Quantum estimation for non-differentiable models

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Abstract
State estimation is a classical problem in quantum information. In optimization
of an estimation scheme, to find a lower bound to the error of the estimator
is a very important step. So far, all the proposed tractable lower bounds use
a derivative of the density matrix. However, sometimes, we are interested in
quantities with singularity, e.g. concurrence etc. In this paper, lower bounds
to a mean square error of an estimator are derived for a quantum estimation
problem without smoothness assumptions. Our main idea is to replace the
derivative by difference, as is done in classical estimation theory. We applied
the inequalities to several examples, and derived an optimal estimator for some
of them.

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1. Introduction

Quantum state estimation is a classical problem in quantum information [12, 16]. It is not
only useful for various purposes, e.g., evaluation of realized quantum information processing
systems, but also is a fundamental problem in its own right.

As is the case in classical estimation theory[4], often, it is assumed that the unknown source
is a member of a parametrized family of quantum states, which is called a *model*, to reduce the
problem to the estimation of the unknown (in general, vector valued) parameter. Sometimes,
we are interested in some physical quantities of the state, e.g. entanglement of the state. In
such cases, the estimation of a function of the unknown parameter is considered.

So far, most of the studies of quantum estimation theory have assumed that the model
is a smooth surface in the space of quantum states, and that the function to be estimated is
differentiable up to the necessary order. Under these smoothness assumptions, tractable lower
bounds to the MSE of the estimator have been studied, and some of them give achievable

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[4] Throughout the paper, the estimation theory of classical probability distributions is called 'classical estimation'.

bounds [12, 15, 16, 25]. Especially, in the asymptotic regime, we have lots of results on achievable bounds.

On the other hand, when there are singularities in the model and/or in the function to be estimated, little has been found out, so far as general theory is concerned. It should be stressed that there are some practically important examples to which the smoothness assumptions do not apply. For example, concurrence, a measure of entanglement, is singular at zero point. Also, considering that state estimation is a fundamental problem of quantum information, it is better studied in the most general setting.

The discrete models, or the models whose parameter takes values in a discrete set, are the only non-differentiable models which have been studied intensively, and there are many results in special cases, mainly by exploiting symmetry. However, there are relatively few results which are valid for all discrete models. To begin with, it is not straightforward even to work out a non-trivial lower bound to the error of the optimal measurement. It is true that the formula in [24, 14], which is a special case of the complementarity theorem of SDP, gives necessary and sufficient conditions for the optimal measurement. However, this formula is far from tractable in many cases, being a system of nonlinear matrix equations and inequalities.

The purpose of the paper is to give the first general treatment of quantum state estimation without the smoothness assumptions, developing quantum versions of the Hammersley–Chapman–Robbins inequality [6, 9], Kshirsagar inequality [18] and Koike inequality [17] in classical statistics. While the lower bounds under the smoothness assumption use the differential of the density matrix, our new inequalities use difference.

The paper is organized as follows. Section 2 is preliminaries. We give a brief review on classical and quantum estimation theory, and set up the problem. In section 3, we state our new inequalities, whose proofs are given in section 5. In section 4, our theory is applied to several examples. Non-asymptotic and asymptotic inequalities are derived, and based on those, optimal estimates are given for some of the examples. In section 6, we state the conclusions and the future problems.

2. Preliminaries

2.1. Classical estimation theory

An important problem of classical estimation is to optimize the estimator of (a function of) the parameter which is assigned for the unknown probability distribution. The error is often evaluated by MSE under the unbiasedness condition. Here, the estimator is said to be unbiased if its expectation equals the true value of (a function of) the parameter.

In many cases, the optimal solution is too hard to obtain. However, a series of tractable lower bounds to mean square errors (MSEs) of unbiased estimators is derived using the first-order and the higher order derivatives of the probability distribution with respect to the parameter of the model. The inequality based on the first-order derivative is called the Cramér–Rao (CR) inequality [20], while those which also exploit the higher order derivatives are called Bhattacharyya inequalities [4]. By definition, the Bhattacharyya inequality is always not worse than the CR inequality.

In general, none of these lower bounds is achievable, but yet there are many cases where one of them can be achieved by some estimators. In the asymptotic limit, an asymptotic CR inequality gives achievable lower bounds in general [1]. Needless to say, these inequalities rely on the smoothness assumptions.

These inequalities can be generalized to the cases with singularity by replacing (resp. higher order) derivatives by (resp. higher order) differences. A difference version of

the CR inequality (resp. Bhattacharyya inequality) is the Hammersley–Chapman–Robbins–Kshirsagar (HCRK) inequality [9, 6, 18] (resp. Koike inequality [17]). By definition, the Koike inequality is always not worse than the HCRK inequality. When the singularity is absent, by taking the difference infinitesimally small, those difference versions reproduce the derivative versions. We can also make an asymptotic version of the HCRK inequality, but unlike the differentiable cases, this bound is not always achievable [22]. See [2] for a more detailed description of the theory which allows singularity.

2.2. Quantum estimation theory with smoothness assumptions (I)

Quantum versions for inequalities under the smoothness assumptions, i.e., quantum Cramér–Rao (QCR) inequality [12, 16, 25] and quantum Bhattacharyya (QB) inequality [5], have already been studied a lot.

One important point is that, due to the non-commutativity of quantum mechanics, there are many quantum versions of those inequalities (quantum Cramér–Rao inequalities). A difficulty is that there is no 'best' QCR inequality. That is, to obtain the tighter lower bound, one must chose a proper version of QCR depending on the estimation problem of interest.

