hat{a}] \\ [\hat{a}^\dagger, \hat{a}^\dagger] & [\hat{a}^\dagger, \hat{a}] \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \otimes \hat{I} = \sigma_z \otimes \hat{I},$$

It is easy to obtain the following:

$$\hat{a}^\dagger \hat{a} |n\rangle = n |n\rangle. \quad (12)$$

So, the photon-number states $|n\rangle$ are eigenstates of $\hat{a}^\dagger \hat{a} = \hat{n}$ with eigenvalue n . Therefore, we can write

$$\hat{n} = \sum_{n=0}^{\infty} n |n\rangle \langle n|. \quad (13)$$

The operator \hat{n} is known as the photon-number operator.

2.3 Position and Quadrature operators

Let us now define the position and momentum quadrature operators as

$$\hat{x} = \frac{\hat{a} + \hat{a}^\dagger}{\sqrt{2}}, \quad \hat{p} = \frac{\hat{a} - \hat{a}^\dagger}{\sqrt{2}i}. \quad (14)$$

By definition, these are Hermitian operators and can be compactly written as

$$\begin{bmatrix} \hat{x} \\ \hat{p} \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -i & i \end{bmatrix} \begin{bmatrix} \hat{a} \\ \hat{a}^\dagger \end{bmatrix}. \quad (15)$$

By rearrangement, we obtain the following:

$$\begin{bmatrix} \hat{a} \\ \hat{a}^\dagger \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & i \\ 1 & -i \end{bmatrix} \begin{bmatrix} \hat{x} \\ \hat{p} \end{bmatrix}. \quad (16)$$

The quadrature operators \hat{x} and \hat{p} are unbounded since \hat{a} and \hat{a}^\dagger are unbounded. From the commutation relations of \hat{a} and \hat{a}^\dagger , we can work out the commutation relations of \hat{x} and \hat{p} . The CCR of the quadrature operators can then be embedded in a matrix as follows:

$$\begin{bmatrix} [\hat{x}, \hat{x}] & [\hat{x}, \hat{p}] \\ [\hat{p}, \hat{x}] & [\hat{p}, \hat{p}] \end{bmatrix} = i \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \otimes \hat{I}. \quad (17)$$

2.4 Eigenvectors of $\hat{x}, \hat{p}, \hat{a}, \hat{a}^\dagger$

In this section, we show that \hat{x} , \hat{p} , and \hat{a}^\dagger do not have normalized eigenvectors, and that the coherent states (which we define later) are the normalized eigenvectors of the annihilation operator.

Proposition 2. *The quadrature operators \hat{x} and \hat{p} do not have normalized eigenvectors.*

Proof. Suppose that $|\psi\rangle$ is an eigenvector of \hat{x} . That is,

$$\hat{x} |\psi\rangle = \lambda |\psi\rangle, \quad (18)$$

where $\lambda \in \mathbb{R}$. Now, we know that $[\hat{x}, \hat{p}] = i\hat{I}$. Next, consider that

$$\langle \psi | [\hat{x}, \hat{p}] | \psi \rangle = \langle \psi | \hat{x} \hat{p} - \hat{p} \hat{x} | \psi \rangle \quad (19)$$

$$= \langle \psi | \lambda \hat{p} - \hat{p} \lambda | \psi \rangle = 0. \quad (20)$$

However, $\langle \psi | i\hat{I} | \psi \rangle = i$. This leads to a contradiction, and implies that \hat{x} cannot have a normalized eigenvector. \square

Following a similar argument, we can prove that \hat{p} cannot have a normalized eigenvectors.

Proposition 3. *The creation operator \hat{a}^\dagger does not have a normalized eigenvector.*

Proof. Suppose that there exists a normalized eigenvector $|\psi\rangle$ such that

$$\hat{a}^\dagger |\psi\rangle = \mu |\psi\rangle \quad \forall \mu \in \mathbb{C}. \quad (21)$$

We can write $|\psi\rangle = \sum_{n=0}^{\infty} c_n |n\rangle$ for $c_n \in \mathbb{C}$ such that $\sum_{n=0}^{\infty} |c_n|^2 = 1$. Then, it follows from (21) that

$$\hat{a}^\dagger |\psi\rangle = \sum_{n=0}^{\infty} c_n \hat{a}^\dagger |n\rangle = \sum_{n=0}^{\infty} c_n \sqrt{n+1} |n+1\rangle \quad (22)$$

$$= \sum_{n=0}^{\infty} c_n \mu |n\rangle. \quad (23)$$

This implies that $c_0 \mu = 0$, $c_0 = c_1 \mu$, $c_1 \sqrt{2} = c_2 \mu$, and so on. If $\mu \neq 0$, then $c_0 = 0$ and this implies $c_n = 0$, where $n \in \mathbb{N}$. If $\mu = 0$, then also $c_0 = 0$ and this implies $c_n = 0$, where $n \in \mathbb{N}$. Therefore, the creation operator \hat{a}^\dagger does not have a normalized eigenvector. \square

Interestingly, the annihilation operator \hat{a} has normalized eigenstates, which are called **coherent states**. Each of the coherent states are parametrized by $\alpha \in \mathbb{C}$. That is, $\hat{a} |\alpha\rangle = \alpha |\alpha\rangle$.

Proposition 4. *The annihilation operator \hat{a} has coherent states $|\alpha\rangle$ as its normalized eigenvectors.*

Proof. Let us suppose that a coherent state $|\alpha\rangle$ is an eigenstate of \hat{a} . Expanding $|\alpha\rangle$ in terms of the number basis, we obtain

$$|\alpha\rangle = \sum_{n=0}^{\infty} c_n |n\rangle \quad \text{for } c_n \in \mathbb{C}. \quad (24)$$

Now apply \hat{a} to $|\alpha\rangle$:

$$\hat{a} |\alpha\rangle = \hat{a} \sum_{n=0}^{\infty} c_n |n\rangle \quad (25)$$

$$= \sum_{n=0}^{\infty} c_n \hat{a} |n\rangle \quad (26)$$

$$= \sum_{n=1}^{\infty} c_n \sqrt{n} |n-1\rangle. \quad (27)$$

To be an eigenstate, $|\alpha\rangle$ should satisfy the following relation:

$$\hat{a} |\alpha\rangle = \alpha |\alpha\rangle \quad (28)$$

$$\sum_{n=1}^{\infty} c_n \sqrt{n} |n-1\rangle = \sum_{n=0}^{\infty} \alpha c_n |n\rangle. \quad (29)$$

Equating coefficients term by term gives the following recursion relation:

$$c_n \sqrt{n} = \alpha c_{n-1}, \quad (30)$$

which gives us the following:

$$c_n = \frac{\alpha^n}{\sqrt{n!}} c_0. \quad (31)$$

Then,

$$|\alpha\rangle = c_0 \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle. \quad (32)$$

From the normalization condition, we can fix the value of c_0 . We thus have,

$$1 = \langle \alpha | \alpha \rangle \quad (33)$$

$$= |c_0|^2 \sum_{n,n'=0}^{\infty} \frac{\alpha^{*n} \alpha^{n'}}{\sqrt{n!n'}} \langle n | n' \rangle \quad (34)$$

$$= |c_0|^2 \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n!} \quad (35)$$

$$= |c_0|^2 e^{|\alpha|^2}. \quad (36)$$

This implies

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle, \quad (37)$$

concluding the proof. □

3 Multiple modes

Earlier in this lecture, we have been concentrating on single mode systems. Now, we move on to study multiple-mode bosonic Hilbert spaces. By tensoring together several separable Hilbert spaces, each corresponding to a bosonic mode, we get a multiple-mode bosonic Hilbert space. Each mode j is equipped with canonical operators \hat{x}_j and \hat{p}_j for $j \in \{1, \dots, m\}$, where m is the number of modes. If $j \neq k$, then $[\hat{x}_j, \hat{p}_k] = 0$, since these operators are acting on different Hilbert spaces. Now, we can encode these canonical commutation relations as

$$[\hat{x}_j, \hat{p}_k] = i\delta_{j,k}\hat{I}. \quad (38)$$

To write the relations compactly, we define the vector of the canonical operators as

$$\hat{r} = \begin{bmatrix} \hat{x}_1 \\ \hat{p}_1 \\ \vdots \\ \hat{x}_n \\ \hat{p}_n \end{bmatrix} \quad (39)$$

Then, the CCR can be encoded in the following matrix:

$$[\hat{r}, \hat{r}^\dagger] = \begin{bmatrix} [\hat{x}_1, \hat{x}_1] & [\hat{x}_1, \hat{p}_1] & \dots \\ [\hat{p}_1, \hat{x}_1] & [\hat{p}_1, \hat{p}_1] & \dots \\ \vdots & \vdots & \ddots \end{bmatrix} = i\Omega, \quad (40)$$

where $\Omega = \bigoplus_{j=1}^n \Omega_1 = I_n \otimes \Omega_1$ with

$$\Omega_1 = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}. \quad (41)$$

Ω is a special matrix, called the symplectic form, which realizes a symplectic inner product via $x^T \Omega y$. Some properties of the symplectic form are the following:

- $\Omega^T = -\Omega$
- $\Omega^T \Omega = -\Omega^2 = I_{2n}$. That is, Ω is an orthogonal matrix.
- Commutator matrix $i\Omega$ is involutory, that is, $(i\Omega)^2 = I$.

One can also use a different order for vectors of canonical operators as

$$\hat{s} = \begin{bmatrix} \hat{x}_1 \\ \vdots \\ \hat{x}_n \\ \hat{p}_1 \\ \vdots \\ \hat{p}_n \end{bmatrix}. \quad (42)$$

In this case,

$$[\hat{s}, \hat{s}^\dagger] = iJ, \quad (43)$$

where

$$J = \begin{bmatrix} 0_n & I_n \\ -I_n & 0_n \end{bmatrix} = \Omega_1 \otimes I_n. \quad (44)$$

Another convention often used in the literature is the following:

$$\hat{a} = \begin{bmatrix} \hat{a}_1 \\ \hat{a}_1^\dagger \\ \vdots \\ \hat{a}_n \\ \hat{a}_n^\dagger \end{bmatrix}. \quad (45)$$

Then, $\hat{a} = U\hat{r}$, where the unitary U is defined as

$$U = \bigoplus_{j=1}^n u = I_n \otimes u, \quad (46)$$

with

$$u = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & i \\ 1 & -i \end{bmatrix}. \quad (47)$$

Then,

$$\left[\hat{\underline{a}}, \hat{\underline{a}}^\dagger \right] = \left[U \hat{r}, \hat{r}^\dagger U^\dagger \right] \quad (48)$$

$$= U \left[\hat{r}, \hat{r}^\dagger \right] U^\dagger \quad (49)$$

$$= U i (I_n \otimes \Omega_1) U^\dagger \quad (50)$$

$$= i (I_n \otimes u) (I_n \otimes \Omega_1) (I_n \otimes u^\dagger) \quad (51)$$

$$= i I_n \otimes u \Omega_1 u^\dagger \quad (52)$$

$$= I_n \otimes \sigma_z \quad (53)$$

$$= \bigoplus_{i=1}^n \sigma_z. \quad (54)$$

This implies,

$$\left[\hat{\underline{a}}, \hat{\underline{a}}^\dagger \right] = I_n \otimes \sigma_z. \quad (55)$$

One can also define another order

$$\bar{\hat{\underline{a}}} = \begin{bmatrix} \hat{a}_1 \\ \hat{a}_1^\dagger \\ \vdots \\ \hat{a}_n \\ \hat{a}_n^\dagger \end{bmatrix}. \quad (56)$$

However, we do not go into the details of this convention.

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1 Overview

In the last lecture, we developed the background required to study single-mode bosonic systems. We studied creation, annihilation, position, and momentum operators and their properties. We then extended the above for multiple-mode bosonic systems, and introduced the canonical symplectic form.

In this lecture, we will introduce the mean vector in Section 2.1 and the covariance matrix of a bosonic state in Section 2.2. We will then derive constraints that are fulfilled by a covariance matrix of a bosonic state in Section 3.

2 Mean vector and covariance matrix

Consider the vector \hat{r} of canonical quadrature operators for an m -mode bosonic system:

$$\hat{r} \equiv (\hat{x}_1, \hat{p}_1, \dots, \hat{x}_m, \hat{p}_m)^T, \quad (1)$$

where \hat{x} refers to the position-quadrature operator and \hat{p} refers to the momentum-quadrature operator.

2.1 Mean vector

For a state ρ of multiple modes, the mean vector \bar{r} is given by

$$\bar{r} = (\bar{x}_1, \bar{p}_1, \dots, \bar{x}_m, \bar{p}_m), \quad (2)$$

where the components of the mean vector are defined as follows:

$$\bar{x}_1 = \text{Tr}[\hat{x}_1\rho] = \text{Tr}\left[\left(\hat{x}_1 \otimes \hat{I} \otimes \dots \otimes \hat{I}\right)\rho\right], \quad (3)$$

$$\bar{p}_1 = \text{Tr}[\hat{p}_1\rho] = \text{Tr}\left[\left(\hat{I} \otimes \hat{p}_1 \otimes \hat{I} \otimes \dots \otimes \hat{I}\right)\rho\right], \quad (4)$$

$$\bar{x}_j = \text{Tr}[\hat{x}_j\rho] = \langle \hat{x}_j \rangle_\rho, \quad (5)$$

$$\bar{p}_j = \text{Tr}[\hat{p}_j\rho] = \langle \hat{p}_j \rangle_\rho, \quad (6)$$

where \hat{I} is the identity operator and $j \in \{1, 2, \dots, m\}$. Then, as a shorthand we can write the mean vector as

$$\bar{r} = \text{Tr}[\hat{r}\rho] = (\text{Tr}[\hat{x}_1\rho], \text{Tr}[\hat{p}_1\rho], \dots, \text{Tr}[\hat{x}_m\rho], \text{Tr}[\hat{p}_m\rho])^T \quad (7)$$

Just like classical probability distributions need not have a finite mean, a quantum state need not have a finite mean.

2.2 Covariance matrix

Let us denote the covariance matrix of a quantum state by σ , and let the entries be given by σ_{jk} . Let \hat{r}_j be the j th element of \hat{r} , where $j \in \{1, \dots, 2m\}$, and m is the number of modes of the quantum state considered. Let us define $\hat{r}_j^c = \hat{r}_j - \langle \hat{r}_j \rangle_\rho$. Then, the covariance matrix elements are defined as

$$\sigma_{jk} = \text{Tr} [(\hat{r}_j^c \hat{r}_k^c + \hat{r}_k^c \hat{r}_j^c) \rho] \quad (8)$$

$$= \text{Tr} [\{\hat{r}_j^c, \hat{r}_k^c\} \rho] \quad (9)$$

$$= \langle \{\hat{r}_j^c, \hat{r}_k^c\} \rangle_\rho, \quad (10)$$

where $\sigma_{jk} \in \mathbb{R}$ and $k \in \{1, \dots, 2m\}$.

Now, consider the total photon number operator

$$\hat{N} = \sum_{j=1}^m \hat{n}_j, \quad (11)$$

where $\hat{n}_j = \hat{a}_j^\dagger \hat{a}_j$. Let us define finite-energy state as the states that fulfill the following constraint:

$$\text{Tr} [\hat{N} \rho] < \infty. \quad (12)$$

Proposition 1. *A state has finite energy iff the elements of \bar{r} and σ are finite, that is $\bar{r}_j < \infty$ and $\sigma_{jk} < \infty$.*

Proof. Let us first prove that if the state ρ has finite energy then the elements of its mean vector \bar{r} and covariance matrix σ are finite. The definition of a finite-energy state implies

$$\text{Tr} [\hat{n}_j \rho] < \infty. \quad (13)$$

Then observe that,

$$\text{Tr} [\hat{n}_j \rho] = \frac{1}{2} \text{Tr} [(\hat{x}_j^2 + \hat{p}_j^2 - 1) \rho] < \infty. \quad (14)$$

This implies, $\text{Tr} [\hat{x}_j^2 \rho], \text{Tr} [\hat{p}_j^2 \rho] < \infty$. Then, we conclude the following:

$$|\bar{x}_j| = |\text{Tr} [\hat{x}_j \rho]| \quad (15)$$

$$= |\text{Tr} [\hat{x}_j \sqrt{\rho} \sqrt{\rho}]| \quad (16)$$

$$\leq \sqrt{\text{Tr} [\hat{x}_j \sqrt{\rho} \sqrt{\rho} \hat{x}_j] \cdot \text{Tr} [\sqrt{\rho} \sqrt{\rho}]} \quad (17)$$

$$= \sqrt{\text{Tr} [\hat{x}_j^2 \rho]} < \infty. \quad (18)$$

The first inequality follows from the Cauchy-Schwarz inequality. Similarly, $|\bar{p}_j| = |\text{Tr} [\hat{p}_j \rho]| < \infty$. Therefore, we can conclude that finite-energy states have finite mean vector.

Now, let us prove that the elements of a covariance matrix of finite-energy states are finite. First let us consider the diagonal terms:

$$\sigma_{jj} = 2 \operatorname{Tr} \left[(\hat{r}_j^c)^2 \rho \right] \quad (19)$$

$$= 2 \operatorname{Tr} \left[(\hat{r}_j - \langle \hat{r}_j \rangle)^2 \rho \right] \quad (20)$$

$$= 2 \operatorname{Tr} \left[\hat{r}_j^2 \rho + \langle \hat{r}_j \rangle^2 \rho - 2 \hat{r}_j \langle \hat{r}_j \rangle \rho \right] \quad (21)$$

$$= 2 \operatorname{Tr} \left[\hat{r}_j^2 \rho - \langle \hat{r}_j \rangle^2 \rho \right] \quad (22)$$

$$= 2 \left[\langle \hat{r}_j^2 \rangle_\rho - \langle \hat{r}_j \rangle_\rho^2 \right] \quad (23)$$

$$< \infty. \quad (24)$$

Now, the first term of (23) is finite as seen previously, and the second term is finite since the mean vector of the finite-energy state is finite. Therefore, we conclude that the diagonal elements of a covariance vector of a finite-energy state are finite. Now, we consider the off-diagonal elements σ_{jk} , where $j \neq k$.

$$|\sigma_{jk}| = |\langle \hat{r}_j^c \hat{r}_k^c + \hat{r}_k^c \hat{r}_j^c \rangle_\rho| \quad (25)$$

$$\leq |\langle \hat{r}_j^c \hat{r}_k^c \rangle_\rho| + |\langle \hat{r}_k^c \hat{r}_j^c \rangle_\rho| \quad (26)$$

Now, consider

$$|\langle \hat{r}_j^c \hat{r}_k^c \rangle_\rho| = |\operatorname{Tr} [\sqrt{\rho} \hat{r}_j^c \hat{r}_k^c \sqrt{\rho}]| \quad (27)$$

$$\leq \sqrt{\operatorname{Tr} \left[(\hat{r}_j^c)^2 \rho \right] \operatorname{Tr} \left[(\hat{r}_k^c)^2 \rho \right]} \quad (28)$$

$$< \infty \quad (29)$$

The first inequality follows from the Cauchy–Schwarz inequality, and the second inequality follows from (19). Now, let us prove the converse. That is, if the state is a finite-energy state, then the covariance matrix is finite.

To prove the opposite implication, consider that

$$\operatorname{Tr} (\hat{N} \rho) = \sum_{j=1}^m \operatorname{Tr} [\hat{n}_j \rho] \quad (30)$$

$$= \sum_{j=1}^m [\operatorname{Tr} [\hat{x}_j^2 \rho] + \operatorname{Tr} [\hat{p}_j^2 \rho] - 1] \quad (31)$$

$$< \infty \quad (32)$$

The last inequality follows from the assumed finiteness of the elements of the mean vector and covariance matrix. \square

Instead of writing all the $2m \times 2m$ elements of the covariance matrix, we condense it to write the covariance matrix as follows:

$$\sigma = \operatorname{Tr} \left[\left\{ (\hat{r} - \bar{r}), (\hat{r} - \bar{r})^\dagger \right\} \rho \right], \quad (33)$$

where,

$$\left\{ (\hat{r} - \bar{r}), (\hat{r} - \bar{r})^\dagger \right\} = \begin{bmatrix} \{\hat{r}_1 - \bar{r}_1, \hat{r}_1 - \bar{r}_1\} & \{\hat{r}_1 - \bar{r}_1, \hat{r}_2 - \bar{r}_2\} & \dots \\ \{\hat{r}_2 - \bar{r}_2, \hat{r}_1 - \bar{r}_1\} & \{\hat{r}_2 - \bar{r}_2, \hat{r}_2 - \bar{r}_2\} & \dots \\ \vdots & \vdots & \ddots \end{bmatrix}. \quad (34)$$

Then,

$$\sigma = \begin{bmatrix} \text{Tr} [\{\hat{r}_1 - \bar{r}_1, \hat{r}_1 - \bar{r}_1\} \rho] & \text{Tr} [\{\hat{r}_1 - \bar{r}_1, \hat{r}_2 - \bar{r}_2\} \rho] & \dots \\ \text{Tr} [\{\hat{r}_2 - \bar{r}_2, \hat{r}_1 - \bar{r}_1\} \rho] & \text{Tr} [\{\hat{r}_2 - \bar{r}_2, \hat{r}_2 - \bar{r}_2\} \rho] & \dots \\ \vdots & \vdots & \ddots \end{bmatrix}. \quad (35)$$

3 Constraints on covariance matrix

In this section, we establish certain properties of the covariance matrix. We first prove that the covariance matrix (CM) of a vector of random variables is Hermitian and positive semi-definite (PSD). Next, we prove that the covariance matrix of a quantum state fulfills a stronger constraint, that is $\sigma + i\Omega \geq 0$, and that the covariance matrix is positive definite.

3.1 CM of vector of random variables is PSD

Consider a covariance matrix Σ for a vector of random variables. We now prove that the covariance matrix is positive semi-definite.

Proposition 2. *The covariance matrix of a vector of random variables is Hermitian and PSD, that is, $\Sigma = \Sigma^\dagger$ and $\Sigma \geq 0$.*

Proof. That the covariance matrix is Hermitian follows from the definition. We now give a proof that the covariance matrix is PSD. Let X be a vector of random variables. Then, $X = [X_1, X_2, \dots, X_m]^T$, where X_i is a random variable and has realizations in \mathbb{C} . Then,

$$\Sigma = \mathbb{E} \left[(X - \mathbb{E}(X)) (X - \mathbb{E}(X))^\dagger \right]. \quad (36)$$

Now, let \underline{w} be a constant vector in \mathbb{C}^m . Consider then

$$\underline{w}^\dagger \Sigma \underline{w} = \underline{w}^\dagger \mathbb{E} \left[(X - \mathbb{E}(X)) (X - \mathbb{E}(X))^\dagger \right] \underline{w} \quad (37)$$

$$= \mathbb{E} \left[\underline{w}^\dagger (X - \mathbb{E}(X)) (X - \mathbb{E}(X))^\dagger \underline{w} \right] \quad (38)$$

$$= \mathbb{E} \left[|\underline{w}^\dagger (X - \mathbb{E}(X))|^2 \right] \geq 0. \quad (39)$$

Since this holds for all $w \in \mathbb{C}^m$, it follows that $\Sigma \geq 0$. \square

3.2 Uncertainty principle of covariance matrix

Now, we derive an important constraint on the covariance matrix of a quantum state. This is the **uncertainty principle** for the covariance matrix.

Theorem 3. *The covariance matrix σ of a quantum state fulfills the following constraint:*

$$\sigma + i\Omega \geq 0. \quad (40)$$

Proof. Consider the following $(2m \times 2m)$ complex matrix given by

$$\tau = 2 \operatorname{Tr} \left[(\hat{r} - \bar{r}) (\hat{r} - \bar{r})^\dagger \rho \right]. \quad (41)$$

We first prove that τ is PSD, and then deduce the statement of the theorem. Let $\underline{w} \in \mathbb{C}^{2m}$. Then,

$$\underline{w}^\dagger \tau \underline{w} = 2 \operatorname{Tr} \underline{w}^\dagger \left[(\hat{r} - \bar{r}) (\hat{r} - \bar{r})^\dagger \rho \right] \underline{w} \quad (42)$$

$$= 2 \operatorname{Tr} \left[\underline{w}^\dagger (\hat{r} - \bar{r}) (\hat{r} - \bar{r})^\dagger \underline{w} \rho \right] \quad (43)$$

$$= 2 \operatorname{Tr} \left[\hat{O} \hat{O}^\dagger \rho \right] \quad (44)$$

$$\geq 0, \quad (45)$$

where $\hat{O} = \underline{w}^\dagger (\hat{r} - \bar{r})$. Since $\hat{O}^\dagger \hat{O}$ is PSD and so is ρ , we arrive at the last inequality. Now, the above argument holds for all $\underline{w} \in \mathbb{C}^{2m}$, and so we conclude that τ is PSD.