However, if either the parameter of the model is scalar valued, or a scalar-valued function of the parameter is to be estimated, an SLD QCR (defined later) gives a tighter lower bound than any other QCR. Also, in this case, an SLD QCR gives the asymptotically achievable lower bound to the error of estimators, as in the classical estimation theory.

Now, we state the mathematical detail of the theory. Let $\mathcal{H}$ be a separable Hilbert space describing the physical system of interest. Denote the set of linear operators on $\mathcal{H}$ and the set of density operators, by $\mathcal{L}(\mathcal{H})$ and by $\mathcal{S}(\mathcal{H})(\subset \mathcal{L}(\mathcal{H}))$, respectively. Let Θ be a parameter space which is a subset of the set $\mathbb{R}$ of real numbers, and assume that the density matrix for the system of interest is a member of a parametrized family of states, $\{\rho_\theta; \theta \in \Theta\}$, which is called a *model*. Throughout the paper, except as otherwise noted, we assume

$$\rho_\theta > 0, \tag{1}$$

or the density matrix ρ_θ has its reverse.

The model is said to be differentiable (resp. non-differentiable), if the map $\theta \mapsto \rho_\theta$ is differentiable (resp. not differentiable). We would like to estimate $g(\theta)$ by measuring the system where $g(\theta)$ is a function of θ. An estimator of $g(\theta)$ is a measurement whose output is an estimate, i.e., a POVM M which takes values on $g(\mathbb{R})$.

2.2.1. Non-asymptotic theory with the smoothness assumptions.
In a non-asymptotic setting, we often impose an unbiasedness condition on estimators, which is defined as follows:

Definition 1. *The bias $b(M, \theta)$ of an estimator M at θ is defined by*

$$b(M, \theta) = \int_{\gamma \in g(\Theta)} (\gamma - g(\theta)) \operatorname{Tr}(\rho_\theta M(\mathrm{d}\gamma)).$$

If $b(M, \theta) \equiv 0$, M is said to be unbiased at θ. If M is unbiased at any θ, M is said to be unbiased.

The classical CR inequality uses a *logarithmic derivative* $l_\theta(x)$ which is defined as

$$l_\theta(x) := \frac{\mathrm{d}}{\mathrm{d}\theta} \log p(x, \theta),$$

or as the solution to the equation

$$p(x, \theta)l_\theta(x) = \frac{\mathrm{d}p(x, \theta)}{\mathrm{d}\theta}.$$

There are many quantum analogues of a logarithmic derivative, due to the non-commutativity of quantum mechanics. Among those, a symmetric logarithmic derivative (SLD) and a right logarithmic derivative (RLD) are most frequently used.

Definition 2. *An SLD $L_\theta^S \in \mathcal{L}(\mathcal{H})$ is defined as a solution to the equation*

$$\frac{\mathrm{d}}{\mathrm{d}\theta}\rho_\theta = \frac{\rho_\theta L_\theta^S + L_\theta^S \rho_\theta}{2}, \qquad L_\theta^S = \left(L_\theta^S\right)^\dagger.$$

An RLD $L_\theta^R \in \mathcal{L}(\mathcal{H})$ defined as a solution to the equation

$$\frac{\mathrm{d}}{\mathrm{d}\theta}\rho_\theta = \rho_\theta L_\theta^R. \tag{2}$$

An SLD and an RLD are uniquely defined since ρ_θ is invertible by assumption (1). The performance of an estimator M of $g(\theta)$ is evaluated by the MSE

$$V_\theta(M) = \int_{\gamma \in g(\Theta)} (\gamma - g(\theta))^2 \operatorname{Tr}(\rho_\theta M(\mathrm{d}\gamma)).$$

If the bias $b(M,\theta)$ is exactly zero, MSE is equal to what is called variance. An SLD and an RLD quantum Cramér–Rao inequality are stated as follows:

Proposition 1 [12]**.** *If an estimator M is unbiased, it holds that*

$$V_\theta(M) \geqslant (g'(\theta))^2 / J_\theta^S \geqslant (g'(\theta))^2 / J_\theta^R \tag{3}$$

where

$$J_\theta^S = \operatorname{Tr}\left(\rho_\theta \left(L_\theta^S\right)^2\right), \qquad J_\theta^R = \operatorname{Tr}\left(\rho_\theta L_\theta^R \left(L_\theta^R\right)^\dagger\right).$$

The equality in the first inequality in (3) holds if and only if M gives the spectral decomposition of a Hermitian matrix T such that $T - g(\theta)I \in \operatorname{span}\{L_\theta^S\}$, where I is the identity on $\mathcal{H}$.

The proof of the proposition is reviewed in section 5.

See [20] for the classical version of the theory, [12, 16, 25] for the quantum theory.

2.2.2. Asymptotic theory with the smoothness assumptions. Assuming that n identical independent samples $\rho_\theta^{\otimes n}$ of unknown states ρ_θ are given, let us analyse the behaviour of estimators as n tends to infinity. An estimator is a POVM M living in $\mathcal{H}^{\otimes n}$. If the smoothness assumptions hold, the mean square error converges to zero with the order of $O(1/n)$. Therefore, we focus on the coefficient of the $1/n$-term.

In asymptotic analysis, the unbiasedness condition is replaced by asymptotic unbiasedness defined as follows.

Definition 3. *For the sequence M_n of estimators of $g(\theta)$, if the bias $b(M_n, \theta)$ satisfies*

$$b(M_n, \theta) = o(1/\sqrt{n}), \qquad \frac{\mathrm{d}}{\mathrm{d}x}b(M_n, x)\bigg|_{x=\theta} = o(1/\sqrt{n}),$$

M_n is said to be asymptotically unbiased at θ. If M_n is unbiased at any $\theta \in \Theta$, M is said to be asymptotically unbiased.

The asymptotic quantum Cramér–Rao (AQCR) inequality is stated as follows:

Proposition 2 [7, 10, 8]**.** *Assume that M_n is asymptotically unbiased. Then, we have*

$$\lim_{n\to\infty} nV_\theta(M_n) \geqslant (g'(\theta))^2 / J_\theta^S \geqslant (g'(\theta))^2 / J_\theta^R. \tag{4}$$

Especially, the first inequality is achieved by some asymptotically unbiased estimators.

2.3. Quantum estimation theory with smoothness assumptions (II)

In this subsection, we review quantum estimation theory for vector-valued parameters with smoothness assumptions. For simplicity, here we concentrate on the estimation of the parameter itself, and do not treat the estimation of $g(\theta)$.

Let us denote by m the dimension of the parameter $\theta = (\theta^1, \ldots, \theta^m)$ ($m = 1$ if θ is scalar), and define SLD $L_{i,\theta}^S$ of θ^i and RLD $L_{i,\theta}^R$ as the solution to the equations

$$\frac{\partial}{\partial \theta^i} \rho_\theta = \frac{1}{2}\left(L_{i,\theta}^S \rho_\theta + \rho_\theta L_{i,\theta}^S\right) = \rho_\theta L_{i,\theta}^R.$$

Define also matrices J_θ^S and J_θ^R by

$$J_{\theta,i,j}^S = \tfrac{1}{2} \operatorname{Tr} \rho_\theta \left(L_{i,\theta}^S L_{j,\theta}^S + L_{j,\theta}^S L_{i,\theta}^S\right), \qquad J_{\theta,i,j}^R = \operatorname{Tr} \rho_\theta L_{j,\theta}^R \left(L_{i,\theta}^R\right)^\dagger,$$

respectively.

Proposition 3 [16]. *Assume that the estimator M is unbiased (for each θ^i). Then, for any real valued positive matrix G, we have*

$$\operatorname{Sp} G V_\theta(M) \geqslant \operatorname{Sp} G \left(J_\theta^S\right)^{-1}, \qquad \operatorname{Sp} G V_\theta(M) \geqslant \operatorname{Sp} G \left(J_\theta^R\right)^{-1} + \operatorname{Spabs} \operatorname{Im} G \left(J_\theta^R\right)^{-1}.$$

The proof is reviewed in section 5. Here, Sp is the trace over the vector space $\mathbb{C}^m$, and Spabs A is the sum of absolute values of eigenvalues of A. Typically, G is chosen to be $\operatorname{diag}(g_1, \ldots, g_m)$, and in that case $\operatorname{Sp} G V_\theta(M)$ is a weighted sum of MSE of the estimators of components of θ.

Different from the scalar-valued parameter case, we cannot say which one is better in general. However, if $\left[L_{i,\theta}^S, L_{j,\theta}^S\right] = 0$, SLD QCR gives a better lower bound, and is asymptotically achievable by the estimator based on the simultaneous spectral decomposition of SLD. If LSD are not commutative, RLD QCR will often be useful.

3. New inequalities for non-differentiable models

3.1. Non-asymptotic theory without the smoothness assumptions

If ρ_θ and/or the function $g(\theta)$ are not differentiable with respect to θ, then the inequality (3) does not make any sense. In classical statistics, Hammersley [9] and Chapman and Robbins [6] have derived an inequality using the one-sided difference in place of the derivative, and Kshirsagar [18] improved it by the two-sided difference. We generalize their idea to the quantum theory. The proofs of the theorems are given in section 5.

Let $\mathcal{F}$ be the linear space of $\mathbb{R}$-valued functions of $\theta \in \Theta$. For $f(\theta) \in \mathcal{F}$ and for $\delta \in \mathbb{R}$, let Δ_δ be a linear operator defined by

$$\Delta_\delta^t f(\theta) = \frac{f(\theta + t\delta) - f(\theta - (1 - t)\delta)}{\delta}.$$

We next define operators, which are analogues of SLD and RLD.

Definition 4. *For $\delta \in \mathbb{R}$, define $L_{\theta,\delta}^{S,t}\left(= \left(L_{\theta,\delta}^{S,t}\right)^\dagger\right)$ and $L_{\theta,\delta}^{R,t}$ by*

$$\Delta_\delta^t \rho_\theta = \frac{\rho_\theta L_{\theta,\delta}^{S,t} + L_{\theta,\delta}^{S,t} \rho_\theta}{2}, \qquad \Delta_\delta^t \rho_\theta = \rho_\theta L_{\theta,\delta}^{R,t}. \tag{5}$$

($L_{\theta,\delta}^{S,t}$ and $L_{\theta,\delta}^R$ are uniquely defined since ρ_θ is invertible by the assumption (1).)

Remark 1. If ρ_θ is differentiable with θ, then $L_{\theta,\delta}^{S,t} \to L_\theta^S$ and $L_{\theta,\delta}^{R,t} \to L_\theta^R$ as $\delta \to 0$ since $\Delta_\delta^t \rho_\theta \to (d/d\theta)\rho_\theta$ as $\delta \to 0$.