Now, consider that

$$2\hat{r}_j \hat{r}_k = \{\hat{r}_j, \hat{r}_k\} + [\hat{r}_j, \hat{r}_k]. \quad (46)$$

This implies,

$$2(\hat{r} - \bar{r})(\hat{r} - \bar{r})^\dagger = \left\{ (\hat{r} - \bar{r}), (\hat{r} - \bar{r})^\dagger \right\} + \left[(\hat{r} - \bar{r}), (\hat{r} - \bar{r})^\dagger \right] \quad (47)$$

$$= \left\{ (\hat{r} - \bar{r}), (\hat{r} - \bar{r})^\dagger \right\} + \left[\hat{r}, \hat{r}^\dagger \right] \quad (48)$$

Then, we obtain the following:

$$\tau = 2 \operatorname{Tr} \left[\left((\hat{r} - \bar{r}) (\hat{r} - \bar{r})^\dagger \right) \rho \right] \quad (49)$$

$$= \operatorname{Tr} \left[\left\{ (\hat{r} - \bar{r}), (\hat{r} - \bar{r})^\dagger \right\} \rho \right] + \operatorname{Tr} \left[\left[\hat{r}, \hat{r}^\dagger \right] \rho \right] \quad (50)$$

$$= \sigma + i\Omega \geq 0. \quad (51)$$

The last inequality follows from $\tau \geq 0$. □

Now, we prove that σ is PSD. Note that the eigenvalues of a matrix do not change under a transpose. So, if they are positive, then they remain positive after the transpose of the matrix. Then,

$$\sigma + i\Omega \geq 0, \quad (52)$$

implies

$$(\sigma + i\Omega)^T \geq 0. \quad (53)$$

which in turn implies,

$$\sigma - i\Omega \geq 0. \quad (54)$$

Then combining (54) with (52), we obtain that $\sigma \geq 0$. That is, σ is a PSD.

3.3 CM of quantum states is positive definite

We now prove that a quantum covariance matrix is in fact positive definite. This makes them more special and easier to work mathematically than classical covariance matrices.

Proposition 4. *A quantum covariance matrix is positive definite.*

Proof. We prove this statement by contradiction. Let us assume that the quantum covariance matrix is not positive definite. That is, \exists a real, non-zero vector $\psi \in \mathbb{R}^{2m}$, such that $\sigma|\psi\rangle = 0$. Then, for $\varepsilon \in \mathbb{R}$, set $\psi(\varepsilon) = (I + \varepsilon i\Omega)\psi$. By invoking the following assumption $\sigma\psi = 0$, and the following facts: $\psi^T\Omega\psi = 0 \forall \psi \in \mathbb{R}^{2m}$ and $(i\Omega)^2 = I$, we find that

$$\begin{aligned} & \psi(\varepsilon)^\dagger (\sigma + i\Omega) \psi(\varepsilon) \\ &= \psi^T (I + \varepsilon i\Omega) (\sigma + i\Omega) (I + \varepsilon i\Omega) \psi \end{aligned} \quad (55)$$

$$= \psi^T (I + \varepsilon i\Omega) (i\Omega + \varepsilon\sigma i\Omega + \varepsilon I) \psi \quad (56)$$

$$= \psi^T (i\Omega + \varepsilon\sigma i\Omega + \varepsilon I + \varepsilon i\Omega (i\Omega + \varepsilon\sigma i\Omega + \varepsilon I)) \psi \quad (57)$$

$$= \psi^T (i\Omega + \varepsilon\sigma i\Omega + 2\varepsilon I + \varepsilon^2\Omega^T\sigma\Omega + \varepsilon^2 i\Omega) \psi \quad (58)$$

$$= \psi^T (2\varepsilon I + \varepsilon^2\Omega^T\sigma\Omega) \psi \quad (59)$$

$$= 2\varepsilon\psi^T\psi + \varepsilon^2 (\Omega\psi)^T \sigma (\Omega\psi) \quad (60)$$

Now, suppose that $(\Omega\psi)^T \sigma (\Omega\psi) = 0$. Then picking $\varepsilon < 0$, implies that $2\varepsilon\psi^T\psi < 0$, which contradicts the fact that $\sigma + i\Omega \geq 0$ for any quantum covariance matrix σ .

Now, suppose that $(\Omega\psi)^T \sigma (\Omega\psi) > 0$. Then pick $\varepsilon < 0$ and such that

$$|\varepsilon| \leq \frac{2\psi^T\psi}{(\Omega\psi)^T \sigma (\Omega\psi)}. \quad (61)$$

This implies,

$$2\varepsilon\psi^T\psi + \varepsilon^2 (\Omega\psi)^T \sigma (\Omega\psi) < 0, \quad (62)$$

and there exists $\psi(\varepsilon)$ such that

$$\psi(\varepsilon)^\dagger (\sigma + i\Omega) \psi(\varepsilon) < 0, \quad (63)$$

again contradicting the assumption that $\sigma + i\Omega \geq 0$. Hence, σ must be positive definite. \square

3.4 Uncertainty principle for a single-mode bosonic state

The covariance matrix of a single-mode bosonic state is given as

$$\sigma = \begin{bmatrix} 2\langle(\hat{x}^c)^2\rangle_\rho & \langle\{\hat{x}^c, \hat{p}^c\}\rangle_\rho \\ \langle\{\hat{x}^c, \hat{p}^c\}\rangle_\rho & 2\langle(\hat{p}^c)^2\rangle_\rho \end{bmatrix} = \begin{bmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{bmatrix}. \quad (64)$$

The 2×2 matrix σ is the covariance matrix of a single-mode bosonic system if and only if the following constraint holds

$$\sigma + i\Omega \geq 0 \iff \det(\sigma) \geq 1 \text{ and } \sigma > 0. \quad (65)$$

The forward direction of the above statement is easy to prove. We have already shown

$$\sigma + i\Omega \geq 0 \implies \sigma > 0. \tag{66}$$

Now we prove that

$$\sigma + i\Omega \geq 0 \implies \det(\sigma) \geq 1. \tag{67}$$

The constraint $\sigma + i\Omega \geq 0$ implies that

$$\det(\sigma + i\Omega) = \sigma_{11}\sigma_{22} - (\sigma_{12}^2 + 1) \geq 0. \tag{68}$$

We thus see that $\det(\sigma) \geq 1$.

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1 Overview

In the previous lecture, we considered finite-energy states, defined the covariance matrix, and studied constraints that the covariance matrix should satisfy. Lastly, we also stated and proved the uncertainty principle for bosonic quantum states.

In this lecture, we consider generic transformations of quantum states. We study the effects of these transformations on the mean vector and covariance matrix of the state in consideration. We will define the unitary displacement operator and study its properties. Lastly, we will define another set of Hamiltonians that are quadratic in the quadrature operators, which generate another class of transformations. The study of those transformations will be completed in the following lectures.

2 Generic transformations of quantum states

In this section, we study generic transformations on quantum states and their effect on the mean vector and covariance matrix of the states.

2.1 The Displacement Operator

Suppose that we would like to shift the mean vector of an n -mode quantum state by a vector $\bar{r} \in \mathbb{R}^{2n}$. To do so, we define the **unitary displacement operator**.

Definition 1. *The unitary displacement operator $\hat{D}_{\bar{r}}$ is defined as*

$$\hat{D}_{\bar{r}} = e^{i\bar{r}^T \Omega \hat{r}} \quad (1)$$

where \hat{r} is the vector of quadrature operators as defined in earlier lectures, and Ω is the symplectic form that captures the canonical commutation relations between the quadrature operators.

Lemma 2. *The displacement of an n -mode state is a tensor product of single-mode displacements.*

$$\hat{D}_{\bar{r}} = \hat{D}_{\bar{r}_1} \otimes \hat{D}_{\bar{r}_2} \otimes \dots \otimes \hat{D}_{\bar{r}_n} \quad (2)$$

with $\bar{r}_j = (\bar{x}_j \ \bar{p}_j)^T$.

Proof. Note that

$$\bar{r}^T \Omega \hat{r} = \sum_{j,k=1}^{2n} \bar{r}_j \Omega_{jk} \hat{r}_k \quad (3)$$

$$= \sum_{j=1}^n (\bar{x}_j \hat{p}_j - \bar{p}_j \hat{x}_j). \quad (4)$$

Due to this component-wise expression, we have that

$$e^{i\bar{r}^T \Omega \hat{r}} = \exp \left(i \sum_{j=1}^n (\bar{x}_j \hat{p}_j - \bar{p}_j \hat{x}_j) \right) \quad (5)$$

and thus that

$$\hat{D}_{\bar{r}} = \hat{D}_{\bar{r}_1} \otimes \hat{D}_{\bar{r}_2} \otimes \dots \otimes \hat{D}_{\bar{r}_n}, \quad (6)$$

concluding the proof. \square

Further, we can think of $\bar{r}^T \Omega \hat{r}$ as a Hamiltonian. From the above analysis we note that

$$\left(\bar{r}^T \Omega \hat{r} \right)^\dagger = \bar{r}^T \Omega \hat{r}. \quad (7)$$

Since $\bar{r}^T \Omega \hat{r}$ is a Hamiltonian, it follows that $e^{i\bar{r}^T \Omega \hat{r}}$ is indeed unitary, as stated in Definition 1.

2.2 Inverse of the displacement operator

Observe that

$$\hat{D}_{\bar{r}}^\dagger = \left(e^{i\bar{r}^T \Omega \hat{r}} \right)^\dagger = e^{-i\bar{r}^T \Omega \hat{r}} = \hat{D}_{-\bar{r}}. \quad (8)$$

This implies that the displacement can be inverted by displacing in the opposite way.

2.3 Commutation Relations between Displacement Operators

Suppose that we have two displacement operators \hat{D}_{r_1} and \hat{D}_{r_2} for $r_1, r_2 \in \mathbb{R}^{2n}$. What is the commutation relation between the two displacement operators? In what follows, we prove the following equation:

$$\hat{D}_{r_1+r_2} = \hat{D}_{r_1} \hat{D}_{r_2} e^{ir_1^T \Omega r_2 / 2}. \quad (9)$$

To prove this, we first need the following result.

Lemma 3. *When X and Y commute with $[X, Y]$, the following equality holds*

$$e^X e^Y = e^{X+Y + \frac{1}{2}[X, Y]}. \quad (10)$$

Proof. The starting point is the celebrated **Baker–Campbell–Hausdorff formula**

$$e^X Y e^{-X} = Y + [X, Y] + \frac{1}{2!} [X, [X, Y]] + \frac{1}{3!} [X, [X, [X, Y]]] + \dots \quad (11)$$

In the case that X and Y both commute with $[X, Y]$, the above simplifies to the following for $s \in \mathbb{R}$.

$$e^{sX} Y e^{-sX} = Y + s[X, Y]. \quad (12)$$

Define $g(s) = e^{sX} e^{sY}$. By differentiating with respect to s , one obtains

$$\frac{dg(s)}{ds} = \frac{d}{ds} \left(e^{sX} e^{sY} \right) \quad (13)$$

$$= X e^{sX} e^{sY} + e^{sX} Y e^{sY} \quad (14)$$

$$= X g(s) + e^{sX} Y e^{-sX} e^{sX} e^{sY} \quad (15)$$

$$= \left(X + e^{sX} Y e^{-sX} \right) g(s) \quad (16)$$

$$= \left(X + Y + s[X, Y] \right) g(s). \quad (17)$$

The solution to this differential equation is

$$g(s) = e^{s(X+Y) + \frac{s^2}{2}[X, Y]} = e^{sX} e^{sY}. \quad (18)$$

$\forall s \in \mathbb{R}$ such that X and Y commute with $[X, Y]$. The second equality in the above follows from the definition of $g(s)$.

Set $s = 1$ to yield

$$e^X e^Y = e^{X+Y + \frac{1}{2}[X, Y]}, \quad (19)$$

concluding the proof. \square

Lemma 4.

$$\hat{D}_{r_1+r_2} = \hat{D}_{r_1} \hat{D}_{r_2} e^{ir_1^T \Omega r_2 / 2}. \quad (20)$$

Proof. Set $X = e^{ir_1^T \Omega \hat{r}}$ and $Y = e^{ir_2^T \Omega \hat{r}}$.

We evaluate $[X, Y]$ as a first step.

$$[X, Y] = \left[ir_1^T \Omega \hat{r}, ir_2^T \Omega \hat{r} \right] \quad (21)$$

$$= - \left[r_1^T \Omega \hat{r}, r_2^T \Omega \hat{r} \right] \quad (22)$$

$$= - \left[\sum_{jk} r_{1,j} \Omega_{jk} \hat{r}_k, \sum_{lm} r_{2,l} \Omega_{lm} \hat{r}_m \right] \quad (23)$$

$$= - \sum_{jklm} r_{1,j} r_{2,l} \Omega_{jk} \Omega_{lm} \left[\hat{r}_k, \hat{r}_m \right] \quad (24)$$

$$= - \sum_{jklm} r_{1,j} r_{2,l} \Omega_{jk} \Omega_{lm} i \Omega_{km} \quad (25)$$

$$= -i \sum_{jklm} r_{1,j} \Omega_{jk} \Omega_{km} \Omega_{lm} r_{2,l} \quad (26)$$

$$= i \sum_{jklm} r_{1,j} \Omega_{jk} \Omega_{km} \Omega_{ml} r_{2,l} \quad (27)$$

$$= i r_1^T \Omega \Omega \Omega r_2 \quad (28)$$

$$= -i r_1^T \Omega r_2. \quad (29)$$

In the above, the first four equalities follow from algebraic manipulation and expanding X and Y in terms of their components. The fifth equality follows from application of the canonical commutation relation. The sixth equality again is algebraic manipulation, and the seventh equality follows from Ω being antisymmetric. The eighth equality follows from observing the expression to describe matrix multiplication. The final equality follows from the involutory nature of $i\Omega$, i.e. $\Omega^2 = -I$.

$[X, Y] = -i r_1^T \Omega r_2$ is a scalar, and hence commutes with both X and Y . Because of this, we can apply the above Lemma 3.

$$\hat{D}_{r_1} \hat{D}_{r_2} = e^{i r_1^T \Omega \hat{r}} e^{i r_2^T \Omega \hat{r}} \quad (30)$$

$$= e^{(i r_1^T \Omega \hat{r} + i r_2^T \Omega \hat{r} - i/2 r_1^T \Omega r_2)} \quad (31)$$

$$= e^{i(r_1+r_2)^T \Omega \hat{r}} e^{-\frac{i}{2} r_1^T \Omega r_2} \quad (32)$$

$$= \hat{D}_{r_1+r_2} e^{-\frac{i}{2} r_1^T \Omega r_2}. \quad (33)$$

We can now write

$$\hat{D}_{r_1+r_2} = \hat{D}_{r_1} \hat{D}_{r_2} e^{\frac{i}{2} r_1^T \Omega r_2} \quad (34)$$

which completes the proof. \square

Corollary 5.

$$\hat{D}_{r_1} \hat{D}_{r_2} = \hat{D}_{r_2} \hat{D}_{r_1} e^{-i r_1^T \Omega r_2} \quad (35)$$

Proof. Apply Lemma 4 twice to get

$$\hat{D}_{r_1} \hat{D}_{r_2} e^{\frac{i}{2} r_1^T \Omega r_2} = \hat{D}_{r_1+r_2} \quad (36)$$

$$= \hat{D}_{r_2} \hat{D}_{r_1} e^{\frac{i}{2} r_2^T \Omega r_1} \quad (37)$$

$$= \hat{D}_{r_2} \hat{D}_{r_1} e^{\frac{i}{2} r_1^T \Omega^T r_2} \quad (38)$$

$$= \hat{D}_{r_2} \hat{D}_{r_1} e^{-\frac{i}{2} r_1^T \Omega r_2}. \quad (39)$$

The first equality is a statement of Lemma 4. The second equality comes from once more applying Lemma 4. The third and fourth equalities come from considering the transpose of the argument of the exponential. \square

2.4 Connection to traditional single-mode displacement operator

Definition 6. In quantum optics, we define the single-mode displacement operator as follows:

$$D(\alpha) \equiv \exp(\alpha \hat{a}^\dagger - \alpha^* \hat{a}) \quad (40)$$

To see its connection to the displacement operator discussed so far, consider that for $\alpha \in \mathbb{C}$ and $\alpha = \alpha_R + i\alpha_I$,

$$D(\alpha) \equiv \exp(\alpha \hat{a}^\dagger - \alpha^* \hat{a}) \quad (41)$$

$$= \exp\left([\alpha_R + i\alpha_I] \hat{a}^\dagger - [\alpha_R - i\alpha_I] \hat{a}\right) \quad (42)$$

$$= \exp\left(\alpha_R [\hat{a}^\dagger - \hat{a}] + i\alpha_I [\hat{a} + \hat{a}^\dagger]\right) \quad (43)$$

$$= \exp\left(-i\sqrt{2}\alpha_R \left[\frac{\hat{a} - \hat{a}^\dagger}{\sqrt{2}i}\right] + i\sqrt{2}\alpha_I \left[\frac{\hat{a} + \hat{a}^\dagger}{\sqrt{2}}\right]\right) \quad (44)$$

$$= \exp\left(i\sqrt{2}[\alpha_I \hat{x} - \alpha_R \hat{p}]\right). \quad (45)$$

It is important to keep in mind that there is a factor of $\sqrt{2}$ that must be taken care of when going between the two conventions.

To implement an n -mode displacement operator on a quantum state in a lab, one uses an array of highly transmissive beamsplitters and strong local oscillators in coherent states. This point will be returned to later.

2.5 Effect of displacement operator on mean vector of a state

Theorem 7. *The displacement operator $\hat{D}_{\bar{r}}$ shifts the mean vector of an arbitrary state ρ by \bar{r} .*

$$\hat{D}_{\bar{r}}^\dagger \hat{r} \hat{D}_{\bar{r}} = \hat{r} - \bar{r}. \quad (46)$$

Proof. Upon action of a displacement operator $\hat{D}_{\bar{r}}$, the new mean vector of ρ is given by

$$\bar{r}' = \text{Tr}[\hat{r} \hat{D}_{\bar{r}} \rho \hat{D}_{\bar{r}}^\dagger] \quad (47)$$

$$= \text{Tr}[\hat{D}_{\bar{r}}^\dagger \hat{r} \hat{D}_{\bar{r}} \rho] \quad (48)$$

which arises from the definition of the mean vector and the cyclicity of trace.

From the above, we see that the problem of computing the new mean vector has been reduced to computing $\hat{D}_{\bar{r}}^\dagger \hat{r} \hat{D}_{\bar{r}}$, which is the same as computing

$$\hat{D}_{\bar{r}}^\dagger \hat{x}_j \hat{D}_{\bar{r}} \quad \text{and} \quad \hat{D}_{\bar{r}}^\dagger \hat{p}_j \hat{D}_{\bar{r}} \quad \forall j \in \{1, \dots, n\}. \quad (49)$$

We proved earlier in Lemma 2 that the displacement operator for n modes can be written as a tensor product of single-mode displacements. This enables us to write

$$\hat{D}_{\bar{r}}^\dagger \hat{x}_j \hat{D}_{\bar{r}} = \left(\hat{D}_{\bar{r}_1}^\dagger \otimes \dots \otimes \hat{D}_{\bar{r}_n}^\dagger\right) \hat{x}_j \left(\hat{D}_{\bar{r}_1} \otimes \dots \otimes \hat{D}_{\bar{r}_n}\right) \quad (50)$$

$$= \hat{D}_{\bar{r}_j}^\dagger \hat{x}_j \hat{D}_{\bar{r}_j}. \quad (51)$$

For \hat{p}_j , we can similarly write

$$\hat{D}_{\bar{r}}^\dagger \hat{p}_j \hat{D}_{\bar{r}} = \hat{D}_{\bar{r}_j}^\dagger \hat{p}_j \hat{D}_{\bar{r}_j}. \quad (52)$$

We invoke the BCH formula (Lemma 3) to calculate the above.

$$\hat{D}_{\bar{r}_j}^\dagger \hat{x}_j \hat{D}_{\bar{r}_j} = e^{i[\bar{p}_j \hat{x}_j - \bar{x}_j \hat{p}_j]} \hat{x}_j e^{-i[\bar{p}_j \hat{x}_j - \bar{x}_j \hat{p}_j]} \quad (53)$$

$$= \hat{x}_j + \left[i(\bar{p}_j \hat{x}_j - \bar{x}_j \hat{p}_j), \hat{x}_j \right] + \text{higher-order nested commutators that vanish} \quad (54)$$

$$= \hat{x}_j + i \left[-\bar{x}_j \hat{p}_j, \hat{x}_j \right] \quad (55)$$

$$= \hat{x}_j - i\bar{x}_j [\hat{p}_j, \hat{x}_j] \quad (56)$$

$$= \hat{x}_j - i\bar{x}_j(-i) \quad (57)$$

$$= \hat{x}_j - \bar{x}_j. \quad (58)$$

A similar calculation yields

$$\hat{D}_{\bar{r}_j}^\dagger \hat{p}_j \hat{D}_{\bar{r}_j} = \hat{p}_j - \bar{p}_j. \quad (59)$$

Put together, we have

$$\hat{D}_{\bar{r}_j}^\dagger \hat{r} \hat{D}_{\bar{r}_j} = \hat{r} - \bar{r}. \quad (60)$$

$$\implies \bar{r}' = \text{Tr}[\hat{D}_{\bar{r}_j}^\dagger \hat{r} \hat{D}_{\bar{r}_j}] \quad (61)$$

$$= \text{Tr}[(\hat{r} - \bar{r})\rho] \quad (62)$$

$$= \text{Tr}[\hat{r}\rho] - \bar{r}. \quad (63)$$

where we identify $\text{Tr}[\hat{r}\rho]$ as the original mean vector of ρ . \square

2.6 Effect of displacement operator on covariance matrix of a state

Lemma 8. *The covariance matrix of a state ρ is unchanged upon action by a displacement operator.*

This can be easily seen from the definition of the covariance matrix.

3 Quadratic Hamiltonians

The unitary displacement operator constitutes the most general evolution realizable by a Hamiltonian that is linear in the quadrature operators; i.e., the Hamiltonian is a real linear combination of the quadrature operators. It is a natural next step to examine the evolution effected by a quadratic Hamiltonian.

The general form of a quadratic Hamiltonian is as follows:

$$\hat{H} = \frac{1}{2} \hat{r}^T H \hat{r} \quad (64)$$

where H is a real, symmetric $2n \times 2n$ matrix.

In the above, \hat{H} is the Hamiltonian operator, and H is the Hamiltonian matrix.

The Hamiltonian (64) realizes the following evolution:

$$e^{-i\hat{H}t} = e^{-\frac{i}{2} \hat{r}^T H t \hat{r}}. \quad (65)$$

In the above, it is to be noted that the time parameter can be subsumed into the Hamiltonian matrix.