If the model is differentiable both from the left and from the right, we have

$$\lim_{\delta \to 0+} L_{\theta,\delta}^{S,t} = t L_{\theta,t}^{S,+} + (1-t)L_\theta^{S,-}, \qquad \lim_{\delta \to 0+} L_{\theta,\delta}^{R,t} = t L_{\theta,t}^{R,+} + (1-t)L_\theta^{R,-}, \tag{6}$$

where $L_\theta^{S,\pm}$ and $L_\theta^{R,\pm}$ are defined by

$$\lim_{\delta \to 0\pm} \Delta_\delta^1 \rho_\theta = \tfrac{1}{2}\big(\rho_\theta L_\theta^{S,\pm} + L_\theta^{S,\pm}\rho_\theta\big) = \rho_\theta L_\theta^{R,\pm}.$$

(Observe that

$$\Delta_\delta^t \rho_\theta = t\Delta_{t\delta}^1 \rho_\theta + (1-t)\Delta_{(1-t)\delta}^0 \rho_\theta.)$$

If the singular model of our concern is embedded in the larger smooth model, then $L_\theta^{S,\pm}$ and $L_\theta^{R,\pm}$ are calculated from SLD and RLD of the larger model.

Our first result, the quantum Hammersley–Chapman–Robbins–Kshirsagar (QHCRK) inequality, is given in the following theorem:

Theorem 1. *If the estimator M of $g(\theta)$ is unbiased, then*

$$V_\theta(M) \geqslant (\Delta_\delta^t g(\theta))^2 \big/ J_{\theta,\delta}^{S,t} \tag{7}$$

$$\geqslant (\Delta_\delta^t g(\theta))^2 \big/ J_{\theta,\delta}^{R,t} \tag{8}$$

where

$$J_{\theta,\delta}^{S,t} = \mathrm{Tr}\big(\rho_\theta \big(L_{\theta,\delta}^{S,t}\big)^2\big), \qquad J_{\theta,\delta}^{R,t} = \mathrm{Tr}\big(\rho_\theta L_{\theta,\delta}^R \big(L_{\theta,\delta}^{R,t}\big)^\dagger\big).$$

The equality in (7) holds if and only if M gives the spectral decomposition of a Hermitian matrix T such that $T - \theta I \in \mathrm{span}\{L_{\theta,\delta}^{S,t}\}$.

We next present the quantum Koike (QK) inequality which improves QHCRK. For a function $f(\theta)$ of $\theta \in \Theta$, for a real number δ and for an integer $k \geqslant 1$, we define the kth difference operator $\Delta_{\delta,k}$ by

$$\Delta_{\delta,k} f(\theta) = (-1)^k \frac{1}{\delta^k} \sum_{i=0}^k (-1)^i \binom{k}{i} f(\theta + \delta i).$$

Note that, if $f(\theta)$ is k-times differentiable, then $\Delta_{\delta,k} f(\theta) \to (d^k/d\theta^k)f(\theta)$ as $\delta \to 0$. Let us define $L_{\theta,\delta,k}^S$ and $L_{\theta,\delta,k}^R$ as follows:

Definition 5. *Define $L_{\theta,\delta,k}^S$ and $L_{\theta,\delta,k}^R$ by*

$$\Delta_{\delta,k}\rho_\theta = \frac{\rho_\theta L_{\theta,\delta,k}^S + L_{\theta,\delta,k}^S \rho_\theta}{2}\big(L_{\theta,\delta,k}^S = \big(L_{\theta,\delta,k}^S\big)^\dagger\big),$$

$$\Delta_{\delta,k}\rho_\theta = \rho_\theta L_{\theta,\delta,k}^R.$$

Let us define $r \times r$ matrices $K_{\theta,\delta}^S = \big(K_{\theta,\delta,i,j}^S\big)$ and $K_{\theta,\delta}^R = \big(K_{\theta,\delta,i,j}^R\big)$ $(i, j = 1, \ldots, r)$ by

$$K_{\theta,\delta,i,j}^S = \mathrm{Tr}\big(\rho_\theta L_{\theta,\delta,i}^S L_{\theta,\delta,j}^S\big), \qquad K_{\theta,\delta,i,j}^R = \mathrm{Tr}\big(\rho_\theta L_{\theta,\delta,i}^R \big(L_{\theta,\delta,j}^R\big)^\dagger\big),$$

and let $\mathbf{v} = {}^t(\Delta_{\theta,\delta,1}g(\theta), \ldots, \Delta_{\theta,\delta,r}g(\theta))$ be a column vector. We then have the following quantum Koike inequality which generalizes and improves the QHCRK inequality of theorem 1.

Theorem 2. *If an estimator M for $g(\theta)$ is unbiased, then*

$$V_\theta(M) \geqslant {}^t\mathbf{v}\left(K_{\theta,\delta}^S\right)^{-1}\mathbf{v}, \tag{9}$$

$$V_\theta(M) \geqslant {}^t\mathbf{v}\left(K_{\theta,\delta}^R\right)^{-1}\mathbf{v}, \tag{10}$$

where $\left(K_{\theta,\delta}^S\right)^{-1}$ and $\left(K_{\theta,\delta}^R\right)^{-1}$ are generalized inverses. The equality holds if and only if M can be written as an observable T such that $T - \theta I \in \mathrm{span}\left\{L_{\theta,\delta,1}^S, \ldots, L_{\theta,\delta,k}^S\right\}$.

Remark 2. We can derive the Bhattacharyya inequality by theorem 2.

3.2. Asymptotic theory without the smoothness assumptions

If the smoothness assumptions are not valid, MSE $V_\theta(M_n, \theta)$ of appropriate estimators M_n does not necessarily scale in $O(1/n)$. (This point is discussed in [22] in detail in the classical estimation theory.) The convergence rate was expressed by an increasing sequence c_n that goes to infinity as $n \to \infty$.

In this paper, we study the following two cases.

Case 1. The parameter of the model takes discrete values, and each point in the model is isolated, and $g(\theta) = \theta$.
Case 2. The model and the function $g(\theta)$ are continuous,

In case 1, if the model has only two density matrices, the estimation of θ seems quite close to the test of a simple hypothesis about θ. We discuss this point later. In both cases 1 and 2, we use RLD-type inequalities, since SLD-type inequalities are mathematically intractable.

3.2.1. Discrete case.

If the set Θ of parameters is discrete and each element of Θ is isolated (i.e., there is a positive real number c such that, for any θ and $\theta' \in \Theta$, it holds that $\|\rho_\theta - \rho_{\theta'}\|_{\mathrm{tr}} > c$), then the convergence rates of the bias and the variance of appropriate estimators are exponential.

Assume that $\theta, \theta + \delta \in \Theta$, and that there is no element of $\Theta \subset \mathbb{R}$ between θ and $\theta + \delta$. We also assume that $g(\theta) \neq g(\theta + \delta)$. Then, we have the following asymptotic QHCRK (AQHCRK) inequality for the discrete case.

Theorem 3. *Assume that there is n_0 such that, if $n \geqslant n_0$, then $b(M_n, \theta)$ and $b(M_n, \theta + \delta)$ satisfy*

$$\frac{|b(M_n, \theta)|}{|\delta|} \leqslant \frac{|\Delta_\delta g(\theta)|}{3}, \qquad \text{and} \qquad \frac{|b(M_n, \theta + \delta)|}{|\delta|} \leqslant \frac{|\Delta_\delta g(\theta)|}{3}. \tag{11}$$

Then

$$\liminf_{n \to \infty} \frac{1}{n} \log(V_\theta(M_n)) \geqslant -\log\left(1 + \delta^2 J_{\theta,\delta}^{R,1}\right). \tag{12}$$

Proof. Observe

$$\mathrm{Tr}\, \rho_\theta^{-1} \rho_{\theta+\delta}^2 = 1 + \delta^2 J_{\theta,\delta}^{R,1}. \tag{13}$$

Replacing ρ_θ and $\rho_{\theta+\delta}$ in (13) by $\rho_\theta^{\otimes n}$ and $\rho_{\theta+\delta}^{\otimes n}$, we obtain

$$\mathrm{Tr}\left(\rho_\theta^{\otimes n} L_{\theta,\delta}^{R,(n)}\left(L_{\theta,\delta}^{R,(n)}\right)^\dagger\right) = \frac{1}{\delta^2}\left\{\mathrm{Tr}\left(\rho_\theta^{\otimes n}\right)^{-1}\left(\rho_{\theta+\delta}^{\otimes n}\right)^2 - 1\right\} = \frac{1}{\delta^2}\left(\left(\mathrm{Tr}\,\rho_\theta^{-1}\rho_{\theta+\delta}^2\right)^n - 1\right)$$

$$= \frac{1}{\delta^2}\left(\left(1 + \delta^2 J_{\theta,\delta}^{R,1}\right)^n - 1\right), \tag{14}$$

where the last equation is due to (13).

Assumption (11) and formula (28) imply that, for $n \geqslant n_0$,

$$\frac{1}{n} \log V_\theta(M_n) \geqslant \frac{1}{n} 2 \log |\Delta_\delta b(M_n, \theta) + \Delta_\delta g(\theta)| - \frac{1}{n} \log \mathrm{Tr}\big(\rho_{\theta,\delta}^{\otimes n} L_{\theta,\delta}^{R,(n)} \big(L_\delta^{R,(n)}\big)^\dagger\big)$$

$$= \frac{1}{n} 2 \log \left| \frac{b(M_n, \theta + \delta) - b(M_n, \theta)}{\delta} + \Delta_\delta g(\theta) \right| - \frac{1}{n} \frac{\big(1 + \delta^2 J_{\theta,\delta}^{R,1}\big)^n - 1}{\delta^2}$$

$$\geqslant \frac{1}{n} 2 \log \frac{|\Delta_\delta g(\theta)|}{3} - \frac{1}{n} \log \frac{\big(1 + \delta^2 J_{\theta,\delta}^{R,1}\big)^n - 1}{\delta^2}$$

$$\to -\log\big(1 + \delta^2 J_{\theta,\delta}^{R,1}\big) \qquad (n \to \infty).$$

Hence (12) holds.   □

We would like to remark that $\log(1 + \delta^2 J_{\theta,\delta}^{R,1})$ is always not smaller than the relative entropy $D(\rho_{\theta+\delta} \parallel \rho_\theta)$, which is defined as

$$D(\rho_{\theta+\delta} \| \rho_\theta) = \mathrm{Tr}(\rho_{\theta+\delta}(\log \rho_{\theta+\delta} - \log \rho_\theta)).$$

The reason is the following. Consider a model $\Theta = \{\theta, \theta + \delta\}$. Due to the theory of quantum hypothesis testing ([13, 21]), for any $\epsilon > 0$, there is a sequence N_n of POVMs taking values in $\mathbb{R}$ such that

$$\mathrm{Tr}\big(\rho_{\theta+\delta}^{\otimes n} N_n(\theta)\big) \leqslant \frac{|\Delta_\delta g(\theta)|}{3}, \qquad \lim_{n \to \infty} \frac{1}{n} \log \mathrm{Tr}\big(\rho_\theta^{\otimes n} N_n(\theta + \delta)\big) = -D(\rho_{\theta+\delta} \parallel \rho_\theta). \qquad (15)$$