3.1 Effect of quadratic Hamiltonian on mean vector of a state

Theorem 9. *A quadratic Hamiltonian with Hamiltonian matrix H changes the vector \hat{r} of canonical quadrature operators as*

$$e^{i\hat{H}t}\hat{r}e^{-i\hat{H}t} = e^{\Omega H t}\hat{r}. \quad (66)$$

Proof. We will again invoke the BCH formula (Lemma 3) which is restated below for completeness.

$$e^{\hat{X}}\hat{Y}e^{-\hat{X}} = \hat{Y} + [\hat{X}, \hat{Y}] + \frac{1}{2!}[\hat{X}, [\hat{X}, \hat{Y}]] + \frac{1}{3!}[\hat{X}, [\hat{X}, [\hat{X}, \hat{Y}]]] + \dots \quad (67)$$

$$e^{i\hat{H}t}\hat{r}e^{-i\hat{H}t} = \hat{r} + [i\hat{H}t, \hat{r}] + \frac{1}{2!}[i\hat{H}t, [i\hat{H}t, \hat{r}]] + \frac{1}{3!}[i\hat{H}t, [i\hat{H}t, [i\hat{H}t, \hat{r}]]] + \dots \quad (68)$$

Consider $[i\hat{H}t, \hat{r}] = it[\hat{H}, \hat{r}]$ one component at a time.

$$[\hat{H}, \hat{r}_l] = \left[\frac{1}{2} \sum_{jk} \hat{r}_j H_{jk} \hat{r}_k, \hat{r}_l \right] \quad (69)$$

$$= \frac{1}{2} \sum_{jk} H_{jk} (\hat{r}_j \hat{r}_k \hat{r}_l - \hat{r}_l \hat{r}_j \hat{r}_k) \quad (70)$$

$$= \frac{1}{2} \sum_{jk} H_{jk} (\hat{r}_j \hat{r}_k \hat{r}_l - \hat{r}_j \hat{r}_l \hat{r}_k + \hat{r}_j \hat{r}_l \hat{r}_k - \hat{r}_l \hat{r}_j \hat{r}_k) \quad (71)$$

$$= \frac{1}{2} \sum_{jk} H_{jk} (\hat{r}_j [\hat{r}_k, \hat{r}_l] + [\hat{r}_j, \hat{r}_l] \hat{r}_k) \quad (72)$$

$$= \frac{1}{2} \sum_{jk} H_{jk} (\hat{r}_j i\Omega_{kl} + i\Omega_{jl} \hat{r}_k) \quad (73)$$

$$= \frac{i}{2} \sum_{jk} H_{jk} \hat{r}_j \Omega_{kl} + H_{jk} \Omega_{jl} \hat{r}_k \quad (74)$$

$$= \frac{i}{2} \sum_{jk} (-\Omega_{lk}) H_{kj} \hat{r}_j + (-\Omega_{lj}) H_{jk} \hat{r}_k \quad (75)$$

$$= -i[\Omega H \hat{r}]_l \quad (76)$$

In the above, the first two equalities come from the form of \hat{H} . The third equality comes from adding and subtracting the term $\hat{r}_j \hat{r}_l \hat{r}_k$. The fourth equality comes from algebraic simplification, and the fifth equality comes from recognizing that $[\hat{r}_k, \hat{r}_l] = i\Omega_{kl}$. Using the fact that Ω is antisymmetric, we arrive at the final set of equalities.

This implies

$$[i\hat{H}t, \hat{r}] = it[\hat{H}, \hat{r}] \quad (77)$$

$$= it(-i\Omega H \hat{r}) \quad (78)$$

$$= \Omega H t \hat{r}. \quad (79)$$

Using linearity of the commutator,

$$[i\hat{H}t, [i\hat{H}t, \hat{r}]] = [i\hat{H}t, \Omega H t \hat{r}] \quad (80)$$

$$= (\Omega H t)^2 \hat{r} \quad (81)$$

and inductively

$$[i\hat{H}t, \dots [i\hat{H}t, \hat{r}]] = (\Omega H t)^k \hat{r}. \quad (82)$$

In the above, there are $k - 1$ nested commutators, or k commutators in total.

This altogether implies

$$e^{i\hat{H}t} \hat{r} e^{-i\hat{H}t} = \sum_{k=0}^{\infty} \frac{(\Omega H t)^k}{k!} \hat{r} \quad (83)$$

$$= e^{\Omega H t} \hat{r}, \quad (84)$$

concluding the proof. \square

Corollary 10. *A quadratic Hamiltonian with Hamiltonian matrix H changes the mean vector of a state ρ from $\text{Tr}[\hat{r}\rho]$ to $e^{\Omega H t} \text{Tr}[\hat{r}\rho]$.*

Proof. Direct consequence of the above and the following:

$$\bar{r}' = \text{Tr}[\hat{r} e^{-i\hat{H}t} \rho e^{i\hat{H}t}] \quad (85)$$

$$= \text{Tr}[e^{i\hat{H}t} \hat{r} e^{-i\hat{H}t} \rho]. \quad (86)$$

Similar to the procedure with the displacement operator, we have reduced the problem of computing the new mean vector to computing $e^{i\hat{H}t} \hat{r} e^{-i\hat{H}t}$, which was accomplished previously.

Finally we can write the effect on the original mean vector:

$$\bar{r}' = \text{Tr}[e^{i\hat{H}t} \hat{r} e^{-i\hat{H}t} \rho] \quad (87)$$

$$= \text{Tr}[e^{\Omega H t} \hat{r} \rho] \quad (88)$$

$$= e^{\Omega H t} \text{Tr}[\hat{r} \rho], \quad (89)$$

concluding the proof. \square

3.2 Effect of quadratic Hamiltonian on canonical commutation relations

Now that we have seen the effect of a quadratic Hamiltonian on the mean vector of a state, another natural question to ask is the effect of a quadratic Hamiltonian on the canonical commutation relations. In the following, we redefine Ht as H .

Theorem 11. *A quadratic Hamiltonian as defined in (64) leaves the canonical commutation relations unchanged, i.e.*

$$[e^{\Omega H} \hat{r}, (e^{\Omega H} \hat{r})^T] = i\Omega. \quad (90)$$

Proof. For real symmetric H , we have

$$\left[e^{\Omega H} \hat{r}, (e^{\Omega H} \hat{r})^T \right] = e^{\Omega H} [\hat{r}, \hat{r}^T] (e^{\Omega H})^T \quad (91)$$

$$= e^{\Omega H} i\Omega (e^{\Omega H})^T \quad (92)$$

$$= i\Omega. \quad (93)$$

The first equality follows from the linearity of the commutator. The second equality follows by application of the canonical commutation relation. To see the validity of the last equality, consider the following:

$$e^{\Omega H} i\Omega (e^{\Omega H})^T = e^{\Omega H} i\Omega e^{(\Omega H)^T} \quad (94)$$

$$= e^{\Omega H} i\Omega e^{-H\Omega} \quad (95)$$

$$= i\Omega i\Omega e^{\Omega H} i\Omega e^{-H\Omega} \quad (96)$$

$$= i\Omega e^{(i\Omega)\Omega H(i\Omega)} e^{-H\Omega} \quad (97)$$

$$= i\Omega e^{(i\Omega)(i\Omega)H\Omega} e^{-H\Omega} \quad (98)$$

$$= i\Omega e^{H\Omega} e^{-H\Omega} \quad (99)$$

$$= i\Omega. \quad (100)$$

In the above, the first equality can be seen from the functional calculus of matrices. The second equality comes from the antisymmetry of Ω and the symmetry of H . The third equality arises because $(i\Omega)^2 = I$. The fourth equality also follows from the functional calculus of matrices (i.e. $Mf(X)M^{-1} = f(MXM^{-1})$). The fifth equality comes from combining terms and again recognizing that $(i\Omega)^2 = I$. The sixth and last equalities come from algebraic simplification. \square

Definition 12. Any real matrix S for which $S\Omega S^T = \Omega$ is called symplectic; i.e., the action of S preserves the symplectic form Ω .

Corollary 13. The evolution matrix $e^{\Omega H}$ is symplectic.

This is seen from the fact that the evolution $e^{\Omega H}$ preserves the canonical commutation relations.

Lemma 14. All symplectic matrices are invertible and the inverse of symplectic S is given by $S^{-1} = -\Omega S^T \Omega$.

Proof. Consider that

$$S\Omega S^T = \Omega \quad (101)$$

$$\implies S\Omega S^T \Omega^T = \Omega \Omega^T = I \quad (102)$$

$$\implies S^{-1} = \Omega S^T \Omega^T = -\Omega S^T \Omega, \quad (103)$$

concluding the proof. \square

3.3 Necessity for realness of Hamiltonian matrix

In the preceding definition of the standard quadratic Hamiltonian as in (64), we restricted ourselves to only real and symmetric $2n \times 2n$ matrices H . In the following, we will prove that this is indeed the most general consideration and that antisymmetric Hamiltonian matrices H result in a non-Hermitian Hamiltonian.

Lemma 15. *When defining quadratic Hamiltonians, it suffices to restrict ourselves to consider real, symmetric $2n \times 2n$ Hamiltonian matrices.*

Proof. To see this, we consider a general Hamiltonian matrix with symmetric and antisymmetric parts, and arrive at the conclusion that the resulting Hamiltonian is not necessarily Hermitian. This will allow us to conclude that to ensure the Hermiticity of the Hamiltonian operator, the corresponding Hamiltonian matrix must be real and symmetric.

Let H be an arbitrary $2n \times 2n$ matrix. We can write it as

$$H = \frac{H + H^T}{2} + \frac{H - H^T}{2} \quad (104)$$

$$= H^s + H^a \quad (105)$$

where H^s denotes the symmetric part of H , and H^a denotes the antisymmetric part of H . Now consider the operator

$$\frac{1}{2} \hat{r}^T H \hat{r} = \frac{1}{2} \hat{r}^T (H^s + H^a) \hat{r} \quad (106)$$

$$= \frac{1}{2} \hat{r}^T H^s \hat{r} + \frac{1}{2} \hat{r}^T H^a \hat{r}. \quad (107)$$

Focus on the second term in the above.

$$\frac{1}{2} \hat{r}^T H^a \hat{r} = \frac{1}{2} \sum_{jk} \hat{r}_j H_{jk}^a \hat{r}_k \quad (108)$$

$$= \frac{1}{2} \sum_{j < k} \hat{r}_j H_{jk}^a \hat{r}_k + \hat{r}_k H_{kj}^a \hat{r}_j \quad (109)$$

$$= \frac{1}{2} \sum_{j < k} \hat{r}_j H_{jk}^a \hat{r}_k = \hat{r}_k H_{jk}^a \hat{r}_j \quad (110)$$

$$= \frac{1}{2} \sum_{j < k} H_{jk}^a (\hat{r}_j \hat{r}_k - \hat{r}_k \hat{r}_j) \quad (111)$$

$$= \frac{1}{2} \sum_{j < k} H_{jk}^a [\hat{r}_j, \hat{r}_k] \quad (112)$$

$$= \frac{1}{2} \sum_{j < k} H_{jk}^a i \Omega_{jk} \quad (113)$$

$$= \frac{i}{2} \sum_{j < k} H_{jk}^a \Omega_{jk} \quad (114)$$

$$= ic \quad (115)$$

where c is some real number. The key point is that the above term is imaginary.

Thus we see from (107) that if $H^a \neq 0$, then

$$\frac{1}{2}\hat{r}^T H \hat{r} = \frac{1}{2}\hat{r}^T H^s \hat{r} + ic \quad (116)$$

which implies that (107) cannot be Hermitian. We have thus arrived at the desired conclusion. \square

3.4 Obtaining Hamiltonian matrix from symplectic evolution matrix

If $S = e^{\Omega H}$, then S is symplectic for real, symmetric H .

Here, we show a complementary result.

Theorem 16. *If S is diagonalizable with strictly positive eigenvalues, then $H = \Omega^T \ln S$ is symmetric, where \ln denotes the matrix logarithm.*

Proof. Consider that

$$H^T = (\Omega^T \ln S)^T \quad (117)$$

$$= (\ln S)^T \Omega \quad (118)$$

$$= \Omega \Omega^T (\ln S^T) \Omega \quad (119)$$

$$= \Omega \ln (\Omega^T S^T \Omega) \quad (120)$$

$$= \Omega \ln ((-\Omega^T) S^T (-\Omega)) \quad (121)$$

$$= \Omega \ln (\Omega S^T \Omega^T) \quad (122)$$

$$= \Omega \ln S^{-1} \quad (123)$$

$$= -\Omega \ln S \quad (124)$$

$$= \Omega^T \ln S \quad (125)$$

$$= H. \quad (126)$$

Thus we see that $H = H^T$ and that H is real and symmetric.

The first equality comes from the assumption in the theorem. The second equality comes from distributing the transpose operation. The third equality is apparent when one realizes that $\Omega \Omega^T = I$. The fourth equality comes from the functional calculus of matrices. The fifth equality arises from the antisymmetry of Ω . The seventh equality comes from the fact that S is symplectic. \square

Corollary 17. *From any symplectic matrix S that is diagonalizable with strictly positive eigenvalues, we can get its Hamiltonian matrix by using $H = \Omega^T \ln S$.*

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1 Overview

In the previous lecture, we studied transformations of quantum states under evolutions induced by both linear and quadratic Hamiltonians.

In this lecture, we will continue on the same track and proceed to define faithful Gaussian states. Further, we will discuss the most general form that a Gaussian state can take.

2 Quadratic Hamiltonians

2.1 Faithful quantum states

Consider a Hamiltonian of the form

$$\hat{H} = \frac{1}{2} \hat{r}^T H \hat{r} + \hat{r}^T \bar{r}' \quad (1)$$

where $\bar{r}' \in \mathbb{R}^{2n}$ and H is a positive definite $2n \times 2n$ real matrix. A faithful n -mode Gaussian state is defined as follows:

$$\frac{e^{-\beta \hat{H}}}{\text{Tr}[e^{-\beta \hat{H}}]} \text{ for } \beta > 0. \quad (2)$$

The word faithful means that the state is positive definite, which also means that it has full support.

Consider that

$$\hat{H}' \equiv \frac{1}{2} (\hat{r} - \bar{r})^T H (\hat{r} - \bar{r}) \quad (3)$$

$$= \frac{1}{2} (\hat{r}^T H \hat{r} - 2\bar{r}^T H \hat{r} + \|\bar{r}\|_2^2) \quad (4)$$

$$= \frac{1}{2} \hat{r}^T H \hat{r} - \hat{r}^T H \bar{r} + \frac{1}{2} \|\bar{r}\|_2^2. \quad (5)$$

Now if we set $\bar{r} = -H^{-1} \bar{r}'$, we recover the original form of the Hamiltonian in (1) up to an additive constant. That constant term $\|\bar{r}\|_2^2$ can be eliminated after normalization. Furthermore, β can be subsumed into H .

Thus, we take our formal definition of faithful Gaussian states to be as follows:

Definition 1. A *faithful n -mode Gaussian state* is defined as follows:

$$\frac{\exp\left(-\frac{1}{2}(\hat{r} - \bar{r})^T H(\hat{r} - \bar{r})\right)}{\text{Tr}\left[\exp\left(-\frac{1}{2}(\hat{r} - \bar{r})^T H(\hat{r} - \bar{r})\right)\right]}. \quad (6)$$

where $\bar{r} \in \mathbb{R}^{2n}$ and H is a positive definite $2n \times 2n$ real matrix.

It is natural at this point to consider computing the mean vector, covariance matrix, and normalization for a faithful Gaussian state parameterized by \bar{r} and H .

2.2 Simple example of a single-mode state

We will start with perhaps the most simple example possible. Consider a single-mode state with Hamiltonian matrix

$$H = \lambda \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad (7)$$

$\lambda > 0$, and $\bar{r} = 0$.

Then the state is given by

$$\rho = \frac{e^{-\frac{1}{2}\hat{r}^T H \hat{r}}}{\text{Tr}[e^{-\frac{1}{2}\hat{r}^T H \hat{r}}]}. \quad (8)$$

Consider that

$$\frac{1}{2}\hat{r}^T H \hat{r} = \frac{1}{2} \begin{pmatrix} \hat{x} & \hat{p} \end{pmatrix} \begin{pmatrix} \lambda & 0 \\ 0 & \lambda \end{pmatrix} \begin{pmatrix} \hat{x} \\ \hat{p} \end{pmatrix} \quad (9)$$

$$= \frac{\lambda}{2}(\hat{x}^2 + \hat{p}^2). \quad (10)$$

If we now use

$$\hat{n} = \hat{a}^\dagger \hat{a} = \left(\frac{\hat{x} - i\hat{p}}{\sqrt{2}} \right) \left(\frac{\hat{x} + i\hat{p}}{\sqrt{2}} \right) \quad (11)$$

$$= \frac{1}{2}(\hat{x}^2 + \hat{p}^2 + i[\hat{x}, \hat{p}]) \quad (12)$$

$$= \frac{1}{2}(\hat{x}^2 + \hat{p}^2 - 1), \quad (13)$$

then

$$\frac{1}{2}\hat{r}^T H \hat{r} = \lambda(\hat{n} + 1/2). \quad (14)$$

We can use the fact that $\hat{n} = \sum_{n=0}^{\infty} n|n\rangle\langle n|$ to write

$$e^{-\frac{1}{2}\hat{r}^T H \hat{r}} = \sum_{n=0}^{\infty} e^{-\lambda(n+\frac{1}{2})} |n\rangle\langle n| \quad (15)$$

$$= e^{-\frac{\lambda}{2}} \sum_{n=0}^{\infty} e^{-\lambda n} |n\rangle\langle n| \quad (16)$$

$$\implies \text{Tr}[e^{-\frac{1}{2}\hat{r}^T H \hat{r}}] = e^{-\frac{\lambda}{2}} \sum_{n=0}^{\infty} e^{-\lambda n} \quad (17)$$

$$= e^{-\frac{\lambda}{2}} \frac{1}{1 - e^{-\lambda}} \quad (18)$$

$$= \frac{1}{e^{\frac{\lambda}{2}} - e^{-\frac{\lambda}{2}}} \quad (19)$$

$$\equiv z(\lambda). \quad (20)$$

We denote the final quantity as $z(\lambda)$ due to its role as the partition function from statistical mechanics.

2.2.1 Mean vector

We now prove that any state diagonal in the Fock basis has mean vector equal to zero. This follows because

$$\langle n|\hat{x}|n\rangle = \frac{1}{\sqrt{2}} \langle n|\hat{a} + \hat{a}^\dagger|n\rangle \quad (21)$$

$$= \frac{1}{\sqrt{2}} [\langle n|\hat{a}|n\rangle + \langle n|\hat{a}^\dagger|n\rangle] \quad (22)$$

$$= \frac{1}{\sqrt{2}} [\sqrt{n} \langle n|n-1\rangle + \sqrt{n+1} \langle n|n+1\rangle] \quad (23)$$

$$= 0. \quad (24)$$

By a similar calculation, $\langle n|\hat{p}|n\rangle = 0$.

Therefore any state that is diagonal in the Fock (number state) basis has mean vector equal to zero and we can write

$$\text{Tr}[e^{-\frac{1}{2}\hat{r}^T H \hat{r}} \hat{x}] = 0 = \text{Tr}[e^{-\frac{1}{2}\hat{r}^T H \hat{r}} \hat{p}]. \quad (25)$$

2.2.2 Covariance matrix

It is simple to show that $\langle n|\hat{x}\hat{p} + \hat{p}\hat{x}|n\rangle = 0$ and also that

$$\langle n|2\hat{x}^2|n\rangle = 2n + 1 = \langle n|2\hat{p}^2|n\rangle. \quad (26)$$

It follows from

$$\hat{x}\hat{p} + \hat{p}\hat{x} = \frac{1}{2i} \left[(\hat{a} + \hat{a}^\dagger) (\hat{a} - \hat{a}^\dagger) + (\hat{a} - \hat{a}^\dagger) (\hat{a} + \hat{a}^\dagger) \right] \quad (27)$$

$$= \frac{1}{2i} \left[\hat{a}^2 + \hat{a}^\dagger \hat{a} - \hat{a} \hat{a}^\dagger - (\hat{a}^\dagger)^2 + \hat{a}^2 - \hat{a}^\dagger \hat{a} + \hat{a} \hat{a}^\dagger - (\hat{a}^\dagger)^2 \right] \quad (28)$$

$$= \frac{1}{i} \left[\hat{a}^2 - (\hat{a}^\dagger)^2 \right]. \quad (29)$$

Then we find that

$$\langle n | [\hat{x}\hat{p} + \hat{p}\hat{x}] | n \rangle = \frac{1}{i} \langle n | \left[\hat{a}^2 - (\hat{a}^\dagger)^2 \right] | n \rangle \quad (30)$$

$$= \frac{1}{i} \langle n | \hat{a}^2 | n \rangle - \langle n | (\hat{a}^\dagger)^2 | n \rangle \quad (31)$$

$$= \frac{1}{i} \sqrt{n(n-1)} \langle n | n-2 \rangle - \sqrt{(n+1)(n+2)} \langle n | n+2 \rangle \quad (32)$$

$$= 0. \quad (33)$$

Also, we find that

$$\langle n | 2\hat{x}^2 | n \rangle = 2 \langle n | \left(\frac{\hat{a} + \hat{a}^\dagger}{\sqrt{2}} \right)^2 | n \rangle \quad (34)$$

$$= \langle n | \hat{a}^2 + \hat{a}^\dagger \hat{a} + \hat{a} \hat{a}^\dagger + (\hat{a}^\dagger)^2 | n \rangle \quad (35)$$

$$= \langle n | \hat{a}^2 + 2\hat{a}^\dagger \hat{a} + I + (\hat{a}^\dagger)^2 | n \rangle \quad (36)$$

$$= 2n + 1, \quad (37)$$

and similarly,

$$\langle n | 2\hat{p}^2 | n \rangle = 2 \langle n | \left(\frac{\hat{a} - \hat{a}^\dagger}{\sqrt{2}i} \right)^2 | n \rangle \quad (38)$$

$$= -\langle n | \hat{a}^2 - \hat{a}^\dagger \hat{a} - \hat{a} \hat{a}^\dagger + (\hat{a}^\dagger)^2 | n \rangle \quad (39)$$

$$= \langle n | -\hat{a}^2 + 2\hat{a}^\dagger \hat{a} + I - (\hat{a}^\dagger)^2 | n \rangle \quad (40)$$

$$= 2n + 1. \quad (41)$$

This means that

$$\text{Tr} \left[\{ \hat{x}, \hat{p} \} \frac{e^{-\frac{1}{2} \hat{r}^T H \hat{r}}}{z(\lambda)} \right] = 0 \quad (42)$$

and

$$2\text{Tr} \left[\hat{x}^2 \frac{e^{-\frac{1}{2}\hat{r}^T H \hat{r}}}{z(\lambda)} \right] = \frac{1}{z(\lambda)} \text{Tr} \left[2\hat{x}^2 \sum_{n=0}^{\infty} e^{-\lambda(n+\frac{1}{2})} |n\rangle\langle n| \right] \quad (43)$$

$$= \frac{1}{z(\lambda)} \sum_{n=0}^{\infty} e^{-\lambda(n+\frac{1}{2})} 2\text{Tr} [\hat{x}^2 |n\rangle\langle n|] \quad (44)$$

$$= \frac{1}{z(\lambda)} \sum_{n=0}^{\infty} e^{-\lambda(n+\frac{1}{2})} (2n+1) \quad (45)$$

$$= 1 + 2 \frac{e^{-\frac{\lambda}{2}}}{z(\lambda)} \sum_{n=0}^{\infty} e^{-\lambda n} n \quad (46)$$

$$= 1 + 2 \frac{e^{-\frac{\lambda}{2}}}{z(\lambda)} \left[-\frac{d}{d\lambda} \left(\sum_{n=0}^{\infty} e^{-\lambda n} \right) \right] \quad (47)$$

$$= 1 + 2 \frac{e^{-\frac{\lambda}{2}}}{z(\lambda)} \left[-\frac{d}{d\lambda} \left(\frac{1}{1-e^{-\lambda}} \right) \right] \quad (48)$$

$$= 1 + 2 \left(1 - e^{-\lambda} \right) \left[\frac{e^{-\lambda}}{(1-e^{-\lambda})^2} \right] \quad (49)$$

$$= \coth \left(\frac{\lambda}{2} \right) \quad (50)$$

$$\equiv \nu(\lambda) > 1 \text{ for } \lambda > 0 \quad (51)$$

where $\coth x = \frac{e^x + e^{-x}}{e^x - e^{-x}}$.

Similarly, we have

$$2\text{Tr} \left[\hat{p}^2 \frac{e^{-\frac{1}{2}\hat{r}^T H \hat{r}}}{z(\lambda)} \right] = \coth \left(\frac{\lambda}{2} \right). \quad (52)$$

So we have seen that a single-mode state with Hamiltonian matrix $H = \begin{pmatrix} \lambda & 0 \\ 0 & \lambda \end{pmatrix}$ for $\lambda > 0$ has mean vector equal to zero, and covariance matrix σ given by

$$\sigma = \begin{pmatrix} \nu(\lambda) & 0 \\ 0 & \nu(\lambda) \end{pmatrix}, \quad (53)$$

where $\nu(\lambda) = \coth \left(\frac{\lambda}{2} \right)$.

2.2.3 Normalization

The normalization of this state is

$$\text{Tr} [e^{-\frac{1}{2}\hat{r}^T H \hat{r}}] = z(\lambda) = \frac{1}{e^{\frac{\lambda}{2}} - e^{-\frac{\lambda}{2}}}. \quad (54)$$

We can apply our arguments from the previous calculation (specifically (21) and (26)) to conclude that the **mean vector of this state is zero**.

2.3.1 Covariance matrix

The covariance matrix is a diagonal matrix given as

$$\sigma = \bigoplus_{j=1}^n \nu(\lambda_j) \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad (65)$$

where as in the previous, $\nu(\lambda_j) = \coth\left(\frac{\lambda_j}{2}\right) > 1$.