We can regard N_n as an estimator of θ satisfying (11). Indeed, there is n_0 such that, if $n \geqslant n_0$ then

$$\frac{|b(N_n, \theta)|}{|\delta|} = \frac{|\delta| \, \mathrm{Tr}(\rho_\theta^{\otimes n} N_n(\theta + \delta))}{|\delta|} \leqslant \frac{|\Delta_\delta g(\theta)|}{3},$$

$$\frac{|b(N_n, \theta + \delta)|}{|\delta|} = \frac{|\delta| \, \mathrm{Tr}(\rho_{\theta+\delta}^{\otimes n} N_n(\theta))}{|\delta|} \leqslant \frac{|\Delta_\delta g(\theta)|}{3}.$$

Moreover,

$$\frac{1}{n} \log V_\theta(N_n) = \frac{1}{n} \log \big((g(\theta + \delta) - g(\theta))^2 \, \mathrm{Tr}\big(\rho_\theta^{\otimes n} N_n(\theta + \delta)\big)\big)$$

$$\to -D(\rho_{\theta+\delta} \parallel \rho_\theta) \qquad (n \to \infty).$$

Due to (12), we have $D(\rho_{\theta+\delta} \| \rho_\theta) \leqslant \log\big(1 + \delta^2 J_{\theta,\delta}^{R,1}\big)$.

3.2.2. Continuous case.

Let $L_{\theta,\delta}^{R,n,t}$ be the solution to the equation

$$\Delta_\delta^t \rho_\theta^{\otimes n} = \rho_\theta^{\otimes n} L_{\theta,\delta}^{R,n,t}.$$

For $h \in \mathbb{R}$, let $\delta = h/c_n$. Define that

$$J_\theta^{R,t} = \limsup_{h \to +0} \limsup_{n \to \infty} \frac{1}{c_n^2} \mathrm{Tr}\big(\rho_\theta^{\otimes n} L_{\theta,h/c_n}^{R,n,t} \big(L_{\theta,h/c_n}^{R,n,t}\big)^\dagger\big), \qquad g_t'(\theta) = \lim_{\delta \to +0} \Delta_\delta^t g(\theta).$$

If ρ_θ is differentiable from the right (resp. left), $J_\theta^{R,1}$ (resp. $J_\theta^{R,0}$) is equal to J_θ^R where the two-sided derivative in (2) is replaced with the right (resp. left) derivative. This is shown as follows. Replacing δ with $h/\sqrt{n}$ and c_n with $\sqrt{n}$ in (14), we have

$$J_\theta^{R,1} = \limsup_{h \to +0} \limsup_{n \to \infty} \frac{\big(1 + h^2 J_{\theta,h/\sqrt{n}}^R/n\big)^n - 1}{h^2} = \limsup_{h \to +0} \frac{e^{h^2 J_\theta^R} - 1}{h^2} \qquad (16)$$

$$= J_\theta^R.$$

(The left differentiable case is also given in a similar way.)

Next, we define asymptotic unbiasedness for a sequence M_n of estimators of $g(\theta)$ based on measurements of $\rho_\theta^{\otimes n}$ as follows:

Definition 6. *A sequence M_n of estimators of $g(\theta)$ is said to be c_n-unbiased at θ from the right if*

$$c_n b(M_n, \theta + h/c_n) \to 0 \qquad \text{as} \quad n \to \infty$$

for any $h \geqslant 0$ which is small enough. Similarly, M_n is said to be c_n-unbiased at θ from the left if

$$c_n b(M_n, \theta - h/c_n) \to 0 \qquad \text{as} \quad n \to \infty$$

for any $h \geqslant 0$ small enough.

Then, we have the following asymptotic right (resp. left) QHCRK inequality.

Theorem 4. *Assume that M_n is c_n unbiased at θ from the right (resp. from the left), and $J_\theta^{R,1} < \infty$, $|g_1'(\theta)| < \infty$ (resp. $J_\theta^{R,0} < \infty$, $|g_0'(\theta)| < \infty$). Then,*

$$\liminf_{n\to\infty} c_n^2 V_\theta(M_n) \geqslant (g_1'(\theta))^2 / J_\theta^{R,1} \qquad \left(\text{resp. } \liminf_{n\to\infty} c_n^2 V_\theta(M_n) \geqslant (g_0'(\theta))^2 J_\theta^{R,0}\right). \tag{17}$$

The proof is given in section 5.

Remark 3. Due to (16), theorem 4 implies AQCR inequality. Note that this argument is technically much more complicated than the proof of the similar statement in non-asymptotic theory. In fact, it is not straightforward to prove a similar relation between asymptotic SLD-base inequalities, for the absence of the equivalence of equation (14).

3.3. Non-asymptotic theory for a model with a vector-valued parameter

Define an operator $\Delta_{i,\delta}^t$ by

$$\Delta_{i,\delta}^t f(\theta) = \frac{f(\theta^1, \ldots, \theta^i + t\delta, \ldots, \theta^m) - f(\theta^1, \ldots, \theta^i - (1-t)\delta, \ldots, \theta^m)}{\delta},$$

and the difference version of SLD $L_{i,\theta,\delta}^{S,t}$ and RLD $L_{i,\theta,\delta}^{R,t}$ is defined as the solution to the equations

$$\Delta_{i,\delta}^t \rho_\theta = \tfrac{1}{2}\left(L_{i,\theta,\delta}^{S,t} \rho_\theta + \rho_\theta L_{i,\theta,\delta}^{S,t}\right) = \rho_\theta L_{i,\theta,\delta}^{R,t}.$$

The following relation will be useful for further analysis.

For $\mathbf{t} = (t_i, \ldots, t_m)$ ($0 \leqslant t_i \leqslant 1$) and $\boldsymbol{\delta} = (\delta_1, \ldots, \delta_m)$, define matrices $J_{\theta,\boldsymbol{\delta}}^{S,\mathbf{t}}$, $J_{\theta,\boldsymbol{\delta}}^{R,\mathbf{t}}$ by

$$J_{\theta,\boldsymbol{\delta},i,j}^{S,\mathbf{t}} = \tfrac{1}{2}\operatorname{Tr}\rho_\theta\left(L_{i,\theta,\delta_i}^{S,t_i} L_{j,\theta,\delta_j}^{S,t_j} + L_{j,\theta,\delta_j}^{S,t_j} L_{i,\theta,\delta_j}^{S,t_i}\right), \qquad J_{\theta,\boldsymbol{\delta},i,j}^{R,\mathbf{t}} = \operatorname{Tr}\rho_\theta L_{j,\theta,\delta_j}^{R,t_j}\left(L_{i,\theta,\delta_j}^{R,t_i}\right)^\dagger.$$

Analogously to models with scalar parameters, we have the following theorem, which is proven in section 5.

Theorem 5. *If the estimator is unbiased, for any $\boldsymbol{\delta}$ and for any $\mathbf{t}$ such that $0 \leqslant t_i \leqslant 1$, we have*

$$\operatorname{Sp} G V_\theta(M) \geqslant \operatorname{Sp} G \left(J_{\theta,\boldsymbol{\delta}}^{S,\mathbf{t}}\right)^{-1},$$

$$\operatorname{Sp} G V_\theta(M) \geqslant \operatorname{Sp} G \left(J_{\theta,\boldsymbol{\delta}}^{R,\mathbf{t}}\right)^{-1} + \operatorname{Spabs} \operatorname{Im} G \left(J_{\theta,\boldsymbol{\delta}}^{R,\mathbf{t}}\right)^{-1}.$$

4. Examples

In this section, we will demonstrate our theory in several examples.

4.1. Estimation of concurrence

For $-1 < \theta < 1$, let ρ_θ be a density matrix on a 2×2 system given by

$$\rho_\theta = \frac{1+\theta}{2}|\Phi^+\rangle\langle\Phi^+| + \frac{1-\theta}{2}|\Phi^-\rangle\langle\Phi^-|$$

where $|\Phi^\pm\rangle = (|00\rangle \pm |11\rangle)/\sqrt{2}$ are maximally entangled states which are mutually orthogonal. This type of state can be produced by parametric down conversion [19].

Let $g(\theta) = |\theta|$, which is equal to the concurrence [23], a measure of the quantum entanglement between two 2-level systems. At $\theta \neq 0$, we can define the usual SLD and RLD, and both J_θ^S and J_θ^R are given by

$$J_\theta^S = J_\theta^R = \frac{1}{1-\theta^2}.$$

At $\theta = 0$, we have

$$J_{\theta,\delta}^{S,1} = J_{\theta,\delta}^{R,1} = \frac{1}{1-\theta^2}$$

for any $-1 < \delta < 1$. Therefore, the QHCRK inequality is

$$V_\theta(M) \geqslant 1 - \theta^2.$$

In this model, however, there is no unbiased estimator for $g(\theta) = |\theta|$. Therefore, the inequality is nonsense in the non-asymptotic setting.

Let us consider the asymptotic case, where we construct a sequence M_n of estimators of $g(\theta)$, which achieves the asymptotic AQHCRK bound. Here, $c_n = \sqrt{n}$. The AQHCRK inequality for estimators which are $\sqrt{n}$-unbiased from the right is given due to (16)

$$\lim_{n\to\infty} c_n^2 V_\theta(M_n) \geqslant 1 - \theta^2.$$

This bound is achieved by the following scheme.

Step 1. For $i = 1, 2, \ldots, n$, we measure the ith subsystem of $\mathcal{H}^{\otimes n}$ by a two-valued POVM $\{|\Phi^+\rangle\langle\Phi^+|, I - |\Phi^+\rangle\langle\Phi^+|\}$. Let $x_i = 1$ if $|\Phi^+\rangle\langle\Phi^+|$ is observed, and let $x_i = 0$ if $I - |\Phi^+\rangle\langle\Phi^+|$ is observed.

Step 2. Let

$$y = \begin{cases} \sum_{i=1}^n x_i/n & \text{if} \quad \sum_{i=1}^n x_i/n \geqslant -n^{-1/3}, \\ -\sum_{i=1}^n x_i/n & \text{if} \quad \sum_{i=1}^n x_i/n < -n^{-1/3}. \end{cases}$$

The expectation $E_\theta(y)$ of y for $\rho_\theta^{\otimes n}$ is $\theta + o(1/n)$ as $n \to \infty$ so such an estimator M_n is $1/\sqrt{n}$-unbiased at θ from the right, and $V_\theta(M_n) = (1-\theta^2)/n$.

4.2. A discrete model

This example can be regarded as a non-commutative version of the classical model of discrete uniform distributions.