If the covariance matrix elements are given as in (65), then the Hamiltonian is $H = \bigoplus_{j=1}^n \lambda(\nu_j) \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ for $\lambda(\nu) = 2\text{arcoth}(\nu) > 0$.

2.3.2 Normalization

The normalization is given by

$$\text{Tr} \left[\bigotimes_{j=1}^n e^{-\frac{\lambda_j}{2}(\hat{x}_j^2 + \hat{p}_j^2)} \right] = \prod_{j=1}^n \text{Tr} \left[e^{-\frac{\lambda_j}{2}(\hat{x}_j^2 + \hat{p}_j^2)} \right] \quad (66)$$

$$= \prod_{j=1}^n z(\lambda_j) \quad (67)$$

$$= \prod_{j=1}^n \frac{1}{2} \sqrt{\nu_j^2 - 1} \quad (68)$$

$$= \prod_{j=1}^n \sqrt{\text{Det} \left(\frac{\sigma_j + i\Omega_1}{2} \right)} \quad (69)$$

$$= \sqrt{\prod_{j=1}^n \text{Det} \left(\frac{\sigma_j + i\Omega_1}{2} \right)} \quad (70)$$

$$= \sqrt{\text{Det} \left(\frac{\sigma + i\Omega}{2} \right)}. \quad (71)$$

This sequence of steps utilizes the fact that $\sigma + i\Omega = \bigoplus_{j=1}^n \sigma_j + i\Omega_1$ where $\sigma_j = \nu_j \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$. We also used the fact that $\text{Det}(A \oplus B) = \text{Det}(A)\text{Det}(B)$.

To summarize, for multimode states with Hamiltonian matrix $H = \bigoplus_{j=1}^n \lambda_j \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$, the state given by

$$\frac{e^{-\frac{1}{2}\hat{r}^T H \hat{r}}}{\text{Tr}[e^{-\frac{1}{2}\hat{r}^T H \hat{r}}]}$$

has mean vector equal to zero, covariance matrix

$$\sigma = \bigoplus_{j=1}^n \nu(\lambda_j) \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad (72)$$

with $\nu(\lambda_j) = \coth\left(\frac{\lambda_j}{2}\right)$ and normalization

$$\prod_{j=1}^n z(\lambda_j) = \sqrt{\text{Det}\left(\frac{\sigma + i\Omega}{2}\right)}. \quad (73)$$

3 Towards a general Gaussian state

In this section, we work towards establishing the most general form that a Gaussian state can take. We begin with a quadratic Hamiltonian, act upon it by congruence with a symplectic matrix S , and lastly we displace the state to obtain the most general form.

Suppose now that we take such a diagonal Hamiltonian H and act on it by congruence with a symplectic matrix S to produce a new Hamiltonian matrix H' .

$$H' = S^T H S \quad (74)$$

where $S = e^{\Omega A}$ for symmetric and real A . Consider now the state

$$\rho = \frac{e^{-\frac{1}{2}\hat{r}^T H' \hat{r}}}{\text{Tr}\left[e^{-\frac{1}{2}\hat{r}^T H' \hat{r}}\right]} = \frac{e^{-\frac{1}{2}\hat{r}^T S^T H S \hat{r}}}{\text{Tr}\left[e^{-\frac{1}{2}\hat{r}^T S^T H S \hat{r}}\right]} \quad (75)$$

3.1 Mean Vector

In the following, we will show how the mean vector of ρ as defined in (75) is equal to zero.

We have

$$S\hat{r} = e^{\Omega A}\hat{r} = e^{\frac{i}{2}\hat{r}^T A \hat{r}}\hat{r}e^{-\frac{i}{2}\hat{r}^T A \hat{r}} \quad (76)$$

$$(77)$$

and

$$S^{-1}\hat{r} = e^{-\Omega A}\hat{r} = e^{\frac{i}{2}\hat{r}^T (-A) \hat{r}}\hat{r}e^{-\frac{i}{2}\hat{r}^T (-A) \hat{r}} \quad (78)$$

$$= e^{-\frac{i}{2}\hat{r}^T A \hat{r}}\hat{r}e^{\frac{i}{2}\hat{r}^T A \hat{r}}. \quad (79)$$

$$\implies \frac{1}{2} \hat{r}^T S^T H S \hat{r} = \frac{1}{2} (S \hat{r})^T H S \hat{r} \quad (80)$$

$$= \frac{1}{2} \left(e^{\frac{i}{2} \hat{r}^T A \hat{r}} \hat{r} e^{-\frac{i}{2} \hat{r}^T A \hat{r}} \right)^T H \left(e^{\frac{i}{2} \hat{r}^T A \hat{r}} \hat{r} e^{-\frac{i}{2} \hat{r}^T A \hat{r}} \right) \quad (81)$$

$$= e^{\frac{i}{2} \hat{r}^T A \hat{r}} \frac{1}{2} \hat{r}^T H \hat{r} e^{-\frac{i}{2} \hat{r}^T A \hat{r}} \quad (82)$$

$$\implies e^{-\frac{1}{2} \hat{r}^T S^T H S \hat{r}} = e^{\frac{i}{2} \hat{r}^T A \hat{r}} e^{-\frac{1}{2} \hat{r}^T H \hat{r}} e^{-\frac{i}{2} \hat{r}^T A \hat{r}} \quad (83)$$

$$(84)$$

$$\implies \text{mean vector of } \frac{e^{-\frac{1}{2} \hat{r}^T S^T H S \hat{r}}}{\text{Tr} \left[e^{-\frac{1}{2} \hat{r}^T S^T H S \hat{r}} \right]}$$

$$= \text{Tr} \left[\frac{\hat{r} e^{\frac{i}{2} \hat{r}^T A \hat{r}} e^{-\frac{1}{2} \hat{r}^T H \hat{r}} e^{-\frac{i}{2} \hat{r}^T A \hat{r}}}{\text{Tr} \left[e^{-\frac{1}{2} \hat{r}^T H \hat{r}} \right]} \right] \quad (85)$$

$$= \text{Tr} \left[e^{-\frac{i}{2} \hat{r}^T A \hat{r}} \hat{r} e^{\frac{i}{2} \hat{r}^T A \hat{r}} \frac{e^{-\frac{1}{2} \hat{r}^T H \hat{r}}}{\text{Tr} \left[e^{-\frac{1}{2} \hat{r}^T H \hat{r}} \right]} \right] \quad (86)$$

$$= \text{Tr} \left[S^{-1} \hat{r} \frac{e^{-\frac{1}{2} \hat{r}^T H \hat{r}}}{\text{Tr} \left[e^{-\frac{1}{2} \hat{r}^T H \hat{r}} \right]} \right] \quad (87)$$

$$= S^{-1} \cdot 0 = 0. \quad (88)$$

In the above, the second equality arises due to cyclicity of the trace. The third equality follows from (79). S^{-1} can then be pulled out of the trace operation and the final equality follows from the earlier performed calculations in 2.2.1.

3.2 Covariance Matrix

Since the mean vector is zero, the covariance matrix is given by

$$\sigma = \text{Tr} \left[\{ \hat{r}, \hat{r}^T \} e^{\frac{i}{2} \hat{r}^T A \hat{r}} \frac{e^{-\frac{1}{2} \hat{r}^T H \hat{r}}}{\text{Tr} \left[e^{-\frac{1}{2} \hat{r}^T H \hat{r}} \right]} e^{-\frac{i}{2} \hat{r}^T A \hat{r}} \right] \quad (89)$$

$$= \text{Tr} \left[e^{-\frac{i}{2} \hat{r}^T A \hat{r}} \{ \hat{r}, \hat{r}^T \} e^{\frac{i}{2} \hat{r}^T A \hat{r}} \frac{e^{-\frac{1}{2} \hat{r}^T H \hat{r}}}{\text{Tr} \left[e^{-\frac{1}{2} \hat{r}^T H \hat{r}} \right]} \right] \quad (90)$$

$$= \text{Tr} \left[\{ S^{-1} \hat{r}, (S^{-1} \hat{r})^T \} \frac{e^{-\frac{1}{2} \hat{r}^T H \hat{r}}}{\text{Tr} \left[e^{-\frac{1}{2} \hat{r}^T H \hat{r}} \right]} \right] \quad (91)$$

$$= S^{-1} \text{Tr} \left[\{ \hat{r}, \hat{r}^T \} \frac{e^{-\frac{1}{2} \hat{r}^T H \hat{r}}}{\text{Tr} \left[e^{-\frac{1}{2} \hat{r}^T H \hat{r}} \right]} \right] S^{-T} \quad (92)$$

$$= S^{-1} \sigma S^{-T} \quad (93)$$

$$\equiv \sigma'. \quad (94)$$

$$\implies \sigma' = S^{-1} \left(\bigoplus_{j=1}^n \coth \left(\frac{\lambda_j}{2} \right) \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right) S^{-T}. \quad (95)$$

In the above, the first equality arises from the definition of the covariance matrix. The second equality results from the cyclicity of trace. The third equality arises from applying (79). The fourth equality comes from recognizing that S^{-1} and S^{-T} can be taken out of the trace. Finally one can recognize the original covariance matrix and obtain the expression for σ' .

3.3 Normalization

$$\text{Tr} \left[e^{-\frac{1}{2}\hat{r}^T H' \hat{r}} \right] = \text{Tr} \left[e^{\frac{i}{2}\hat{r}^T A \hat{r}} e^{-\frac{1}{2}\hat{r}^T H \hat{r}} e^{-\frac{i}{2}\hat{r}^T A \hat{r}} \right] \quad (96)$$

$$= \text{Tr} \left[e^{-\frac{1}{2}\hat{r}^T H \hat{r}} \right] \quad (97)$$

$$= \sqrt{\text{Det} \left(\frac{\sigma + i\Omega}{2} \right)}. \quad (98)$$

In the above, we used the cyclicity of trace to make the simplification.

For symplectic S , we have the following properties (proved in section 4).

$$\text{Det}(S) = 1 = \text{Det}(S^{-1}) \quad (99)$$

$$= \text{Det}(S^{-T}). \quad (100)$$

Thus we can write

$$\sqrt{\text{Det} \left(\frac{\sigma + i\Omega}{2} \right)} = \sqrt{\text{Det}(S^{-1}) \text{Det} \left(\frac{\sigma + i\Omega}{2} \right) \text{Det}(S^{-T})} \quad (101)$$

$$= \sqrt{\text{Det} \left(S^{-1} \left(\frac{\sigma + i\Omega}{2} \right) S^{-T} \right)} \quad (102)$$

$$= \sqrt{\text{Det} \left(\frac{\sigma' + i\Omega}{2} \right)} \quad (103)$$

where we used that $S\Omega S^T = \Omega$.

3.4 Displacing the state

Now suppose that we act on the new state characterized in the above by a displacement operator $\hat{D}_{\vec{r}} = \exp(i\vec{r}^T \Omega \hat{r})$.

$$\hat{D}_{-\vec{r}} e^{-\frac{1}{2}\hat{r}^T H' \hat{r}} \hat{D}_{\vec{r}} = e^{-\frac{1}{2}[\hat{D}_{-\vec{r}} \hat{r}^T H' \hat{r} \hat{D}_{\vec{r}}]} \quad (104)$$

If we write

$$\hat{r}^T H' \hat{r} = \sum_{jk} \hat{r}_j H'_{jk} \hat{r}_k \quad (105)$$

then we can see that

$$\hat{D}_{-\bar{r}} \hat{r}^T H' \hat{r} \hat{D}_{\bar{r}} = \sum_{jk} \hat{D}_{-\bar{r}} \hat{r}_j \hat{D}_{\bar{r}} H'_{jk} \hat{D}_{-\bar{r}} \hat{r}_k \hat{D}_{\bar{r}} \quad (106)$$

$$= \sum_{jk} (\hat{r}_j - \bar{r}_j) H'_{jk} (\hat{r}_j - \bar{r}_j) \quad (107)$$

which yields

$$\hat{D}_{-\bar{r}} e^{-\frac{1}{2} \hat{r}^T H' \hat{r}} \hat{D}_{\bar{r}} = e^{-\frac{1}{2} [\hat{D}_{-\bar{r}} \hat{r}^T H' \hat{r} \hat{D}_{\bar{r}}]} \quad (108)$$

$$= e^{-\frac{1}{2} (\hat{r} - \bar{r})^T H' (\hat{r} - \bar{r})}. \quad (109)$$

This implies that under this change of the new state (via a displacement operator), the mean vector translates from zero to \bar{r} .

The covariance matrix, on the other hand, remains unchanged because it is invariant to changes in the mean vector alone. By this observation, it also follows that the normalization of the state is unchanged.

This **faithful Gaussian state** can be written as

$$\frac{e^{-\frac{1}{2} (\hat{r} - \bar{r})^T H' (\hat{r} - \bar{r})}}{\sqrt{\text{Det} \left(\frac{\sigma' + i\Omega}{2} \right)}} \quad (110)$$

where

$$H' = S^T \bigoplus_{j=1}^n \lambda_j \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} S \quad (111)$$

and

$$\sigma' = S^{-1} \bigoplus_{j=1}^n \coth \left(\frac{\lambda_j}{2} \right) \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} S^{-T}. \quad (112)$$

Notice the similarity of (110) to the expression for a classical multimode Gaussian density function.

The form of the faithful Gaussian state stated above is actually the **most general form** that a faithful Gaussian quantum state can take.

By everything that we have done in the preceding pages, we can write

$$\frac{e^{-\frac{1}{2} (\hat{r} - \bar{r})^T H' (\hat{r} - \bar{r})}}{\sqrt{\text{Det} \left(\frac{\sigma' + i\Omega}{2} \right)}} = \frac{\hat{D}_{-\bar{r}} \hat{S}_A e^{-\frac{1}{2} \hat{r}^T H \hat{r}} \hat{S}_A^\dagger \hat{D}_{\bar{r}}}{\text{Tr} \left[e^{-\frac{1}{2} \hat{r}^T H \hat{r}} \right]} \quad (113)$$

where

$$H = \bigoplus_{j=1}^n \lambda_j \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad (114)$$

with $\lambda_j > 0$,

$$\hat{S}_A = e^{\frac{i}{2} \hat{r}^T A \hat{r}} \quad (115)$$

and

$$\mathrm{Tr} \left[e^{-\frac{1}{2}\hat{r}^T H \hat{r}} \right] = \sqrt{\mathrm{Det} \left(\frac{\sigma + i\Omega}{2} \right)} \quad (116)$$

$$= \sqrt{\mathrm{Det} \left(\frac{\sigma' + i\Omega}{2} \right)} \quad (117)$$

with $\sigma = \bigoplus_{j=1}^n \nu(\lambda_j) \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ where $\nu(\lambda) = \coth \left(\frac{\lambda}{2} \right)$.

4 Determinant of a symplectic matrix

In the following we prove that the determinant of a symplectic matrix is equal to one.

Lemma 2. *Any symplectic matrix has determinant equal to one.*

Proof. Consider that S is a symplectic matrix. We then have $S\Omega S^T = \Omega$. Beginning with that and taking determinant on both sides, we have the following:

$$\implies \mathrm{Det}(S\Omega S^T) = \mathrm{Det}(\Omega) \quad (118)$$

$$\implies \mathrm{Det}(S)\mathrm{Det}(\Omega)\mathrm{Det}(S^T) = \mathrm{Det}(\Omega) = 1 \quad (119)$$

$$\implies \mathrm{Det}(S)\mathrm{Det}(S^T) = 1 \quad (120)$$

$$\implies \mathrm{Det}(S)^2 = 1 \quad (121)$$

$$\implies \mathrm{Det}(S) = \pm 1. \quad (122)$$

The second line follows from the fact that $\mathrm{Det}(\Omega) = 1$. The fourth line is due to the invariance of the determinant to transposition of its argument.

Now that we have established that $\mathrm{Det}(S) = \pm 1$, we need to eliminate the possibility that $\mathrm{Det}(S) = -1$ to conclude the proof.

Using the fact that any symplectic matrix is invertible (and thus full-rank), it follows that $S^T S$ is a symmetric positive definite matrix. This implies that the eigenvalues of $S^T S + \mathbb{I}$ are greater than one.

Thus

$$S^T S + \mathbb{I} = S^T (S + S^{-T}) \quad (123)$$

$$= S^T (S + \Omega S \Omega^T) \quad (124)$$

which is due to

$$S\Omega S^T = \Omega \quad (125)$$

$$\implies S\Omega S^T \Omega^T = \Omega \Omega^T = \mathbb{I} \quad (126)$$

$$\implies S^{-1} = \Omega S^T \Omega^T \quad (127)$$

$$\implies S^{-T} = \Omega S \Omega^T. \quad (128)$$

Consider that $\Omega = \bigoplus_{j=1}^n \Omega_1 = \mathbb{I} \otimes \Omega_1$. Then, if we write S as follows,

$$S = \sum_{j,k \in \{0,1\}} S_{jk} \otimes |j\rangle\langle k| \quad (129)$$

we get

$$S + \Omega S \Omega^T = \sum_{jk} S_{jk} \otimes |j\rangle\langle k| + (\mathbb{I} \otimes \Omega_1) (S_{jk} \otimes |j\rangle\langle k|) (\mathbb{I}_n \otimes \Omega_1^T) \quad (130)$$

$$= \sum_{jk} S_{jk} \otimes [|j\rangle\langle k| + \Omega_1 |j\rangle\langle k| \Omega_1^T]. \quad (131)$$

Using $\Omega_1 |0\rangle = -|1\rangle$ and $\Omega_1 |1\rangle = |0\rangle$,

$$|j\rangle\langle k| + \Omega_1 |j\rangle\langle k| \Omega_1^T = |j\rangle\langle k| + (-1)^{j+1} (-1)^{k+1} |j \oplus 1\rangle\langle k \oplus 1| \quad (132)$$

$$= |j\rangle\langle k| + (-1)^{j+k} |j \oplus 1\rangle\langle k \oplus 1| \quad (133)$$

$$\implies S + \Omega S \Omega^T = \sum_{jk} S_{jk} \otimes [|j\rangle\langle k| + \Omega_1 |j\rangle\langle k| \Omega_1^T] \quad (134)$$

$$= (S_{00} + S_{11}) \otimes |0\rangle\langle 0| + (S_{01} - S_{10}) \otimes |0\rangle\langle 1| \quad (135)$$

$$+ (-S_{01} + S_{10}) \otimes |1\rangle\langle 0| + (S_{00} + S_{11}) \otimes |1\rangle\langle 1|. \quad (136)$$

Define real matrices C and D as follows:

$$C = S_{00} + S_{11} \quad (137)$$

$$D = S_{01} - S_{10}. \quad (138)$$

$$\implies S + \Omega S \Omega^T = C \otimes |0\rangle\langle 0| + D \otimes |0\rangle\langle 1| - D \otimes |1\rangle\langle 0| + C \otimes |1\rangle\langle 1| \quad (139)$$

$$= (\mathbb{I} \otimes \underline{u}) ([C + iD] \otimes |0\rangle\langle 0| + [C - iD] \otimes |1\rangle\langle 1|) (\mathbb{I} \otimes \underline{u}^\dagger) \quad (140)$$

where $\underline{u} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ i & -i \end{bmatrix}$.

We then get

$$0 < 1 < \text{Det}(S^T S + \mathbb{I}) \quad (141)$$

$$= \text{Det}(S^T (S + \Omega S \Omega^T)) \quad (142)$$

$$= \text{Det}(S^T) \text{Det}(S + \Omega S \Omega^T) \quad (143)$$

$$= \text{Det}(S) \text{Det}(\mathbb{I} \otimes \underline{u}) \text{Det}(C + iD) \text{Det}(C - iD) \text{Det}(\mathbb{I} \otimes \underline{u}^\dagger) \quad (144)$$

$$= \text{Det}(S) \text{Det}(C + iD) \text{Det}(\overline{C + iD}) \quad (145)$$

$$= \text{Det}(S) \text{Det}(C + iD) \overline{\text{Det}(C + iD)} \quad (146)$$

$$= \text{Det}(S) |\text{Det}(C + iD)|^2. \quad (147)$$

Since $\text{Det}(S)|\text{Det}(C + iD)|^2 > 0$, it must be the case that $\text{Det}(S) > 0$.

Thus we can conclude that $\text{Det}(S) \neq -1$ and hence the only remaining possibility, by necessity, is that $\text{Det}(S) = 1$. \square

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1 Overview

In the previous lecture, we defined and studied faithful Gaussian states as thermal states of quadratic Hamiltonians.

In this lecture, we continue the analysis of faithful states as thermal states of quadratic Hamiltonians, and via the Williamson Theorem, we show and prove the form of a general Gaussian state.

2 Recap

In the previous lecture, we defined a faithful Gaussian state to be a thermal state

$$\frac{e^{-\hat{H}}}{\text{Tr}[e^{-\hat{H}}]} \quad (1)$$

of a quadratic Hamiltonian

$$\hat{H} = \frac{1}{2}(\hat{r} - \bar{r})^T H (\hat{r} - \bar{r}) \quad (2)$$

where $\bar{r} \in \mathbb{R}^{2n}$ and H is a $2n \times 2n$ positive definite real matrix.

We showed how to build up a faithful Gaussian state with Hamiltonian matrix

$$H' = S^T H S, \quad (3)$$

$$H = \bigoplus_{j=1}^n \lambda_j \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (4)$$

with $\lambda_j > 0 \forall j \in \{1, \dots, n\}$, S symplectic, and Hamiltonian operator

$$\hat{H}' = \frac{1}{2}(\hat{r} - \bar{r})^T S^T H S (\hat{r} - \bar{r}) \quad (5)$$

$$= \frac{1}{2}(\hat{r} - \bar{r})^T H' (\hat{r} - \bar{r}). \quad (6)$$

This yields a quantum Gaussian state with the following density operator:

$$\rho_G = \frac{e^{-\frac{1}{2}(\hat{r}-\bar{r})^T H' (\hat{r}-\bar{r})}}{\sqrt{\text{Det} \left(\frac{\sigma' + i\Omega}{2} \right)}} \quad (7)$$

where the mean vector of ρ_G is \bar{r} and the covariance matrix is

$$\sigma' = S^{-1}\sigma S^{-T} \quad \text{with} \quad \sigma = \bigoplus_{j=1}^n \coth\left(\frac{\lambda_j}{2}\right) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \quad (8)$$

Also, we noted that ρ_G can be written as

$$\rho_G = \frac{\hat{D}_{-\bar{r}} \hat{S} e^{-\frac{1}{2} \hat{r}^T H' \hat{r}} \hat{S}^\dagger \hat{D}_{\bar{r}}}{\sqrt{\text{Det}\left(\frac{\sigma' + i\Omega}{2}\right)}} \quad (9)$$

where $S = e^{\frac{i}{2} \hat{r}^T (\Omega^T \ln S) \hat{r}}$ and $\hat{D}_{\bar{r}} = \exp(i\bar{r}^T \Omega \hat{r})$.¹

Since H is diagonal,

$$\frac{e^{-\frac{1}{2} \hat{r}^T H \hat{r}}}{\sqrt{\text{Det}\left(\frac{\sigma' + i\Omega}{2}\right)}} = \bigotimes_{j=1}^n \frac{e^{-\lambda_j(\hat{n}_j + \frac{1}{2})}}{z(\lambda_j)} \quad (10)$$

with $z(\lambda_j) = [e^{\lambda_j/2} - e^{-\lambda_j/2}]^{-1}$.

Note that $\frac{e^{-\lambda(\hat{n} + \frac{1}{2})}}{z(\lambda)}$ is typically called the bosonic thermal state, and has mean photon number $\langle \hat{n} \rangle = \frac{1}{2} \langle \hat{x}^2 + \hat{p}^2 - 1 \rangle = \coth\left(\frac{\lambda}{2}\right) - \frac{1}{2}$.

3 Form of a general Gaussian state

Now we will prove, perhaps surprisingly, that the state given in (7) is the most general form that a faithful Gaussian state can take.

Theorem 1. *A Gaussian state given in the form*

$$\rho_G = \frac{e^{-\frac{1}{2}(\hat{r}-\bar{r})^T H'(\hat{r}-\bar{r})}}{\sqrt{\text{Det}\left(\frac{\sigma' + i\Omega}{2}\right)}}, \quad (11)$$

with H' as in (3), is the most general form for any faithful Gaussian state.

Proof. Suppose that the faithful Gaussian state is given by

$$\rho_G = \frac{e^{-\frac{1}{2}(\hat{r}-\bar{r})^T H(\hat{r}-\bar{r})}}{\text{Tr}\left[e^{-\frac{1}{2}(\hat{r}-\bar{r})^T H(\hat{r}-\bar{r})}\right]} \quad (12)$$

where $\bar{r} \in \mathbb{R}^{2n}$ and H is a $2n \times 2n$ real positive definite matrix.

Then, by the Williamson Theorem given below, there exists symplectic S such that

$$H = S^T H_{\text{diag}} S \quad (13)$$

¹Note that for some S , we may need two quadratic evolutions, not one.

where $H_{\text{diag}} = \bigoplus_{j=1}^n \lambda_j \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ for $\lambda_j > 0 \quad \forall j \in \{1, \dots, n\}$ so that we can write ρ_G as

$$\frac{e^{-\frac{1}{2}(\hat{r}-\bar{r})^T S^T H_{\text{diag}} S(\hat{r}-\bar{r})}}{\text{Tr} \left[e^{-\frac{1}{2}(\hat{r}-\bar{r})^T S^T H_{\text{diag}} S(\hat{r}-\bar{r})} \right]} \quad (14)$$

Then by manipulations we have already conducted, there exists a unitary \hat{S} (generated by a quadratic Hamiltonian) and a displacement operator $\hat{D}_{\bar{r}} = \exp(i\bar{r}^T \Omega \hat{r})$ such that ρ_G is given as

$$\propto \hat{D}_{-\bar{r}} \hat{S} e^{-\frac{1}{2} \hat{r}^T H' \hat{r}} \hat{S}^\dagger \hat{D}_{\bar{r}} \quad (15)$$

and the normalization is given by

$$\sqrt{\text{Det} \left(\frac{\sigma' + i\Omega}{2} \right)}, \quad (16)$$

with σ' defined in (8). □

3.1 Williamson Theorem

Theorem 2 (Williamson). *Given a $2n \times 2n$ positive definite real matrix M , there exists a symplectic transformation S such that*

$$SMS^T = D, \quad (17)$$

with

$$D = \bigoplus_{j=1}^n d_j \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (18)$$

and $d_j > 0 \quad \forall j \in \{1, \dots, n\}$. The set $\{d_j\}_{j=1}^n$ is the set of symplectic eigenvalues of M .

Before proving the Williamson Theorem, we recall a standard lemma about the decomposition of real antisymmetric matrices.

Lemma 3. *Let A be a real, full-rank, antisymmetric $2n \times 2n$ matrix (i.e., $A = -A^T$). Then there exists a real orthogonal $2n \times 2n$ matrix O such that*

$$OAO^T = \bigoplus_{j=1}^n c_j \Omega_1, \quad (19)$$

where $\Omega_1 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ and $c_j > 0$.

Proof. Since A is antisymmetric and full rank, it follows that the matrix A^2 is symmetric and negative definite because

$$A^2 = AA = -A^T A < 0 \quad (20)$$

since $A^T A$ is positive definite for any full rank A . Thus there exists an orthogonal transformation O' such that $O' A^2 O'^T = B$ with B diagonal and having strictly negative entries.

Let $|\psi\rangle$ be some eigenvector of A^2 with eigenvalue $b_1 < 0$.

Then

$$\|A|\psi\rangle\|^2 = \langle\psi|A^T A|\psi\rangle = -\langle\psi|A^2|\psi\rangle = -b_1 = |b_1|. \quad (21)$$

So $|\psi'\rangle = \frac{A|\psi\rangle}{\sqrt{|b_1|}}$ is normalized and orthogonal to $|\psi\rangle$ because

$$\langle\psi|\psi'\rangle = \frac{\langle\psi|A\psi\rangle}{\sqrt{|b_1|}} = \frac{(\langle\psi|A\psi\rangle)^T}{\sqrt{|b_1|}} \quad (22)$$

$$= \frac{\langle\psi|A^T\psi\rangle}{\sqrt{|b_1|}} = -\frac{\langle\psi|A\psi\rangle}{\sqrt{|b_1|}} = 0. \quad (23)$$

In the above, we showed that $\langle\psi|\psi'\rangle = -\langle\psi|\psi'\rangle$ and thus $\langle\psi|\psi'\rangle = 0$.

Suppose now that $|\phi\rangle$ is in the subspace orthogonal to $\text{span}\{|\psi\rangle, |\psi'\rangle\}$. This implies that

$$\langle\phi|A\psi\rangle = \langle\phi|\psi'\rangle \sqrt{|b_1|} = 0, \quad (24)$$

$$\langle\phi|A\psi'\rangle = \frac{\langle\phi|A^2\psi\rangle}{\sqrt{|b_1|}} = \frac{\langle\phi|\psi\rangle b_1}{\sqrt{|b_1|}} \quad (25)$$

$$= -\langle\phi|\psi\rangle \sqrt{|b_1|} \quad (26)$$

$$= 0. \quad (27)$$

Furthermore, due to the antisymmetry of A , $\langle\psi|A\psi\rangle = 0 = \langle\psi'|A\psi'\rangle$.

Also,

$$\langle\psi|A\psi'\rangle = \frac{\langle\psi|A^2\psi\rangle}{\sqrt{|b_1|}} = \frac{b_1 \langle\psi|\psi\rangle}{\sqrt{|b_1|}} = -\sqrt{|b_1|}, \quad (28)$$

$$\langle\psi'|A\psi\rangle = \sqrt{|b_1|}, \quad (29)$$

where the second statement above is due to the antisymmetry of A .

Now define the orthogonal matrix O_1 as

$$O_1 = [|\psi'\rangle \quad |\psi\rangle \quad |v_1\rangle \quad \dots \quad |v_{2n-2}\rangle], \quad (30)$$

where $|v_1\rangle, \dots, |v_{2n-2}\rangle$ is a set of orthonormal vectors orthogonal to $|\psi'\rangle$ and $|\psi\rangle$.

Putting everything above together, we conclude that

$$O_1^T A O_1 = \begin{pmatrix} \sqrt{|b_1|} \Omega_1 & 0 \\ 0 & A' \end{pmatrix} \quad (31)$$

and we see that this step gives the first step of the decomposition, after setting $c_1 = \sqrt{|b_1|}$. The matrix A' is antisymmetric, and so this procedure can be repeated exhaustively to complete the decomposition.

□

Proof. **Proof of Williamson Theorem**

Consider the matrix $M^{-\frac{1}{2}} \Omega M^{-\frac{1}{2}}$. It is real and $2n \times 2n$.

Due to the symmetry of M and antisymmetry of Ω , it follows that $M^{-\frac{1}{2}}\Omega M^{-\frac{1}{2}}$ is antisymmetric. Additionally, since both M and Ω are full rank, $M^{-\frac{1}{2}}\Omega M^{-\frac{1}{2}}$ is also full rank.

Thus by invoking Lemma 3 above, there exists a real orthogonal transform O such that

$$OM^{-\frac{1}{2}}\Omega M^{-\frac{1}{2}}O^T = \bigoplus_{j=1}^n d_j^{-1}\Omega_1 \quad \text{with } d_j > 0. \quad (32)$$

Define $\underline{D} = \begin{bmatrix} d_1 & & \\ & \ddots & \\ & & d_n \end{bmatrix}$, an $n \times n$ matrix, and set $D = \underline{D} \otimes I_2$.

Then we have $\bigoplus_{j=1}^n \frac{1}{d_j}\Omega_1 = \underline{D}^{-1} \otimes \Omega_1$. Using this expression, we find that

$$D^{\frac{1}{2}} \left[\bigoplus_{j=1}^n \frac{1}{d_j}\Omega_1 \right] D^{\frac{1}{2}} = \left(\underline{D}^{\frac{1}{2}} \otimes I_2 \right) \left(\underline{D}^{-1} \otimes \Omega_1 \right) \left(\underline{D}^{\frac{1}{2}} \otimes I_2 \right) \quad (33)$$

$$= I_n \otimes \Omega_1 = \Omega. \quad (34)$$

$$\implies D^{\frac{1}{2}}OM^{-\frac{1}{2}}\Omega M^{-\frac{1}{2}}O^T D^{\frac{1}{2}} = \Omega. \quad (35)$$

Now set

$$S \equiv D^{\frac{1}{2}}OM^{-\frac{1}{2}}, \quad (36)$$

and we conclude from (35) that $S\Omega S^T = \Omega$, so that S is symplectic.

Also,

$$SMS^T = \left(D^{\frac{1}{2}}OM^{-\frac{1}{2}} \right) M \left(D^{\frac{1}{2}}OM^{-\frac{1}{2}} \right)^T \quad (37)$$

$$= D^{\frac{1}{2}}OM^{-\frac{1}{2}}MM^{-\frac{1}{2}}O^T D^{\frac{1}{2}} \quad (38)$$

$$= D^{\frac{1}{2}}OO^T D^{\frac{1}{2}} \quad (39)$$

$$= D^{\frac{1}{2}}D^{\frac{1}{2}} \quad (40)$$

$$= D. \quad (41)$$

The statement of the Williamson Theorem is that for a positive definite and real $2n \times 2n$ matrix M , there exists a $2n \times 2n$ symplectic matrix S such that $SMS^T = D$. We have proved by construction of S that such a transform exists. Thus, we have completed the proof of the Williamson Theorem. \square

We can now apply the Williamson Theorem to the Hamiltonian matrix for a faithful Gaussian state.

We recall the form of a Gaussian state

$$\frac{e^{-\hat{H}}}{\text{Tr}[e^{-\hat{H}}]} = \frac{e^{-\frac{1}{2}(\hat{r}-\bar{r})^T H (\hat{r}-\bar{r})}}{\text{Tr}[e^{-\hat{H}}]} \quad (42)$$

$$= \frac{\hat{D}_{-\bar{r}} e^{-\frac{1}{2}\hat{r}^T H \hat{r}} \hat{D}_{\bar{r}}}{\text{Tr}[e^{-\frac{1}{2}\hat{r}^T H \hat{r}}]}. \quad (43)$$

We use the symplectic diagonalization of H as $H = S_H^T (\Lambda \otimes I_2) S_H$ where $\Lambda = \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_j \end{bmatrix}$, and S_H is the transposed inverse of the symplectic transformation that puts H in symplectic normal form.

Then

$$\frac{1}{2} \hat{r}^T H \hat{r} = \frac{1}{2} \hat{r}^T S_H^T (\Lambda \otimes I_2) S_H \hat{r} \quad (44)$$

$$= \frac{1}{2} (S_H \hat{r})^T (\Lambda \otimes I_2) S_H \hat{r}. \quad (45)$$

We can then think of S_H as a coordinate transformation and can define a new set of quadrature operators as $\hat{r}' = S_H \hat{r}$. This is possible since $[\hat{r}', \hat{r}'^T] = i\Omega$.

Then the Hamiltonian

$$\frac{1}{2} \hat{r}'^T H \hat{r}' = \frac{1}{2} \hat{r}'^T (\Lambda \otimes I_2) \hat{r}' \quad (46)$$

is diagonal with respect to this new notation.

Now consider that

$$\frac{1}{2} \hat{r}'^T (\Lambda \otimes I_2) \hat{r}' = \frac{1}{2} \sum_{jk} \hat{r}'_j (\Lambda \otimes I_2)_{jk} \hat{r}'_k \quad (47)$$

$$= \frac{1}{2} \sum_j \lambda_j [\hat{x}_j'^2 + \hat{p}_j'^2]. \quad (48)$$

4 Symplectic decomposition of a positive definite matrix

Given a positive definite M , how can one compute its symplectic matrix S and its symplectic eigenvalues?

To do the task described above, one need only perform the usual eigendecomposition of the matrix $i\Omega M$. Why does this work? By the Williamson Theorem, it follows that

$$M = SDS^T \quad (49)$$

for S symplectic, and where $D = \bigoplus_{j=1}^n d_j \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ is the diagonal matrix of symplectic eigenvalues of M .

Then consider that

$$i\Omega M = i\Omega SDS^T \quad (50)$$

$$= i\Omega S(\underline{D} \otimes I_2) S^T, \quad (51)$$

where $\underline{D} = \begin{bmatrix} d_1 & & \\ & \ddots & \\ & & d_n \end{bmatrix}$.

5 Relation between Hamiltonian matrix and covariance matrix

What is the relationship between the Hamiltonian matrix H and the covariance matrix σ for a general Gaussian state?

Lemma 4. *For a general Gaussian state, the Hamiltonian matrix and covariance matrix are related to each other by*

$$\sigma = \coth\left(\frac{i\Omega H}{2}\right) i\Omega, \quad (67)$$

$$H = 2 \operatorname{arccoth}(i\Omega\sigma) i\Omega, \quad (68)$$

which can be seen as a generalization of what was found for the diagonal case.

Proof. Start with positive definite matrix H . The symplectic diagonalization is

$$H = S^T \bigoplus_{j=1}^n \lambda_j \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} S = S^T D S. \quad (69)$$

An earlier argument established that the covariance matrix is

$$\sigma = S^{-1} \bigoplus_{j=1}^n \coth\left(\frac{\lambda_j}{2}\right) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} S^{-T} \quad (70)$$

$$= S^{-1} \coth\left(\frac{D}{2}\right) S^{-T} \quad (71)$$

Then consider that, from previous reasoning,

$$\frac{1}{2} i\Omega H = \frac{1}{2} S^{-1} (I_n \otimes U) (\underline{D} \otimes -\sigma_Z) (I_n \otimes U^\dagger) S \quad (72)$$

$$\implies \coth\left(\frac{i\Omega H}{2}\right) \quad (73)$$

$$= S^{-1} (I_n \otimes U) \left[\coth\left(\frac{\underline{D} \otimes -\sigma_Z}{2}\right) \right] (I_n \otimes U^\dagger) S \quad (74)$$

$$= S^{-1} (I_n \otimes U) \left[\coth\left(\frac{D}{2}\right) \otimes -\sigma_Z \right] (I_n \otimes U^\dagger) S \quad (75)$$

$$= S^{-1} \left[\coth\left(\frac{D}{2}\right) \otimes -\sigma_Y \right] S \quad (76)$$

$$= S^{-1} \left[\coth\left(\frac{D}{2}\right) \otimes i\Omega_1 \right] S \quad (77)$$

$$= S^{-1} \left[\coth\left(\frac{D}{2}\right) \otimes I_2 \right] [I_n \otimes i\Omega_1] S \quad (78)$$

$$= S^{-1} \coth\left(\frac{D}{2}\right) i\Omega S \quad (79)$$

$$= S^{-1} \coth\left(\frac{D}{2}\right) S^{-T} i\Omega \quad (80)$$

$$= \sigma i\Omega. \quad (81)$$

In the above chain of steps, the first equality is due to the functional calculus of matrices. The second equality is due to the coth function being odd. By simplifying and using properties of Ω , one can simplify towards the end. Summarizing the above, we have shown that

$$\coth\left(\frac{i\Omega H}{2}\right) = \sigma i\Omega \tag{82}$$

which implies that

$$\coth\left(\frac{i\Omega H}{2}\right) i\Omega = \sigma i\Omega(i\Omega) = \sigma. \tag{83}$$

And thus we are done.

A similar proof can be constructed to yield the reverse result, i.e.

$$H = 2\operatorname{arccoth}(i\Omega\sigma)i\Omega, \tag{84}$$

concluding the proof. □

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1 Overview

In the last lecture, we represented faithful Gaussian states as thermal states of quadratic Hamiltonians and discussed the Williamson theorem.

In this lecture, we first review a method to find the symplectic eigenvalues of a positive definite matrix. We then derive a relation between the Hamiltonian matrix and the covariance matrix corresponding to a faithful Gaussian state. Finally, we determine formulas for the purity and von Neumann entropy of a Gaussian state. We point readers to [Ser17] for background on some of the topics covered in this lecture.

2 Symplectic eigenvalues of a positive definite matrix

In this section, we discuss a method to find the symplectic eigenvalues of a positive definite matrix M .

Let Ω denote the real, canonical, anti-symmetric form defined as

$$\Omega = I_n \otimes \Omega_1, \tag{1}$$

where

$$\Omega_1 = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \tag{2}$$

which encodes the canonical commutation relations of the quadrature operators. Note that $\Omega\Omega^T = -\Omega^2 = I$.

Let S denote a symplectic matrix such that $S\Omega S^T = \Omega$. It follows that such a matrix S is invertible with inverse given by $S^{-1} = \Omega S^T \Omega^T$. We begin by showing that $\Omega S = S^{-T} \Omega$. This is a direct consequence of the fact that S^T is symplectic, which can be seen from the following steps:

$$S\Omega S^T = \Omega, \tag{3}$$

$$\Rightarrow S\Omega S^T \Omega = -I, \tag{4}$$

$$\Rightarrow S\Omega S^T \Omega S = -S, \tag{5}$$

$$\Rightarrow S^{-1} S\Omega S^T \Omega S = -S^{-1} S, \tag{6}$$

$$\Rightarrow \Omega S^T \Omega S = -I, \tag{7}$$

$$\Rightarrow S^T \Omega S = \Omega. \tag{8}$$

It then follows that

$$\Omega S = S^{-T} \Omega. \quad (9)$$

As discussed in the previous lecture, a positive definite $2n \times 2n$ matrix M has the following symplectic decomposition:

$$M = SDS^T, \quad (10)$$

where $d_j > 0$ for all $j \in \{1, \dots, n\}$,

$$D = \bigoplus_{j=1}^n d_j \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = D_n \otimes I_2, \quad (11)$$

and

$$D_n = \text{diag}(d_1, d_2, \dots, d_n). \quad (12)$$

We now establish a connection between the symplectic eigenvalues of a positive definite matrix M and the eigenvalues of the matrix $i\Omega M$. Consider the following chain of equalities:

$$i\Omega M = i\Omega SDS^T \quad (13)$$

$$= i\Omega S(D_n \otimes I_2)S^T \quad (14)$$

$$= S^{-T}(i\Omega)(D_n \otimes I_2)S^T \quad (15)$$

$$= S^{-T}(I_n \otimes i\Omega_1)(D_n \otimes I_2)S^T \quad (16)$$

$$= S^{-T}(D_n \otimes i\Omega_1)S^T \quad (17)$$

$$= S^{-T}(D_n \otimes -\sigma_Y)S^T \quad (18)$$

$$= \underbrace{S^{-T}(I_n \otimes U_2)}_B (D_n \otimes -\sigma_Z) \underbrace{(I_n \otimes U_2^\dagger)}_{B^{-1}} S^T. \quad (19)$$

The first equality follows from (10). The second equality follows from (11). The third equality follows from (9). The fourth equality follows from the definition of Ω as defined in (1). The last two equalities follow from the fact that

$$i\Omega_1 = -\sigma_Y = U_2(-\sigma_Z)U_2^\dagger, \quad (20)$$

where

$$U_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ i & -i \end{bmatrix}. \quad (21)$$

From (19) and from the fact that $D_n \otimes -\sigma_Z = \text{diag}(-d_1, d_1, -d_2, d_2, \dots, -d_n, d_n)$, it follows that the usual eigendecomposition of $i\Omega M$ is given by $B(D_n \otimes -\sigma_Z)B^{-1}$, where

$$B = S^{-T}(I_n \otimes U_2) \quad (22)$$

is the matrix of eigenvectors. We note that S^{-T} can be expressed in terms of Ω and S . Since $S\Omega S^T = \Omega$, it follows that $S\Omega S^T \Omega^T = \Omega \Omega^T$. Since $\Omega \Omega^T = I$, $S^{-1} = \Omega S^T \Omega^T$. Therefore, $S^{-T} = \Omega S \Omega^T$.

Therefore, a method to find the symplectic eigenvalues of a positive definite matrix M is as follows. We first find the usual eigendecomposition of the matrix $i\Omega M$, and the corresponding eigenvalues provide the information of symplectic eigenvalues of the matrix M . Moreover, the symplectic matrix S corresponding to the transformation $M = SDS^T$, can be found from the eigenvector matrix $B = S^{-T}(I_n \otimes U_2) = \Omega S \Omega^T (I_n \otimes U_2)$ as defined in (22), i.e., $S = B^{-T}(I_n \otimes U_2^T) = \Omega^T B (I_n \otimes U_2^\dagger) \Omega$.

3 Relationship between the Hamiltonian matrix and the covariance matrix for a faithful Gaussian state

In this section, we derive the following relations between the Hamiltonian matrix and the covariance matrix corresponding to a faithful Gaussian state:

$$\sigma = \coth\left(\frac{i\Omega H}{2}\right) i\Omega, \quad (23)$$

$$H = 2 \operatorname{arccoth}(i\Omega \sigma) i\Omega. \quad (24)$$

As discussed in the previous lecture, a positive definite matrix H can be represented in the following symplectic diagonalized form:

$$H = S^T \bigoplus_{j=1}^n \lambda_j \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} S, \quad (25)$$

where $\lambda_j > 0, \forall j \in \{1, \dots, n\}$.

Moreover, the corresponding covariance matrix σ can be written as

$$\sigma = S^{-1} \bigoplus_{j=1}^n \coth\left(\frac{\lambda_j}{2}\right) \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} S^{-T}, \quad (26)$$

where $\nu_j \equiv \coth(\lambda_j/2)$ for $j \in \{1, \dots, n\}$ are the symplectic eigenvalues of σ .

From (19) and (25), it follows that

$$\frac{1}{2} i\Omega H = \frac{1}{2} S^{-1} (I_n \otimes U_2) (D_n \otimes -\sigma_Z) (I_n \otimes U_2^\dagger) S, \quad (27)$$

where $D_n = \operatorname{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$.

Consider the following chain of equalities:

$$\coth\left(\frac{i\Omega H}{2}\right) = S^{-1} (I_n \otimes U_2) \coth\left(\frac{D_n \otimes -\sigma_Z}{2}\right) (I_n \otimes U_2^\dagger) S \quad (28)$$

$$= S^{-1} (I_n \otimes U_2) (\coth(D_n/2) \otimes -\sigma_Z) (I_n \otimes U_2^\dagger) S \quad (29)$$

$$= S^{-1} (\coth(D_n/2) \otimes i\Omega_1) S \quad (30)$$

$$= S^{-1} (\coth(D_n/2) \otimes I_2) (I_n \otimes i\Omega_1) S \quad (31)$$

$$= S^{-1} (\coth(D_n/2) \otimes I_2) i\Omega S \quad (32)$$

$$= S^{-1} (\coth(D_n/2) \otimes I_2) S^{-T} i\Omega \quad (33)$$

$$= \sigma i\Omega. \quad (34)$$

The first equality follows from (27). The second equality follows from the fact that $\coth(\cdot)$ is an odd function. The third equality follows from (20). The fifth equality follows from (1). The sixth equality follows from (9). The last equality follows from (26).

Therefore, we get

$$\coth\left(\frac{i\Omega H}{2}\right)i\Omega = \sigma(i\Omega)(i\Omega) \quad (35)$$

$$= \sigma. \quad (36)$$

Similarly, the relation in (24) can be derived.

4 Uncertainty relation and symplectic eigenvalues of a covariance matrix

Previously, we proved that the following uncertainty relation holds for any n -mode quantum state that has a finite covariance matrix σ :

$$\sigma + i\Omega \geq 0. \quad (37)$$

We now discuss the restriction imposed by the uncertainty relation in (37) on the symplectic eigenvalues of σ . Let S be the symplectic matrix diagonalizing σ as

$$S\sigma S^T = D = \bigoplus_{j=1}^n d_j \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}. \quad (38)$$

We now prove that (37) implies $d_j \geq 1, \forall j$. Consider the following chain of inequalities:

$$\sigma + i\Omega \geq 0 \quad (39)$$

$$\Rightarrow S(\sigma + i\Omega)S^T \geq 0 \quad (40)$$

$$\Rightarrow S\sigma S^T + iS\Omega S^T \geq 0 \quad (41)$$

$$\Rightarrow D + i\Omega \geq 0 \quad (42)$$

$$\Rightarrow \bigoplus_{j=1}^n d_j \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + i \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \geq 0 \quad (43)$$

$$\Rightarrow \bigoplus_{j=1}^n \begin{bmatrix} d_j & i \\ -i & d_j \end{bmatrix} \geq 0 \quad (44)$$

$$\Rightarrow \begin{bmatrix} d_j & i \\ -i & d_j \end{bmatrix} \geq 0, \forall j. \quad (45)$$

Since the eigenvalues of $\begin{bmatrix} d_j & i \\ -i & d_j \end{bmatrix}$ are $d_j + 1$ and $d_j - 1$, it follows from (45) that $d_j \geq 1, \forall j$.

Thus, any quantum covariance matrix σ (i.e., obeying (37)) has all of its symplectic eigenvalues greater than or equal to one.

5 Purification of a Gaussian state

In this section, we study Gaussian purifications of Gaussian states. We begin by determining the mean vector and covariance matrix for a tensor product of two Gaussian states.

5.1 Tensor product of two Gaussian states

Let \bar{r}_A denote the mean vector and σ_A denote the covariance matrix of a Gaussian state ρ_A . Let \bar{r}_B denote the mean vector and σ_B denote the covariance matrix of a Gaussian state ρ_B . Then the mean vector of the tensor product state $\rho_A \otimes \rho_B$ is given by

$$\bar{r}_{AB} \equiv \begin{bmatrix} \bar{r}_A \\ \bar{r}_B \end{bmatrix}. \quad (46)$$

Moreover, the covariance matrix of $\rho_A \otimes \rho_B$ is given by

$$\sigma_{AB} \equiv \sigma_A \oplus \sigma_B = \begin{bmatrix} \sigma_A & 0 \\ 0 & \sigma_B \end{bmatrix}. \quad (47)$$

Similarly, if the mean vector of a Gaussian state is $\begin{bmatrix} \bar{r}_A \\ \bar{r}_B \end{bmatrix}$ and the covariance matrix is $\begin{bmatrix} \sigma_A & 0 \\ 0 & \sigma_B \end{bmatrix}$, then the Gaussian state is a tensor product of two Gaussian states.

5.2 Gaussian purifications of Gaussian states

A thermal state with mean number of photons $\bar{n} \geq 0$ can be expressed in the photon-number basis as follows.

$$\theta(\bar{n}) = \frac{1}{\bar{n} + 1} \sum_{n=0}^{\infty} \left(\frac{\bar{n}}{\bar{n} + 1} \right)^n |n\rangle\langle n|. \quad (48)$$

Alternatively,

$$\theta(\lambda) = \frac{1}{z(\lambda)} \sum_{n=0}^{\infty} \exp(-\lambda(n + 1/2)) |n\rangle\langle n|, \quad (49)$$

where $z(\lambda) = (e^{\lambda/2} - e^{-\lambda/2})^{-1}$ for $\lambda > 0$ (note that $\lambda = \ln(1 + 1/\bar{n})$).

A purification of the thermal state $\theta_A(\bar{n})$ is given by the following two-mode squeezed vacuum (TMS) state:

$$|\psi_{\text{TMS}}(\bar{n})\rangle_{AR} = \frac{1}{\sqrt{\bar{n} + 1}} \sum_{n=0}^{\infty} \sqrt{\left(\frac{\bar{n}}{\bar{n} + 1} \right)^n} |n\rangle_A |n\rangle_R, \quad (50)$$

where R is a reference system.

The covariance matrix of the two-mode squeezed vacuum state $|\psi_{\text{TMS}}(\bar{n})\rangle_{AR}$ is given by

$$\begin{bmatrix} 2\bar{n} + 1 & 0 & 2\sqrt{\bar{n}(\bar{n} + 1)} & 0 \\ 0 & 2\bar{n} + 1 & 0 & -2\sqrt{\bar{n}(\bar{n} + 1)} \\ 2\sqrt{\bar{n}(\bar{n} + 1)} & 0 & 2\bar{n} + 1 & 0 \\ 0 & -2\sqrt{\bar{n}(\bar{n} + 1)} & 0 & 2\bar{n} + 1 \end{bmatrix}, \quad (51)$$

which can be written in the following compact form:

$$\begin{bmatrix} (2\bar{n} + 1)I & 2\sqrt{\bar{n}(\bar{n} + 1)}\sigma_Z \\ 2\sqrt{\bar{n}(\bar{n} + 1)}\sigma_Z & (2\bar{n} + 1)I \end{bmatrix}. \quad (52)$$

By the Williamson theorem, any n -mode Gaussian state ρ can be written as

$$\rho = \hat{D}_{-\bar{r}} \hat{S} \left[\bigotimes_{j=1}^n \theta_{A_j}(\bar{n}_j) \right] \hat{S}^\dagger \hat{D}_{\bar{r}}, \quad (53)$$

where \hat{S} is a unitary generated by a quadratic Hamiltonian. Then a Gaussian purification of ρ is given by

$$\left[\hat{D}_{-\bar{r}} \hat{S} \right]_{A^n} \bigotimes_{j=1}^n |\psi_{\text{TMS}}(\bar{n}_j)\rangle_{A_j R_j}. \quad (54)$$

The mean vector of this purification is $\begin{bmatrix} \bar{r} \\ 0 \end{bmatrix}$. Moreover, the covariance matrix of this purification is

$$\begin{bmatrix} \sigma & S \bigoplus_{j=1}^n 2\sqrt{\bar{n}_j(\bar{n}_j + 1)}\sigma_Z \\ \left(\bigoplus_{j=1}^n 2\sqrt{\bar{n}_j(\bar{n}_j + 1)}\sigma_Z \right) S^T & \bigoplus_{j=1}^n (2\bar{n}_j + 1)I_2 \end{bmatrix}. \quad (55)$$

One can arrive at this conclusion from the fact that

$$\sigma = S \left(\bigoplus_{j=1}^n (2\bar{n}_j + 1)I_2 \right) S^T \quad (56)$$

and the covariance matrix for $\bigotimes_{j=1}^n |\psi_{\text{TMS}}(\bar{n}_j)\rangle_{A_j R_j}$ is

$$\begin{bmatrix} \bigoplus_{j=1}^n (2\bar{n}_j + 1)I_2 & \bigoplus_{j=1}^n 2\sqrt{\bar{n}_j(\bar{n}_j + 1)}\sigma_Z \\ \bigoplus_{j=1}^n 2\sqrt{\bar{n}_j(\bar{n}_j + 1)}\sigma_Z & \bigoplus_{j=1}^n (2\bar{n}_j + 1)I_2 \end{bmatrix}. \quad (57)$$

We note that the symplectic matrix for the unitary evolution $\hat{S}_{A^n} \otimes I_{R^n}$ is given by

$$\begin{bmatrix} S & 0 \\ 0 & I \end{bmatrix}. \quad (58)$$

6 Purity of a quantum state

The purity of a quantum state ρ is defined as $\text{Tr}\{\rho^2\}$. We now show that $\text{Tr}\{\rho^2\} \leq 1$. Consider the following spectral decomposition of the state ρ :

$$\rho = \sum_x \lambda_x |\phi_x\rangle\langle\phi_x|. \quad (59)$$

Then

$$\text{Tr}\{\rho^2\} = \sum_x \lambda_x^2. \quad (60)$$

Since $\lambda_x \leq 1 \Rightarrow \lambda_x^2 \leq 1$ and since $\sum_x \lambda_x = 1 \Rightarrow \sum_x \lambda_x^2 \leq 1$. Therefore, if a state is pure, then $\text{Tr}\{\rho^2\} = 1$.

We now show that if $\text{Tr}\{\rho^2\} = 1$, then the state is pure. Consider that

$$1 = \text{Tr}\{\rho^2\} \quad (61)$$

$$= \sum_x \lambda_x^2. \quad (62)$$

Moreover, $\text{Tr}\{\rho\} = \sum_x \lambda_x = 1 \Rightarrow \text{Tr}\{\rho\}^2 = \sum_{x,y} \lambda_x \lambda_y = 1$.

Consider the following chain of inequalities:

$$\Rightarrow 0 = \text{Tr}\{\rho^2\} - \text{Tr}\{\rho\}^2 \quad (63)$$

$$= \sum_x \lambda_x^2 - \left[\sum_{x,y} \lambda_x \lambda_y \right] \quad (64)$$

$$= \sum_x \lambda_x^2 - \left[\sum_x \lambda_x^2 + \sum_{x \neq y} \lambda_x \lambda_y \right] \quad (65)$$

$$= \sum_{x \neq y} \lambda_x \lambda_y. \quad (66)$$

Since $\lambda_x, \lambda_y \geq 0$, the only possibility to satisfy (66) is that $\lambda_x = 1$ and $\lambda_y = 0, \forall y \neq x$. Thus, $\text{Tr}\{\rho^2\} = 1$ implies that ρ is a pure state.

6.1 Purity of a Gaussian state

In this section, we calculate the purity for Gaussian states. From the Williamson decomposition of an n -mode Gaussian state as defined in (53) and from the fact that the purity is invariant under unitary transformations, we get

$$\text{Tr}\{\rho^2\} = \prod_{j=1}^n \text{Tr}\{\theta^2(\bar{n}_j)\}. \quad (67)$$

Consider the following chain of equalities:

$$\mathrm{Tr}\{\theta^2(\bar{n}_j)\} = \frac{1}{(\bar{n}_j + 1)^2} \sum_{n=0}^{\infty} \left(\frac{\bar{n}_j}{\bar{n}_j + 1} \right)^{2n} \quad (68)$$

$$= \frac{1}{(\bar{n}_j + 1)^2} \frac{1}{1 - (\bar{n}_j/(\bar{n}_j + 1))^2} \quad (69)$$

$$= \frac{1}{(\bar{n}_j + 1)^2 - \bar{n}_j^2} \quad (70)$$

$$= \frac{1}{2\bar{n}_j + 1} \quad (71)$$

$$= \frac{1}{\nu_j} , \quad (72)$$

where ν_j denotes the symplectic eigenvalue of $\theta(\bar{n}_j)$. The first equality follows from the definition of a thermal state as defined in (48). The second equality follows from the sum of an infinite geometric series.

Therefore,

$$\mathrm{Tr}\{\rho^2\} = \prod_{j=1}^n \frac{1}{\nu_j} \quad (73)$$

$$= \sqrt{\prod_{j=1}^n \frac{1}{\nu_j^2}} \quad (74)$$

$$= \frac{1}{\sqrt{\prod_{j=1}^n \nu_j^2}} \quad (75)$$

$$= \frac{1}{\mathrm{Det}(\sigma)} . \quad (76)$$

The last equality follows from (26) and from the fact that for any symplectic matrix S , $\mathrm{Det}(S) = 1$.

Therefore, the purity of a Gaussian state is

$$\mathrm{Tr}\{\rho^2\} = \frac{1}{\sqrt{\mathrm{Det}(\sigma)}} , \quad (77)$$

which implies that a Gaussian state is pure if and only if $\mathrm{Det}(\sigma) = 1$. Since $\nu_j \geq 1$, an equivalent condition for the purity of a Gaussian state is that all symplectic eigenvalues are equal to one.

7 Entropy of a Gaussian state

In this section, we find an expression for the von Neumann entropy of a Gaussian state.

The von Neumann entropy of a quantum state ρ is defined as

$$S(\rho) \equiv -\mathrm{Tr}\{\rho \ln \rho\} . \quad (78)$$

We begin by expressing a thermal state with the mean photon number \bar{n} in the following form:

$$\theta(\bar{n}) = \frac{1}{\bar{n} + 1} \sum_{n=0}^{\infty} \left(\frac{\bar{n}}{\bar{n} + 1} \right)^n |n\rangle\langle n| \quad (79)$$

$$= \frac{1}{\bar{n} + 1} \left(\frac{\bar{n}}{\bar{n} + 1} \right)^{\hat{n}}. \quad (80)$$

Consider the following chain of equalities:

$$- \text{Tr}\{\theta(\bar{n}) \ln \theta(\bar{n})\} = - \text{Tr} \left\{ \theta(\bar{n}) \ln \frac{1}{\bar{n} + 1} \left(\frac{\bar{n}}{\bar{n} + 1} \right)^{\hat{n}} \right\} \quad (81)$$

$$= - \text{Tr} \left\{ \theta(\bar{n}) \ln \left(\frac{1}{\bar{n} + 1} \right) \right\} - \text{Tr} \left\{ \theta(\bar{n}) \hat{n} \ln \left(\frac{\bar{n}}{\bar{n} + 1} \right) \right\} \quad (82)$$

$$= \ln(\bar{n} + 1) - \ln \left(\frac{\bar{n}}{\bar{n} + 1} \right) \text{Tr}\{\theta(\bar{n}) \hat{n}\} \quad (83)$$

$$= \ln(\bar{n} + 1) - \ln \left(\frac{\bar{n}}{\bar{n} + 1} \right) \bar{n} \quad (84)$$

$$= (\bar{n} + 1) \ln(\bar{n} + 1) - \bar{n} \ln \bar{n} \quad (85)$$

$$\equiv g(\bar{n}). \quad (86)$$

From unitary invariance and additivity of the von Neumann entropy, we get

$$S(\rho) = S \left(\bigotimes_{j=1}^n \theta(\bar{n}_j) \right), \quad (87)$$

where ρ is an n -mode Gaussian state as defined in (53). Therefore,

$$S(\rho) = \sum_{j=1}^n S(\theta(\bar{n}_j)) \quad (88)$$

$$= \sum_{j=1}^n g(\bar{n}_j) \quad (89)$$

We now derive an alternative formula for the von Neumann entropy of faithful Gaussian states. Let

$$\rho = \frac{1}{\sqrt{\text{Det}[(\sigma + i\Omega)/2]}} \exp \left(-\frac{1}{2} (\hat{r} - \bar{r})^T H (\hat{r} - \bar{r}) \right) \quad (90)$$

$$= \hat{D}_{-\bar{r}} \left[\frac{\exp \left(-\frac{1}{2} \hat{r}^T H \hat{r} \right)}{\sqrt{\text{Det}[(\sigma + i\Omega)/2]}} \right] \hat{D}_{\bar{r}} \quad (91)$$

and let

$$\rho_0 = \frac{\exp \left(-\frac{1}{2} \hat{r}^T H \hat{r} \right)}{\sqrt{\text{Det}[(\sigma + i\Omega)/2]}}. \quad (92)$$

Then from unitary invariance of the von Neumann entropy, we get

$$S(\rho) = S(\rho_0) \quad (93)$$

$$= -\text{Tr}\{\rho_0 \ln \rho_0\} \quad (94)$$

$$= -\text{Tr}\left\{\rho_0 \ln \frac{\exp(-\frac{1}{2}\hat{r}^T H \hat{r})}{\sqrt{\text{Det}[(\sigma + i\Omega)/2]}}\right\} \quad (95)$$

$$= -\text{Tr}\left\{\rho_0 \ln \frac{1}{\sqrt{\text{Det}[(\sigma + i\Omega)/2]}}\right\} - \text{Tr}\{\rho_0 \ln \exp(-\frac{1}{2}\hat{r}^T H \hat{r})\} \quad (96)$$

$$= \frac{1}{2} \ln \text{Det}[(\sigma + i\Omega)/2] + \frac{1}{2} \text{Tr}\{\rho_0 \hat{r}^T H \hat{r}\} . \quad (97)$$

We now focus on the second term of the aforementioned equation.

$$\text{Tr}\{\rho_0 \hat{r}^T H \hat{r}\} = \text{Tr}\{\rho_0 \sum_{j,k} \hat{r}_j H_{j,k} \hat{r}_k\} \quad (98)$$

$$= \sum_{j,k} H_{j,k} \text{Tr}\{\rho_0 \hat{r}_j \hat{r}_k\} \quad (99)$$

$$= \frac{1}{2} \sum_{j,k} H_{j,k} \text{Tr}\{\rho_0 (\{\hat{r}_j, \hat{r}_k\} + [\hat{r}_j, \hat{r}_k])\} \quad (100)$$

$$= \frac{1}{2} \sum_{j,k} H_{j,k} (\sigma_{j,k} + i\Omega_{j,k}) \quad (101)$$

$$= \frac{1}{2} \sum_{j,k} H_{j,k} \sigma_{j,k} - \frac{i}{2} \sum_{j,k} H_{j,k} \Omega_{k,j} \quad (102)$$

$$= \frac{1}{2} \text{Tr}\{H\sigma\} - \frac{i}{2} \text{Tr}\{H\Omega\} \quad (103)$$

$$= \frac{1}{2} \text{Tr}\{H\sigma\}, \quad (104)$$

where we used the fact that $\text{Tr}\{H\Omega\} = 0$, which holds because H is symmetric and Ω is antisymmetric.

Therefore,

$$S(\rho) = \frac{1}{2} \ln \text{Det}[(\sigma + i\Omega)/2] + \frac{1}{4} \text{Tr}\{H\sigma\} . \quad (105)$$

Moreover, from (24) it follows that

$$S(\rho) = \frac{1}{2} \ln \text{Det}[(\sigma + i\Omega)/2] + \frac{1}{2} \text{Tr}\{\text{arccoth}(i\Omega\sigma)i\Omega\sigma\} . \quad (106)$$

This latter expression is valid for pure Gaussian states, with the expression $\text{Tr}\{\text{arccoth}(i\Omega\sigma)i\Omega\sigma\}$ understood in a limiting sense.

References

- [Ser17] Alessio Serafini. *Quantum Continuous Variables: A Primer of Theoretical Methods*. CRC Press, 2017.

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1 Overview

In the last lecture, we reviewed a method to find the symplectic eigenvalues of a positive definite matrix. We then derived a relation between the Hamiltonian matrix and the covariance matrix corresponding to a faithful Gaussian state. Finally, we reviewed the conditions for the purity of a Gaussian state and found an expression for the von Neumann entropy of a Gaussian state

In this lecture, we find the quantum relative entropy and the Rényi entropies for faithful Gaussian states. We point readers to [Ser17] for background on topics covered in this lecture.

2 Relative entropy of faithful Gaussian states

The quantum relative entropy $D(\rho||\tau)$ of a density operator ρ and a positive definite operator τ is defined as follows:

$$D(\rho||\tau) = \text{Tr}\{\rho(\ln \rho - \ln \tau)\} . \quad (1)$$

This is the formula for the finite-dimensional case, and it turns out to be legitimate for faithful Gaussian states.

In the last lecture we showed that

$$\text{Tr}\{\rho \ln \rho\} = -\frac{1}{2} \ln \text{Det}[(\sigma_\rho + i\Omega)/2] - \frac{1}{4} \text{Tr}\{H_\rho \sigma_\rho\} \quad (2)$$

We now calculate $-\text{Tr}\{\rho \ln \tau\}$. Consider that

$$\rho = \hat{D}_{-\bar{r}_\rho} \rho_0 \hat{D}_{\bar{r}_\rho}, \quad (3)$$

where ρ_0 has zero mean and the covariance matrix is σ_ρ . Then using cyclicity of trace and functional calculus of $\ln(\cdot)$, we find that

$$-\text{Tr}\{\rho \ln \tau\} = -\text{Tr}\{\rho_0 \ln \hat{D}_{\bar{r}_\rho} \tau \hat{D}_{-\bar{r}_\rho}\}. \quad (4)$$

Let

$$\tau = \frac{\exp[-(1/2)(\hat{r} - \bar{r}_\tau)^T H_\tau (\hat{r} - \bar{r}_\tau)]}{\sqrt{\text{Det}[(\sigma_\tau + i\Omega)/2]}}. \quad (5)$$

Then

$$\hat{D}_{\bar{r}_\rho} \tau \hat{D}_{-\bar{r}_\rho} = \frac{\exp[-(1/2)(\hat{r} - \delta)^T H_\tau (\hat{r} - \delta)]}{\sqrt{\text{Det}[(\sigma_\tau + i\Omega)/2]}} \quad (6)$$

with $\delta = \bar{r}_\tau - \bar{r}_\rho$. Therefore,

$$\begin{aligned} & -\text{Tr}\{\rho_0 \ln \hat{D}_{\bar{r}_\rho} \tau \hat{D}_{-\bar{r}_\rho}\} \\ &= -\text{Tr}\left\{\rho_0 \ln \frac{1}{\sqrt{\text{Det}[(\sigma_\tau + i\Omega)/2]}}\right\} + \text{Tr}\left\{\rho_0 \left(\frac{1}{2}(\hat{r} - \delta)^T H_\tau (\hat{r} - \delta)\right)\right\} \end{aligned} \quad (7)$$

$$= \frac{1}{2} \ln \text{Det}[(\sigma_\tau + i\Omega)/2] + \frac{1}{2} \text{Tr}\{\rho_0 (\hat{r} - \delta)^T H_\tau (\hat{r} - \delta)\} . \quad (8)$$

We now focus on the second term.

$$\begin{aligned} & \frac{1}{2} \sum_{j,k} \text{Tr}\{\rho_0 (\hat{r}_j - \delta_j)(\hat{r}_k - \delta_k)\} H_{j,k}^T \\ &= \frac{1}{2} \sum_{j,k} (\text{Tr}\{\rho_0 \hat{r}_j \hat{r}_k\} - \text{Tr}\{\rho_0 \hat{r}_k\} \delta_j - \text{Tr}\{\rho_0 \hat{r}_j\} \delta_k + \text{Tr}\{\rho_0\} \delta_j \delta_k) H_{j,k}^T \end{aligned} \quad (9)$$

$$= \frac{1}{2} \sum_{j,k} (\text{Tr}\{\rho_0 \hat{r}_j \hat{r}_k\} + \delta_j \delta_k) H_{j,k}^T \quad (10)$$

$$= \frac{1}{2} \sum_{j,k} \text{Tr}\{\rho_0 \hat{r}_j \hat{r}_k\} H_{j,k}^T + \frac{1}{2} \delta^T H_\tau \delta \quad (11)$$

$$= \frac{1}{4} \text{Tr}\{\sigma_\rho H_\tau\} + \frac{1}{2} \delta^T H_\tau \delta . \quad (12)$$

From (8) and (12), we get

$$-\text{Tr}\{\rho \ln \tau\} = \frac{1}{2} \ln \text{Det}[(\sigma_\tau + i\Omega)/2] + \frac{1}{4} \text{Tr}\{\sigma_\rho H_\tau\} + \frac{1}{2} \delta^T H_\tau \delta , \quad (13)$$

where $\delta = \bar{r}_\tau - \bar{r}_\rho$.

Therefore, the quantum relative entropy of two Gaussian states ρ and τ is given by

$$D(\rho||\tau) = \frac{1}{2} \left[\ln \left(\frac{\text{Det}[(\sigma_\tau + i\Omega)/2]}{\text{Det}[(\sigma_\rho + i\Omega)/2]} \right) + \frac{1}{2} \text{Tr}\{\sigma_\rho (H_\tau - H_\rho)\} + \delta^T H_\tau \delta \right] \quad (14)$$

$$= \frac{1}{2} \left[\ln \left(\frac{\text{Det}[\sigma_\tau + i\Omega]}{\text{Det}[\sigma_\rho + i\Omega]} \right) + \frac{1}{2} \text{Tr}\{\sigma_\rho (H_\tau - H_\rho)\} + \delta^T H_\tau \delta \right] . \quad (15)$$

The aforementioned expression is finite whenever τ is faithful.

3 Computing Rényi entropies and powers of Gaussian states

In this section, we first find Rényi entropies of Gaussian states in terms of symplectic eigenvalues. We then find the power of Gaussian states in terms of the mean vector and the covariance matrix.

3.1 Rényi entropies of Gaussian states

The quantum Rényi entropy of a quantum state ρ is defined as

$$S_\alpha(\rho) = \frac{1}{1-\alpha} \ln \text{Tr}\{\rho^\alpha\}, \quad (16)$$

for $\alpha \in (0, 1) \cup (1, \infty)$. Moreover,

$$\lim_{\alpha \rightarrow 1} S_\alpha(\rho) = S(\rho). \quad (17)$$

Our goal is to find $\text{Tr}\{\rho^\alpha\}$. Using the fact that

$$\rho = \hat{D}_{-\bar{r}} \hat{S} \left(\bigotimes_{j=1}^n \theta(\bar{n}_j) \right) \hat{S}^\dagger \hat{D}_{\bar{r}}, \quad (18)$$

we find that

$$\text{Tr}\{\rho^\alpha\} = \prod_{j=1}^n \text{Tr}\{\theta(\bar{n}_j)^\alpha\}. \quad (19)$$

Consider the following chain of equalities:

$$\text{Tr}\{\theta(\bar{n})^\alpha\} = \frac{1}{(\bar{n}+1)^\alpha} \sum_{n=0}^{\infty} \left(\frac{\bar{n}}{\bar{n}+1} \right)^{\alpha n} \quad (20)$$

$$= \frac{1}{(\bar{n}+1)^\alpha} \frac{1}{1 - (\bar{n}/(\bar{n}+1))^\alpha} \quad (21)$$

$$= \frac{1}{(\bar{n}+1)^\alpha - \bar{n}^\alpha}, \quad (22)$$

which implies that

$$\text{Tr}\{\rho^\alpha\} = \prod_{j=1}^n \frac{1}{(\bar{n}_j+1)^\alpha - \bar{n}_j^\alpha}. \quad (23)$$

In terms of symplectic eigenvalues $\nu_j = 2\bar{n}_j + 1$, $\text{Tr}\{\rho^\alpha\}$ is given by

$$\text{Tr}\{\rho^\alpha\} = \prod_{j=1}^n \frac{2^\alpha}{(\nu_j+1)^\alpha - (\nu_j-1)^\alpha}. \quad (24)$$

Therefore, from (16) and (24), it follows that

$$S_\alpha(\rho) = \frac{1}{1-\alpha} \sum_{j=1}^n \ln \left(\frac{2^\alpha}{(\nu_j+1)^\alpha - (\nu_j-1)^\alpha} \right). \quad (25)$$

The Rényi entropy can also be expressed as

$$S_\alpha(\rho) = \frac{\alpha}{1-\alpha} \ln \text{Tr}\{\rho^\alpha\}^{1/\alpha} \quad (26)$$

$$= \frac{\alpha}{1-\alpha} \ln \|\rho\|_\alpha . \quad (27)$$

Therefore,

$$S_\infty(\rho) = -\ln \|\rho\|_\infty \equiv S_{\min}(\rho) \quad (28)$$

We now find $S_\infty(\rho)$ using the fact that $\|\theta(\bar{n})\|_\infty = 1/(\bar{n} + 1)$. Consider the following chain of equalities:

$$S_\infty(\rho) = -\ln \left\| \bigotimes_{j=1}^n \theta(\bar{n}_j) \right\|_\infty \quad (29)$$

$$= -\ln \prod_{j=1}^n \|\theta(\bar{n}_j)\|_\infty \quad (30)$$

$$= \sum_{j=1}^n -\ln(1/(\bar{n}_j + 1)) \quad (31)$$

$$= \sum_{j=1}^n \ln(\bar{n}_j + 1) \quad (32)$$

$$= \sum_{j=1}^n \ln[(\nu_j + 1)/2] . \quad (33)$$

In general, the following relation holds for the Rényi entropy:

$$S_\alpha(\rho) \geq S_\beta(\rho), \quad (34)$$

for $\alpha \leq \beta$.

We now find the difference between $S(\rho)$ and $S_\infty(\rho)$. Consider the following chain of inequalities:

$$S(\rho) - S_\infty(\rho) = \sum_{j=1}^n g(\bar{n}_j) - \ln(\bar{n}_j + 1) \quad (35)$$

$$= \sum_{j=1}^n (\bar{n}_j + 1) \ln(\bar{n}_j + 1) - \bar{n}_j \ln \bar{n}_j - \ln(\bar{n}_j + 1) \quad (36)$$

$$= \sum_{j=1}^n \ln[((\bar{n}_j + 1)/\bar{n}_j)^{\bar{n}_j}] \quad (37)$$

$$\leq \sum_{j=1}^n \ln(e) \quad (38)$$

$$= n . \quad (39)$$

Therefore, the difference between $S(\rho)$ and $S_\infty(\rho)$ never exceeds the number of modes.

3.2 Power of Gaussian state

Let

$$\rho = \frac{1}{\sqrt{\text{Det}[(\sigma + i\Omega)/2]}} \exp\left(-\frac{1}{2}(\hat{r} - \bar{r})^T H (\hat{r} - \bar{r})\right) \quad (40)$$

$$= \hat{D}_{-\bar{r}} \left[\frac{\exp(-\frac{1}{2}\hat{r}^T H \hat{r})}{\sqrt{\text{Det}[(\sigma + i\Omega)/2]}} \right] \hat{D}_{\bar{r}}. \quad (41)$$

Therefore,

$$\rho^\alpha \propto \hat{D}_{-\bar{r}} \exp(-(1/2)\hat{r}^T \alpha H \hat{r}) \hat{D}_{\bar{r}}. \quad (42)$$

Let $H_{(\alpha)} = \alpha H$. Then there exists a corresponding $\sigma_{(\alpha)}$ such that

$$\frac{\rho^\alpha}{\text{Tr}\{\rho^\alpha\}} = \frac{\hat{D}_{-\bar{r}} \exp(-(1/2)\hat{r}^T H_{(\alpha)} \hat{r}) \hat{D}_{\bar{r}}}{\sqrt{\text{Det}[(\sigma_{(\alpha)} + i\Omega)/2]}} \quad (43)$$

$$= \frac{\exp(-(1/2)(\hat{r} - \bar{r})^T H_{(\alpha)} (\hat{r} - \bar{r}))}{\sqrt{\text{Det}[(\sigma_{(\alpha)} + i\Omega)/2]}}. \quad (44)$$

To determine $\sigma_{(\alpha)}$ in terms of σ , we use the following formulas derived in the previous lecture:

$$\sigma = \coth(i\Omega H/2)i\Omega, \quad (45)$$

$$H = 2 \operatorname{arccoth}(i\Omega\sigma)i\Omega. \quad (46)$$

Consider that

$$\sigma_{(\alpha)} = \coth(i\Omega H_{(\alpha)}/2)i\Omega \quad (47)$$

$$= \coth(i\Omega\alpha H/2)i\Omega \quad (48)$$

$$= \coth(i\Omega\alpha/2[2 \operatorname{arccoth}(\sigma i\Omega)]i\Omega) \quad (49)$$

$$= \coth(\alpha \operatorname{arccoth}(\sigma i\Omega))i\Omega. \quad (50)$$

For $|x| > 1$, we have that

$$\coth(\alpha \operatorname{arccoth}(x)) = \frac{(1 + 1/x)^\alpha + (1 - 1/x)^\alpha}{(1 + 1/x)^\alpha - (1 - 1/x)^\alpha}. \quad (51)$$

Since eigenvalues of $\sigma i\Omega$ are either greater than 1 or less than -1 , by using (51) we find that

$$\sigma_{(\alpha)} = \frac{(I + (\sigma i\Omega)^{-1})^\alpha + (I - (\sigma i\Omega)^{-1})^\alpha}{(I + (\sigma i\Omega)^{-1})^\alpha - (I - (\sigma i\Omega)^{-1})^\alpha} i\Omega, \quad (52)$$

which implies that

$$\frac{\rho^\alpha}{\text{Tr}\{\rho^\alpha\}} = \frac{\exp(-(1/2)(\hat{r} - \bar{r})^T H_{(\alpha)} (\hat{r} - \bar{r}))}{\sqrt{\text{Det}[(\sigma_{(\alpha)} + i\Omega)/2]}}. \quad (53)$$

Moreover,

$$\text{Tr}\{\rho^\alpha\} = \text{Tr} \left\{ \left(\frac{\exp(-(1/2)(\hat{r} - \bar{r})^T H(\hat{r} - \bar{r}))}{\sqrt{\text{Det}[(\sigma + i\Omega)/2]}} \right)^\alpha \right\} \quad (54)$$

$$= \frac{1}{(\text{Det}[(\sigma + i\Omega)/2])^{\alpha/2}} \text{Tr}\{\exp(-(1/2)(\hat{r} - \bar{r})^T \alpha H(\hat{r} - \bar{r}))\} \quad (55)$$

$$= \frac{1}{(\text{Det}[(\sigma + i\Omega)/2])^{\alpha/2}} \sqrt{\text{Det}[(\sigma_{(\alpha)} + i\Omega)/2]} . \quad (56)$$

We now focus on two special cases: $\alpha = 2$ and $\alpha = 1/2$. For $\alpha = 2$, we have

$$\frac{(1 + 1/x)^\alpha + (1 - 1/x)^\alpha}{(1 + 1/x)^\alpha - (1 - 1/x)^\alpha} = \frac{1}{2}(x + x^{-1}) \quad (57)$$

Therefore,

$$\sigma_{(2)} = \frac{1}{2}(\sigma i\Omega + (\sigma i\Omega)^{-1})i\Omega \quad (58)$$

$$= \frac{1}{2}(\sigma + i\Omega\sigma^{-1}i\Omega) \quad (59)$$

$$= \frac{1}{2}(\sigma + \Omega\sigma^{-1}\Omega^T) , \quad (60)$$

which implies that

$$\frac{\rho^2}{\text{Tr}\{\rho^2\}} = \frac{\exp(-(1/2)(\hat{r} - \bar{r})^T 2H(\hat{r} - \bar{r}))}{\sqrt{\text{Det}[(1/2)(\sigma + \Omega\sigma^{-1}\Omega^T) + i\Omega]/2]} . \quad (61)$$

Moreover, the purity of the Gaussian state ρ is given by

$$\text{Tr}\{\rho^2\} = \frac{1}{\text{Det}[(\sigma + i\Omega)/2]} \sqrt{\text{Det}[(1/2)(\sigma + \Omega\sigma^{-1}\Omega^T) + i\Omega]/2} , \quad (62)$$

which further reduces (after many steps) to

$$\text{Tr}\{\rho^2\} = \frac{1}{\sqrt{\text{Det}(\sigma)}} . \quad (63)$$

We note that the same expression for the purity of a Gaussian state was derived in the previous lecture by using a different approach.

Let $\alpha = 1/2$. Consider that

$$\frac{\rho^{1/2}}{\text{Tr}\{\rho^{1/2}\}} = \frac{\exp(-(1/2)(\hat{r} - \bar{r})^T H_{(1/2)}(\hat{r} - \bar{r}))}{\sqrt{\text{Det}[(\sigma_{(1/2)} + i\Omega)/2]}} , \quad (64)$$

where $H_{(1/2)} = 1/2H$. Moreover, for $\alpha = 1/2$, we have

$$\frac{(1 + 1/x)^\alpha + (1 - 1/x)^\alpha}{(1 + 1/x)^\alpha - (1 - 1/x)^\alpha} = (1 + \sqrt{1 - 1/x^2})x , \quad (65)$$

which implies that

$$\sigma_{(1/2)} = (I + \sqrt{I - (\sigma i\Omega)^{-2}})(\sigma i\Omega)i\Omega \quad (66)$$

$$= (\sqrt{I + (\sigma\Omega)^{-2}} + I)\sigma . \quad (67)$$

Therefore,

$$\text{Tr}\{\rho^{1/2}\} = \frac{1}{(\text{Det}[(\sigma + i\Omega)/2])^{1/4}} \sqrt{\text{Det}[(\sqrt{I + (\sigma\Omega)^{-2}} + I)\sigma + i\Omega]/2]} . \quad (68)$$

References

- [Ser17] Alessio Serafini. *Quantum Continuous Variables: A Primer of Theoretical Methods*. CRC Press, 2017.

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1 Overview

In the last lecture we derived the formulas for the Rényi entropies, purity, and the entropy of Gaussian states.

In this lecture we derive the formulas for various overlap measures of two Gaussian states such as Holevo fidelity, Uhlmann fidelity, Petz-Rényi relative entropy, and sandwiched Rényi relative entropy.

2 Overlap formulas for Gaussian states

In quantum information, we are often interested in finding out how close two states are. A simple overlap formula between two states ρ and τ is $\text{Tr}[\rho\tau]$. More generally, we compute overlap formulas of the following kind:

$$F_H(\rho, \tau) = \text{Tr} \left[\sqrt{\rho} \sqrt{\tau} \right]^2 \quad (1)$$

$$F(\rho, \tau) = \left\| \sqrt{\rho} \sqrt{\tau} \right\|_1^2 = \text{Tr} \left[\sqrt{\sqrt{\tau} \rho \sqrt{\tau}} \right]^2 \quad (2)$$

F_H represents the Holevo fidelity whereas F represents the Uhlmann fidelity. Generalizing the above, we are interested in Rényi overlaps of the following kind:

$$Q_\alpha(\rho, \tau) = \text{Tr} \left[\rho^\alpha \tau^{1-\alpha} \right], \quad (3)$$

$$\tilde{Q}_\alpha(\rho, \tau) = \text{Tr} \left[\left(\tau^{\frac{1-\alpha}{2\alpha}} \rho \tau^{\frac{1-\alpha}{2\alpha}} \right)^\alpha \right] \quad (4)$$

$$= \text{Tr} \left[\left(\rho^{\frac{1}{2}} \tau^{\frac{1-\alpha}{\alpha}} \rho^{\frac{1}{2}} \right)^\alpha \right], \quad (5)$$

where $\alpha \in (0, 1) \cup (1, \infty)$. Here, Q represents the Petz-Rényi relative entropy while \tilde{Q} represents the sandwiched Rényi relative entropy. Note that $Q_{\alpha=\frac{1}{2}}(\rho, \tau) = \sqrt{F_H(\rho, \tau)}$ and $\tilde{Q}_{\alpha=\frac{1}{2}}(\rho, \tau) = \sqrt{F(\rho, \tau)}$. The reason these overlap functions are interesting is because we can bound the operationally meaningful trace distance between two states as

$$F_H(\rho, \tau) \leq F(\rho, \tau), \quad (6)$$

$$1 - \sqrt{F(\rho, \tau)} \leq 1 - \sqrt{F_H(\rho, \tau)} \leq \frac{1}{2} \|\rho - \tau\|_1 \leq \sqrt{1 - F(\rho, \tau)} \leq \sqrt{1 - F_H(\rho, \tau)}. \quad (7)$$

As we do not possess a general formula for the trace distance between Gaussian states, the above relation proves useful in bounding it. For simplicity in calculating these expressions, we will restrict ourselves to consider only zero-mean states.

2.1 Simple overlap of Gaussian states

Let us first consider the simple overlap formula $\text{Tr}[\rho\tau]$ for states

$$\rho = \frac{1}{\sqrt{\text{Det}\left(\frac{\sigma_\rho + i\Omega}{2}\right)}} \exp\left(-\frac{1}{2}\hat{r}^T H_\rho \hat{r}\right), \quad (8)$$

$$\tau = \frac{1}{\sqrt{\text{Det}\left(\frac{\sigma_\tau + i\Omega}{2}\right)}} \exp\left(-\frac{1}{2}\hat{r}^T H_\tau \hat{r}\right). \quad (9)$$

Thus we obtain

$$\text{Tr}[\rho\tau] = \frac{1}{\sqrt{\text{Det}\left(\frac{\sigma_\rho + i\Omega}{2}\right)\text{Det}\left(\frac{\sigma_\tau + i\Omega}{2}\right)}} \text{Tr}\left[e^{-\frac{1}{2}\hat{r}^T H_\rho \hat{r}} e^{-\frac{1}{2}\hat{r}^T H_\tau \hat{r}}\right] \quad (10)$$

We now wish to simplify the RHS of the above expression involving the product of two quadratic exponentials. In order to do so, we note the general result that for complex symmetric matrices H_1 and H_2 , there exists another complex symmetric matrix H_3 such that if H_3 satisfies the relation

$$e^{-\frac{1}{2}\hat{r}^T H_1 \hat{r}} e^{-\frac{1}{2}\hat{r}^T H_2 \hat{r}} = e^{-\frac{1}{2}\hat{r}^T H_3 \hat{r}}, \quad (11)$$

then it also satisfies

$$e^{-i\Omega H_1} e^{-i\Omega H_2} = e^{-i\Omega H_3}. \quad (12)$$

The latter relation is useful in finding a form for H_3 . Inverting the expression, we obtain

$$e^{i\Omega H_3} = e^{i\Omega H_2} e^{i\Omega H_1} \quad (13)$$

For simplicity in notations, define

$$W_3 = (I + e^{i\Omega H_3}) (I - e^{i\Omega H_3})^{-1}, \quad (14)$$

$$\sigma_3 = -W_3 i\Omega. \quad (15)$$

The latter implies that

$$\sigma_3 = \coth\left(\frac{i\Omega H_3}{2}\right) i\Omega. \quad (16)$$

Also, we note that

$$\sigma_1 = \coth\left(\frac{i\Omega H_1}{2}\right) i\Omega, \quad (17)$$

$$\sigma_2 = \coth\left(\frac{i\Omega H_2}{2}\right) i\Omega. \quad (18)$$

Using these, we can arrive at the final form of σ_3 and H_3 as (see page 13, Ref. [1])

$$\sigma_3 = -i\Omega + (\sigma_2 + i\Omega)(\sigma_1 + \sigma_2)^{-1}(\sigma_1 + i\Omega), \quad (19)$$

$$H_3 = 2i\Omega \text{arccoth}(\sigma_3 i\Omega), \quad (20)$$

from which we can obtain

$$\sqrt{\text{Det} \left(\frac{\sigma_3 + i\Omega}{2} \right)} = \sqrt{\text{Det} \left(\left(\frac{\sigma_2 + i\Omega}{2} \right) \left(\frac{\sigma_1 + \sigma_2}{2} \right)^{-1} \left(\frac{\sigma_1 + i\Omega}{2} \right) \right)} \quad (21)$$

Note that σ_3 is complex symmetric. It can be shown that (see Prop. 11, Ref. [1])

$$\text{Tr} \left[e^{-\frac{1}{2} \hat{r}^T H_3 \hat{r}} \right] = \sqrt{\text{Det} \left(\frac{\sigma_3 + i\Omega}{2} \right)} \quad (22)$$

Thus finally we can simplify the expression for the overlap as

$$\text{Tr} [\rho\tau] = \frac{1}{\sqrt{\text{Det} \left(\frac{\sigma_\rho + i\Omega}{2} \right) \text{Det} \left(\frac{\sigma_\tau + i\Omega}{2} \right)}} \frac{\sqrt{\text{Det} \left(\frac{\sigma_\rho + i\Omega}{2} \right) \text{Det} \left(\frac{\sigma_\tau + i\Omega}{2} \right)}}{\sqrt{\text{Det} \left(\frac{\sigma_\rho + \sigma_\tau}{2} \right)}} \quad (23)$$

$$= \frac{1}{\sqrt{\text{Det} \left(\frac{\sigma_\rho + \sigma_\tau}{2} \right)}} \quad (24)$$

$$= \frac{2^n}{\sqrt{\text{Det}(\sigma_\rho + \sigma_\tau)}} \quad (25)$$

We note that the overlap expression is not a function of the Hamiltonian matrix which implies that it is valid for pure (coherent) states also.

If the mean vectors of the states are represented by \underline{r}_ρ and \underline{r}_τ , then it can be shown that the overlap expression is

$$\text{Tr}[\rho\tau] = \frac{2^n}{\sqrt{\text{Det}(\sigma_\rho + \sigma_\tau)}} \exp[-\underline{\delta}^T (\sigma_\rho + \sigma_\tau)^{-1} \underline{\delta}] \quad (26)$$

where $\underline{\delta} = \underline{r}_\rho - \underline{r}_\tau$.

2.2 Petz-Rényi relative entropy of Gaussian states

Having computed an expression for the simple overlap formula, we now move on to compute the Petz-Rényi overlap of Gaussian states, defined as

$$Q_\alpha(\rho, \tau) = \text{Tr} [\rho^\alpha \tau^{1-\alpha}]. \quad (27)$$

We will restrict ourselves to first consider the case when $\alpha \in (0, 1)$. For notational simplicity, label the normalization of Gaussian states as

$$Z_\rho \equiv \sqrt{\text{Det} \left(\frac{\sigma_\rho + i\Omega}{2} \right)}, \quad (28)$$

For states ρ and τ as defined in (8) and (9), the Petz-Rényi overlap is

$$Q_\alpha(\rho, \tau) = \frac{1}{(Z_\rho)^\alpha (Z_\tau)^{1-\alpha}} \text{Tr} \left[e^{-\frac{1}{2} \hat{r}^T \alpha H_\rho \hat{r}} e^{-\frac{1}{2} \hat{r}^T (1-\alpha) H_\tau \hat{r}} \right] \quad (29)$$

$$= \frac{Z_\rho(\alpha) Z_\tau(1-\alpha)}{(Z_\rho)^\alpha (Z_\tau)^{1-\alpha}} \text{Tr} \left[\frac{e^{-\frac{1}{2} \hat{r}^T \alpha H_\rho \hat{r}}}{Z_\rho(\alpha)} \frac{e^{-\frac{1}{2} \hat{r}^T (1-\alpha) H_\tau \hat{r}}}{Z_\tau(1-\alpha)} \right] \quad (30)$$

wherein we have used the fact that the Hamiltonian matrix of the exponent of a Gaussian state is the product of that exponent with the original Hamiltonian matrix. Now we can apply the simple overlap that we calculated earlier to obtain

$$Q_\alpha(\rho, \tau) = \frac{Z_{\rho^{(\alpha)}} Z_{\tau^{(1-\alpha)}}}{(Z_\rho)^\alpha (Z_\tau)^{1-\alpha}} \frac{1}{\sqrt{\text{Det} \left(\frac{\sigma_{\rho^{(\alpha)}} + \sigma_{\tau^{(1-\alpha)}}}{2} \right)}}, \quad (31)$$

where

$$Z_{\rho^{(\alpha)}} = \sqrt{\text{Det} \left(\frac{\sigma_{\rho^{(\alpha)}} + i\Omega}{2} \right)}, \quad (32)$$

$$Z_{\tau^{(1-\alpha)}} = \sqrt{\text{Det} \left(\frac{\sigma_{\tau^{(1-\alpha)}} + i\Omega}{2} \right)}, \quad (33)$$

and

$$\sigma_{\rho^{(\alpha)}} = \frac{[I + (\sigma_\rho i\Omega)^{-1}]^\alpha + [I - (\sigma_\rho i\Omega)^{-1}]^\alpha}{[I + (\sigma_\rho i\Omega)^{-1}]^\alpha - [I - (\sigma_\rho i\Omega)^{-1}]^\alpha} i\Omega, \quad (34)$$

$$\sigma_{\tau^{(1-\alpha)}} = \frac{[I + (\sigma_\tau i\Omega)^{-1}]^{1-\alpha} + [I - (\sigma_\tau i\Omega)^{-1}]^{1-\alpha}}{[I + (\sigma_\tau i\Omega)^{-1}]^{1-\alpha} - [I - (\sigma_\tau i\Omega)^{-1}]^{1-\alpha}} i\Omega. \quad (35)$$

Holevo Fidelity: For $\alpha = \frac{1}{2}$ the above expression simplifies to

$$Q_{\frac{1}{2}}(\rho, \tau) = \sqrt{F_H(\rho, \tau)} = \text{Tr} [\sqrt{\rho} \sqrt{\tau}] \quad (36)$$

$$= \frac{Z_{\rho^{(1/2)}} Z_{\tau^{(1/2)}}}{(Z_\rho)^{\frac{1}{2}} (Z_\tau)^{\frac{1}{2}}} \frac{1}{\sqrt{\text{Det} \left(\frac{\sigma_{\rho^{(1/2)}} + \sigma_{\tau^{(1/2)}}}{2} \right)}} \quad (37)$$

where

$$\sigma_{\rho^{(1/2)}} = \left(\sqrt{I + (\sigma_\rho \Omega)^{-2}} + I \right) \sigma_\rho, \quad (38)$$

$$\sigma_{\tau^{(1/2)}} = \left(\sqrt{I + (\sigma_\tau \Omega)^{-2}} + I \right) \sigma_\tau, \quad (39)$$

and

$$Z_{\rho^{(1/2)}} = \sqrt{\text{Det} \left(\frac{\sigma_{\rho^{(1/2)}} + i\Omega}{2} \right)}, \quad (40)$$

$$Z_{\tau^{(1/2)}} = \sqrt{\text{Det} \left(\frac{\sigma_{\tau^{(1/2)}} + i\Omega}{2} \right)}. \quad (41)$$

Now we shall consider the case of $\alpha > 1$. This is interesting because we will have to deal with inverses of Gaussian states which are in general unbounded operators. However, we can find expressions

for overlaps. In order to derive such an expression, note that for $H_1, H_2 > 0$ such that $\sigma_2 > \sigma_1$, we have (see Ref. [1])

$$\text{Tr} \left[e^{-\hat{r}^T H_1 \hat{r}} e^{-\hat{r}^T (-H_2) \hat{r}} \right] = \frac{\sqrt{\text{Det} \left(\frac{\sigma_1 + i\Omega}{2} \right) \text{Det} \left(\frac{\sigma_2 + i\Omega}{2} \right)}}{\sqrt{\text{Det} \left(\frac{\sigma_2 - \sigma_1}{2} \right)}} \quad (42)$$

Now we can consider

$$Q_\alpha(\rho, \tau) = \text{Tr} \left[\rho^\alpha \tau^{1-\alpha} \right] \quad (43)$$

$$= \frac{1}{(Z_\rho)^\alpha (Z_\tau)^{1-\alpha}} \text{Tr} \left[e^{-\frac{1}{2} \hat{r}^T \alpha H_\rho \hat{r}} e^{-\frac{1}{2} \hat{r}^T [-(\alpha-1) H_\tau] \hat{r}} \right] \quad (44)$$

We can apply the above relation to obtain the following, when $\sigma_{\tau(\alpha-1)} > \sigma_{\rho(\alpha)}$

$$\text{Tr} \left[\rho^\alpha \tau^{1-\alpha} \right] = \frac{Z_{\rho(\alpha)} Z_{\tau(\alpha-1)}}{(Z_\rho)^\alpha (Z_\tau)^{1-\alpha}} \frac{1}{\sqrt{\text{Det} \left(\frac{\sigma_{\tau(\alpha-1)} - \sigma_{\rho(\alpha)}}{2} \right)}} \quad (45)$$

where $Z_{\rho(\alpha)}$, $Z_{\tau(\alpha-1)}$, and $\sigma_{\rho(\alpha)}$ and $\sigma_{\tau(1-\alpha)}$ are defined similarly. The above expression simplifies significantly for $\alpha = 2$. In that case, for $\sigma_\tau > \sigma_{\rho(2)}$

$$\text{Tr}[\rho^2 \tau^{-1}] = \frac{Z_{\rho(2)} (Z_\tau)^2}{(Z_\rho)^2} \frac{1}{\sqrt{\text{Det} \left(\frac{\sigma_\tau - \sigma_{\rho(2)}}{2} \right)}} \quad (46)$$

where

$$\sigma_{\rho(2)} = \frac{1}{2} (\sigma_\rho + \Omega \sigma_\rho^{-1} \Omega^T) \quad (47)$$

2.3 Sandwiched Petz-Rényi relative entropy

Let's now consider the sandwiched Petz-Rényi relative entropy:

$$\tilde{Q}_\alpha(\rho, \tau) = \text{Tr} \left[\left(\tau^{\frac{1-\alpha}{2\alpha}} \rho \tau^{\frac{1-\alpha}{2\alpha}} \right)^\alpha \right] \quad (48)$$

$$= \text{Tr} \left[\left(\rho^{\frac{1}{2}} \tau^{\frac{1-\alpha}{\alpha}} \rho^{\frac{1}{2}} \right)^\alpha \right] \quad (49)$$

For states ρ and τ as defined in Eqs. (8) and (9),

$$\tilde{Q}_\alpha(\rho, \tau) = \frac{1}{(Z_\rho)^\alpha (Z_\tau)^{1-\alpha}} \text{Tr} \left[\left(e^{-\frac{1}{2} \hat{r}^T \frac{1}{2} H_\rho \hat{r}} e^{-\frac{1}{2} \hat{r}^T [\beta H_\tau] \hat{r}} e^{-\frac{1}{2} \hat{r}^T \frac{1}{2} H_\rho \hat{r}} \right)^\alpha \right], \quad (50)$$

where $\beta = (1 - \alpha)/\alpha$. We use the fact that

$$e^{-\frac{1}{2} \hat{r}^T \frac{1}{2} H_1 \hat{r}} e^{-\frac{1}{2} \hat{r}^T H_2 \hat{r}} e^{-\frac{1}{2} \hat{r}^T \frac{1}{2} H_1 \hat{r}} = e^{-\frac{1}{2} \hat{r}^T H_3 \hat{r}} \quad (51)$$

where (see Prop. 8, Ref. [1])

$$H_3 = 2i\Omega \text{arccoth}(\sigma_3 i\Omega), \quad (52)$$

$$\sigma_3 = \sigma_1 - \left(\sqrt{I + (\sigma_1 \Omega)^{-2}} \right) \sigma_1 (\sigma_1 + \sigma_2)^{-1} \sigma_1 \left(\sqrt{I + (\Omega \sigma_1)^{-2}} \right). \quad (53)$$

Using this, we find that

$$e^{-\frac{1}{2}\hat{r}^T \frac{1}{2}H_\rho \hat{r}} e^{-\frac{1}{2}\hat{r}^T \beta H_\tau \hat{r}} e^{-\frac{1}{2}\hat{r}^T \frac{1}{2}H_\rho \hat{r}} = e^{-\frac{1}{2}\hat{r}^T H_\zeta \hat{r}}, \quad (54)$$

where

$$H_\zeta = 2i\Omega \operatorname{arccoth}(\sigma_\zeta i\Omega), \quad (55)$$

$$\sigma_\zeta = \sigma_\rho - \left(\sqrt{I + (\sigma_\rho \Omega)^{-2}} \right) \sigma_\rho (\sigma_\rho + \sigma_\tau)^{-1} \sigma_\rho \left(\sqrt{I + (\Omega \sigma_\rho)^{-2}} \right), \quad (56)$$

$$\sigma_{\tau(\beta)} = \frac{[I + (\sigma_\tau i\Omega)^{-1}]^\beta + [I - (\sigma_\tau i\Omega)^{-1}]^\beta}{[I + (\sigma_\tau i\Omega)^{-1}]^\beta - [I - (\sigma_\tau i\Omega)^{-1}]^\beta} i\Omega. \quad (57)$$

Finally, we exponentiate this expression with α from the definition of sandwiched Petz-Rényi overlap. We use the fact that this scales the resultant Hamiltonian matrix by a factor α so as to obtain

$$\operatorname{Tr} \left[e^{-\frac{1}{2}\hat{r}^T \alpha H_\zeta \hat{r}} \right] = \sqrt{\operatorname{Det} \left(\frac{\sigma_{\zeta(\alpha)} + i\Omega}{2} \right)} \quad (58)$$

where

$$\sigma_{\zeta(\alpha)} = \frac{[I + (\sigma_\zeta i\Omega)^{-1}]^\alpha + [I - (\sigma_\zeta i\Omega)^{-1}]^\alpha}{[I + (\sigma_\zeta i\Omega)^{-1}]^\alpha - [I - (\sigma_\zeta i\Omega)^{-1}]^\alpha} i\Omega \quad (59)$$

Thus we obtain our formula for the sandwiched Petz-Rényi overlap as:

$$\tilde{Q}_\alpha(\rho, \tau) = \frac{1}{(Z_\rho)^\alpha (Z_\tau)^{1-\alpha}} \sqrt{\operatorname{Det} \left(\frac{\sigma_{\zeta(\alpha)} + i\Omega}{2} \right)} \quad (60)$$

Fidelity is a special case of sandwiched Petz-Rényi overlap. When $\alpha = \frac{1}{2}$, we have

$$F[\rho, \tau] = \left(\tilde{Q}_{\alpha=\frac{1}{2}}(\rho, \tau) \right)^2 \quad (61)$$

Fidelity: If $\alpha = \frac{1}{2}$, we have $\beta = 1$, and $\tau(\beta) = \tau$. Thus we have

$$\sigma_\zeta = \sigma_\rho - \left(\sqrt{I + (\sigma_\rho \Omega)^{-2}} \right) \sigma_\rho (\sigma_\rho + \sigma_\tau)^{-1} \sigma_\rho \left(\sqrt{I + (\sigma_\rho \Omega)^{-2}} \right), \quad (62)$$

$$\sigma_{\zeta(\alpha=\frac{1}{2})} = \left(\sqrt{I + (\sigma_\zeta \Omega)^{-2}} + I \right) \sigma_\zeta, \quad (63)$$

and thus the fidelity becomes

$$F[\rho, \tau] = \operatorname{Tr} \left[\sqrt{\rho^{\frac{1}{2}} \tau \rho^{\frac{1}{2}}} \right]^2 \quad (64)$$

$$= \frac{\operatorname{Det} \left[\sigma_{\zeta(\frac{1}{2})} \right]}{Z_\rho Z_\tau} \quad (65)$$

Now we will find an expression for the sandwiched Petz-Rényi overlap when $\alpha > 1$. For simplicity, define $\gamma = -\beta > 0$. When $\sigma_{\tau(\gamma)} > \sigma_\rho$, we have

$$\tilde{Q}_\alpha(\rho, \tau) = \frac{1}{(Z_\rho)^\alpha (Z_\tau)^{1-\alpha}} \sqrt{\operatorname{Det} \left(\frac{\sigma_{\zeta(\alpha)} + i\Omega}{2} \right)} \quad (66)$$

where

$$\sigma_{\zeta(\alpha)} = \frac{[I + (\sigma_{\zeta}i\Omega)^{-1}]^{\alpha} + [I - (\sigma_{\zeta}i\Omega)^{-1}]^{\alpha}}{[I + (\sigma_{\zeta}i\Omega)^{-1}]^{\alpha} - [I - (\sigma_{\zeta}i\Omega)^{-1}]^{\alpha}} i\Omega, \quad (67)$$

$$\sigma_{\zeta} = \sigma_{\rho} + \left(\sqrt{I + (\sigma_{\rho}\Omega)^{-2}} \right) \sigma_{\rho} (\sigma_{\tau(\gamma)} - \sigma_{\rho})^{-1} \sigma_{\rho} \left(\sqrt{I + (\sigma_{\rho}\Omega)^{-2}} \right), \quad (68)$$

$$\sigma_{\tau(\gamma)} = \frac{[I + (\sigma_{\tau}i\Omega)^{-1}]^{\gamma} + [I - (\sigma_{\tau}i\Omega)^{-1}]^{\gamma}}{[I + (\sigma_{\tau}i\Omega)^{-1}]^{\gamma} - [I - (\sigma_{\tau}i\Omega)^{-1}]^{\gamma}} i\Omega. \quad (69)$$

References

- [1] K. P. Seshadreesan, L. Lami, and M. M. Wilde, *J. Math. Phys.* **59**, 072204 (2018).

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1 Overview

In the last lecture we derived formulas for various overlap measures of Gaussian states.

In this lecture we discuss quasiprobability distributions and characteristic functions to describe Gaussian states. We will also discuss various properties of displacement operators and how they can be used to describe any state.

2 Characteristic functions and Quasiprobability distributions

While Gaussian states can be described by their covariance matrix and mean vector, an alternative way to visualize them is in the phase space. Wigner functions are well-known quasiprobability distributions that can fully characterize a state. For Gaussian states, the Wigner function is non-negative.

Any quantum mechanical process has three parts: state preparation, subsequent evolution through a channel, and finally measurements. This can be captured via a quasi-probability distribution as

$$\mathrm{Tr}[\Omega \mathcal{N}(\rho)] = \int \underbrace{W(\Omega|\lambda)}_{\text{Measurement}} \underbrace{W_{\mathcal{N}}(\lambda|\lambda')}_{\text{Channel}} \underbrace{W_{\rho}(\lambda')}_{\text{State}} d\lambda d\lambda' \quad (1)$$

If each of the three terms of the integrand are positive, then it means that there is an underlying classical description of the quantum physical experiment.

3 Displacement operators

Recall that we defined the displacement operator as

$$\hat{D}_{-r} = e^{-ir^T \Omega \hat{r}} \quad (2)$$

where

$$r = \begin{pmatrix} x \\ p \end{pmatrix} \quad (3)$$

Alternatively, we can define the displacement operator using complex numbers and mode creation and annihilation operators as

$$\hat{D}_{\alpha} = e^{\alpha \hat{a}^{\dagger} - \alpha^* \hat{a}} \quad (4)$$

where

$$\alpha = \frac{x + ip}{\sqrt{2}} \quad (5)$$

Then

$$\hat{D}_{-r} = \hat{D}_\alpha \quad (6)$$

Coherent states are displaced states of the vacuum as

$$\hat{D}_\alpha |0\rangle = |\alpha\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_n \frac{\alpha^n}{\sqrt{n!}} |n\rangle \quad (7)$$

Successive displacements are equivalent to a single displacement up to an overall phase factor as

$$\hat{D}_\alpha \hat{D}_\beta = e^{\frac{1}{2}(\alpha\beta^* - \alpha^*\beta)} \hat{D}_{\alpha+\beta} \quad (8)$$

This allows us to compute the overlap of two coherent states. The overlap of two coherent states is always strictly positive and is given as

$$\langle\beta|\alpha\rangle = \langle 0|\hat{D}_{-\beta}\hat{D}_\alpha|0\rangle \quad (9)$$

$$= \langle 0|\hat{D}_{\alpha-\beta}|0\rangle e^{\frac{1}{2}(\alpha\beta^* - \alpha^*\beta)} \quad (10)$$

$$= \langle 0|\alpha - \beta\rangle e^{\frac{1}{2}(\alpha\beta^* - \alpha^*\beta)} \quad (11)$$

$$= e^{-\frac{1}{2}|\alpha-\beta|^2} e^{\frac{1}{2}(\alpha\beta^* - \alpha^*\beta)} \quad (12)$$

Coherent states together form an overcomplete basis as

$$\hat{I} = \frac{1}{\pi} \int d^2\alpha |\alpha\rangle\langle\alpha| \quad (13)$$

This fact can be used to evaluate the traces of trace-class operators. For any trace-class operator, we have

$$\text{Tr}[\hat{O}] = \sum_{m=0}^{\infty} \langle m|\hat{O}|m\rangle \quad (14)$$

$$= \sum_{m=0}^{\infty} \langle m|\frac{1}{\pi} \int d^2\alpha |\alpha\rangle\langle\alpha|\hat{O}|m\rangle \quad (15)$$

$$= \frac{1}{\pi} \int d^2\alpha \sum_{m=0}^{\infty} \langle m|\alpha\rangle\langle\alpha|\hat{O}|m\rangle \quad (16)$$

$$= \frac{1}{\pi} \int d^2\alpha \sum_{m=0}^{\infty} \langle\alpha|\hat{O}|m\rangle\langle m|\alpha\rangle \quad (17)$$

$$= \frac{1}{\pi} \int_{\mathbb{C}} d^2\alpha \langle\alpha|\hat{O}|\alpha\rangle \quad (18)$$

3.1 Mean vector of coherent states

The above result can be used to evaluate the mean vector and covariance matrix of a coherent state. Alternatively, there is a simpler derivation:

$$\text{Tr} [\hat{x}|\alpha\rangle\langle\alpha|] = \langle\alpha|\hat{x}|\alpha\rangle \quad (19)$$

$$= \langle\alpha|\frac{\hat{a} + \hat{a}^\dagger}{\sqrt{2}}|\alpha\rangle \quad (20)$$

$$= \frac{\langle\alpha|(\hat{a}|\alpha\rangle) + (\langle\alpha|\hat{a}^\dagger)|\alpha\rangle}{\sqrt{2}} \quad (21)$$

$$= \frac{\langle\alpha|\alpha\rangle + \langle\alpha|\alpha^*\rangle}{\sqrt{2}} \quad (22)$$

$$= \frac{2\text{Re}\{\alpha\}}{\sqrt{2}} \quad (23)$$

Alternatively, we can use

$$\text{Tr} [\hat{x}|\alpha\rangle\langle\alpha|] = \text{Tr} [\hat{x}\hat{D}_\alpha|0\rangle\langle 0|\hat{D}_{-\alpha}] \quad (24)$$

$$= \text{Tr} [\hat{D}_{-\alpha}\hat{x}\hat{D}_\alpha|0\rangle\langle 0|] \quad (25)$$

$$= \text{Tr} [\hat{D}_r\hat{x}\hat{D}_{-r}|0\rangle\langle 0|] \quad (26)$$

$$= \text{Tr} [(\hat{x} + x)|0\rangle\langle 0|] \quad (27)$$

$$= \langle 0|\hat{x}|0\rangle + x \quad (28)$$

$$= x \quad (29)$$

$$= \sqrt{2}\text{Re}(\alpha) \quad (30)$$

Similarly, we can find the expectation value of momentum quadrature also. Thus we obtain that for a coherent state $|\alpha\rangle$, the mean vector \bar{r} is

$$\bar{r} = \begin{pmatrix} \sqrt{2}\text{Re}(\alpha) \\ \sqrt{2}\text{Im}(\alpha) \end{pmatrix}, \quad (31)$$

3.2 Covariance matrix of coherent states

We now calculate the covariance matrix of coherent states. We note that

$$\text{Tr} [\hat{x}^2|\alpha\rangle\langle\alpha|] = \text{Tr} [\hat{x}^2\hat{D}_\alpha|0\rangle\langle 0|\hat{D}_{-\alpha}] \quad (32)$$

$$= \text{Tr} [\hat{D}_r\hat{x}^2\hat{D}_{-r}|0\rangle\langle 0|] \quad (33)$$

$$= \text{Tr} [(\hat{x} + x)^2|0\rangle\langle 0|] \quad (34)$$

$$= \text{Tr} [(\hat{x}^2 + 2x\hat{x} + x^2)|0\rangle\langle 0|] \quad (35)$$

$$= 1/2 + x^2 \quad (36)$$

Therefore we have

$$2 \operatorname{Tr} [(\hat{x} - x)^2 |\alpha\rangle\langle\alpha|] = 1 \quad (37)$$

Similarly, we can find the other covariance matrix elements also to find that the covariance matrix σ is

$$\sigma = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \quad (38)$$

We note that the covariance matrix of coherent states is the same as that of the vacuum state.

3.3 Trace of a displacement operator

The displacement operator is not trace class, but it is useful to consider its trace in a generalized sense as follows:

$$\operatorname{Tr}[\hat{D}(\beta)] = \pi \delta^2(\beta), \beta \in \mathbb{C}, \quad (39)$$

which turns out to be a key tool in continuous-variable quantum information.

To prove this, we will first find out $\langle\alpha|\hat{D}(\beta)|\alpha\rangle$. This is

$$\langle\alpha|\hat{D}(\beta)|\alpha\rangle = \langle 0|\hat{D}^\dagger(\alpha)\hat{D}(\beta)\hat{D}(\alpha)|0\rangle \quad (40)$$

$$= \langle 0|\hat{D}^\dagger(\alpha)\exp(\beta\hat{a}^\dagger - \beta^*\hat{a})\hat{D}(\alpha)|0\rangle \quad (41)$$

$$= \langle 0|\exp[\hat{D}^\dagger(\alpha)(\beta\hat{a}^\dagger - \beta^*\hat{a})\hat{D}(\alpha)]|0\rangle \quad (42)$$

$$= \langle 0|\exp[\beta(\hat{a}^\dagger + \alpha) - \beta^*(\hat{a} + \alpha)]|0\rangle \quad (43)$$

Now we use the results that

$$D^\dagger(\alpha)\hat{a}^\dagger D(\alpha) = \hat{a}^\dagger + \alpha^*, \quad (44)$$

$$D^\dagger(\alpha)\hat{a} D(\alpha) = \hat{a} + \alpha \quad (45)$$

so as to obtain

$$\langle\alpha|\hat{D}(\beta)|\alpha\rangle = e^{\beta\alpha^* - \beta^*\alpha} \langle 0|\hat{D}(\beta)|0\rangle \quad (46)$$

$$= e^{\beta\alpha^* - \beta^*\alpha} \langle 0|\beta\rangle \quad (47)$$

$$= e^{\beta\alpha^* - \beta^*\alpha} e^{-\frac{1}{2}|\beta|^2} \quad (48)$$

Using the above result, we can find an expression for the trace of a displacement operator as

$$\operatorname{Tr}[\hat{D}(\beta)] = \frac{1}{\pi} \int d^2\alpha \langle\alpha|\hat{D}(\beta)|\alpha\rangle \quad (49)$$

$$= \frac{e^{-\frac{|\beta|^2}{2}}}{\pi} \int d^2\alpha e^{\beta\alpha^* - \beta^*\alpha} \quad (50)$$

To simplify, redefine

$$\alpha = x + iy, \quad \beta = u + iv, \quad (51)$$

so that $\beta\alpha^* - \beta^*\alpha = 2i(vx - uy)$. Now we have

$$\text{Tr}[\hat{D}(\beta)] = \frac{e^{-\frac{|\beta|^2}{2}}}{\pi} \int \int dx dy e^{2ivx - 2iuy} \quad (52)$$

$$= \frac{e^{-\frac{|\beta|^2}{2}}}{\pi} \int dx e^{2ivx} \int dy e^{-2iuy} \quad (53)$$

$$= \frac{e^{-\frac{|\beta|^2}{2}}}{\pi} 2\pi \delta(2v) 2\pi \delta(2u) \quad (54)$$

$$= \frac{e^{-\frac{|\beta|^2}{2}}}{\pi} \pi^2 \delta(v) \delta(u) \quad (55)$$

$$= \pi \delta^2(\beta) \quad (56)$$

as the exponential factor $e^{-\frac{|\beta|^2}{2}}$ is equal to one when the delta function is nonzero at $\beta = 0$.

3.4 Hilbert-Schmidt inner product of displacement operators

Now we will find the Hilbert-Schmidt inner product of displacement operators. Using the above relation, this is

$$\text{Tr}[\hat{D}(\alpha)\hat{D}(-\beta)] = e^{\frac{1}{2}(-\alpha\beta^* + \alpha^*\beta)} \text{Tr}[\hat{D}(\alpha - \beta)] \quad (57)$$

$$= e^{\frac{1}{2}(-\alpha\beta^* + \alpha^*\beta)} \pi \delta^2(\alpha - \beta) \quad (58)$$

$$= \pi \delta^2(\alpha - \beta) \quad (59)$$

wherein again, we use the fact that the exponential factor $e^{\frac{1}{2}(-\alpha\beta^* + \alpha^*\beta)}$ is equal to one when the delta function is nonzero at $\alpha = \beta$.

In terms of real variables, we can write this orthogonality relation as

$$\text{Tr} [\hat{D}_r \hat{D}_{-s}] = 2\pi \delta^2(r - s) \quad (60)$$

where

$$\alpha = \frac{x_r + ip_r}{\sqrt{2}}, \quad \beta = \frac{x_s + ip_s}{\sqrt{2}}. \quad (61)$$

Generalizing to n modes, the orthogonality relations are as follows:

$$\text{Tr} [\hat{D}(\underline{\alpha}) \hat{D}(-\underline{\beta})] = \pi^n \delta^{2n}(\underline{\alpha} - \underline{\beta}), \quad (62)$$

$$\text{Tr} [\hat{D}_{\underline{r}} \hat{D}_{-\underline{s}}] = (2\pi)^n \delta^{2n}(\underline{r} - \underline{s}). \quad (63)$$

4 Characteristic functions

We define the symmetrically ordered Weyl characteristic function of a state ρ as

$$\chi_\rho(\alpha) = \text{Tr}[\hat{D}(\alpha)\rho] \quad \forall \alpha \in \mathbb{C} \quad (64)$$

This characteristic function is finite for all $\alpha \in \mathbb{C}$ if ρ is trace class. To see this we use the Hölder inequality to have

$$\left| \text{Tr} \left[\hat{D}(\alpha) \rho \right] \right| \leq \left\| \hat{D}(\alpha) \right\|_{\infty} \|\rho\|_1 = \|\rho\|_1 < \infty. \quad (65)$$

Using the Weyl characteristic function, we can write the state as

$$\rho = \frac{1}{\pi} \int d^2\alpha \chi_{\rho}(\alpha) \hat{D}(-\alpha). \quad (66)$$

To prove this, we note that

$$\rho = \left[\frac{1}{\pi} \int d^2\alpha |\alpha\rangle\langle\alpha| \right] \rho \left[\frac{1}{\pi} \int d^2\beta |\beta\rangle\langle\beta| \right] \quad (67)$$

$$= \frac{1}{\pi^2} \int \int d^2\alpha d^2\beta \langle\alpha|\rho|\beta\rangle |\alpha\rangle\langle\beta|. \quad (68)$$

So we only have to show that

$$|\alpha\rangle\langle\beta| = \frac{1}{\pi} \int d^2\gamma \text{Tr} \left[|\alpha\rangle\langle\beta| \hat{D}_{\gamma} \right] \hat{D}_{-\gamma} \quad (69)$$

This can be rewritten as

$$|0\rangle\langle 0| = \frac{1}{\pi} \int d^2\gamma \text{Tr} \left[|\alpha\rangle\langle\beta| \hat{D}_{\gamma} \right] \hat{D}_{-\alpha} \hat{D}_{-\gamma} \hat{D}_{\beta} \quad (70)$$

$$= \frac{1}{\pi} \int d^2\gamma \langle\beta - \gamma|\alpha\rangle e^{\gamma\beta^* - \gamma^*\beta} \hat{D}_{-\alpha} \hat{D}_{-\gamma} \hat{D}_{\beta} \quad (71)$$

$$= \frac{1}{\pi} \int d^2\gamma e^{-\frac{1}{2}|\beta - \alpha - \gamma|^2} \hat{D}_{\beta - \alpha - \gamma} \quad (72)$$

$$= \frac{1}{\pi} \int d^2\gamma e^{-\frac{1}{2}|\gamma|^2} \hat{D}_{\gamma} \quad (73)$$

We will prove this in the next lecture.