Define 2×2 matrices σ_1, σ_2 and 0_2 as

$$\sigma_1 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 1 & 1/2 \\ 1/2 & 1 \end{pmatrix}, \qquad 0_2 = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}.$$

Let $\mathcal{H}$ be an infinite-dimensional Hilbert space spanned by $|1\rangle, |2\rangle, |3\rangle, \ldots$. For $\theta \in \Theta \, (= \mathbb{N}$: the set of natural numbers), let $\rho_\theta \in \mathcal{S}(\mathcal{H})$ be a density operator of the form

$$\rho_\theta = \begin{cases} \theta^{-1} \operatorname{diag}(\underbrace{\sigma_2, \ldots, \sigma_2}_{(\theta-1)/2}, \sigma_1, 0_2, 0_2, \ldots) & \text{if } \theta \text{ is odd,} \\ \theta^{-1} \operatorname{diag}(\underbrace{\sigma_2, \ldots, \sigma_2}_{\theta/2}, 0_2, 0_2, \ldots) & \text{if } \theta \text{ is even} \end{cases}$$

where $\operatorname{diag}(\cdots)$ means the diagonal matrix.

Remark 4. Though ρ_θ is not invertible on $\mathcal{H}$, assumption (1) essentially applies to this example. Indeed, for the achievability of the lower bound, it is sufficient to consider the subspace $\mathcal{H}'_\theta (\subset \mathcal{H})$ supported by ρ_θ.

4.2.1. One-sample analysis. When θ is even, there is an estimator of θ which minimizes variance. Define a Hermitian matrix T by

$$T = \operatorname{diag}(T_1, T_3, T_5, \ldots)$$

where, for an odd number i,

$$T_i = \begin{pmatrix} 2i - 1 & 1/2 \\ 1/2 & 2i + 1/2. \end{pmatrix}.$$

Let the spectral decomposition, described by M, be the estimator of θ. Since

$$\operatorname{Tr}(\rho_\theta T) = \theta \qquad \text{for any } \theta,$$

M is an unbiased estimator.

If θ is even, then M is optimum. The proof is as follows. Define $\Lambda_0, \Lambda_1, \ldots, \Lambda_{\theta-1}$ by

$$\rho_k = \frac{\rho_\theta \Lambda_k + \Lambda_k \rho_\theta}{2} \qquad (k = 0, 1, \ldots, \theta - 1),$$

that is,

$$\Lambda_i = \begin{cases} \dfrac{\theta}{\theta - i} \operatorname{diag}(\underbrace{1, \ldots, 1}_{\theta-i}, 0, 0, \ldots) & \text{if } i \text{ is even,} \\ \dfrac{\theta}{\theta - i} \operatorname{diag}\left(\underbrace{1, \ldots, 1}_{\theta-i-2}, \begin{pmatrix} -1/6 & 1/3 \\ 1/3 & 5/6 \end{pmatrix}, 0, 0, \ldots\right) & \text{if } i \text{ is odd.} \end{cases}$$

Since

$$\begin{aligned} \Delta_{-1,k}\rho_\theta &= \frac{\rho_\theta L^S_{\theta,-1,k} + L^S_{\theta,-1,k}\rho_\theta}{2} \\ &= \frac{\rho_\theta\left((-1)^k \sum_{i=0}^k (-1)^i \binom{k}{i}\Lambda_i\right) + \left((-1)^k \sum_{i=0}^k (-1)^i \binom{k}{i}\Lambda_i\right)\rho_\theta}{2}, \end{aligned}$$

we have

$$L^S_{\theta,-1,k} = (-1)^k \sum_{i=0}^k (-1)^i \binom{k}{i}\Lambda_i.$$

That is, there is a triangle matrix U with nonzero diagonal elements such that $\left(L^S_{\theta,-1,0}, L^S_{\theta,-1,1}, \ldots, L^S_{\theta,-1,\theta-1}\right) = U^t(\Lambda_0, \Lambda_1, \ldots, \Lambda_{\theta-1})$. This means that $\left\{L^S_{\theta,-1,k}\right\}$ and $\{\Lambda_k\}$ have a one-to-one correspondence. Since T is an element of $\operatorname{span}\{\Lambda_0, \Lambda_1, \ldots, \Lambda_{\theta-1}\}$, $T - \theta \in \operatorname{span}\left\{L^S_{\theta,-1,1}, \ldots, L^S_{\theta,-1,\theta-1}\right\}$. Hence the equality in (9) holds.

By direct calculation, the MSE of M is given by

$$V_\theta(M) = \begin{cases} \theta^2/3 - 7/12 + 1/(2\theta) & \text{if } \theta \text{ is odd,} \\ \theta^2/3 - 7/12 & \text{if } \theta \text{ is even.} \end{cases}$$

When θ is odd, a similar argument of $L^S_{\theta,-1,k}$ implies that the best estimator should be given by the spectral decomposition of T' of the form

$$T' = \text{diag}(T_1, T_3, \ldots, T_{\theta-2}, T'_\theta, T_{\theta+2,\ldots})$$

where

$$T'_\theta = \begin{pmatrix} 2\theta - 1 & 0 \\ 0 & 2\theta + 1 \end{pmatrix}.$$

The MSE of the estimator is

$$\theta^2/3 - 7/12 + 1/(4\theta)$$

for odd θ. However, T' depends on the unknown parameter θ. In this sense, there is no estimator which uniformly achieves the QK bound.

4.2.2. Asymptotic analysis. Let us consider the asymptotic setting, $\rho^n_\theta = \rho^{\otimes n}_\theta$. Since this model is discrete and each element ρ_θ is isolated, due to theorem 3, we have the following lower bound to $\liminf_{n\to\infty} \log V_\theta(M_n)$,

$$\log\left(1 + J^{R,1}_{\theta,-1}\right) = \begin{cases} \log(\theta/(\theta-1)) & \text{if } \theta \text{ is odd,} \\ \log(\theta/(\theta-1)) + \log \dfrac{3\theta - 2}{3(\theta-1)} & \text{if } \theta \text{ is even.} \end{cases}$$

Based on an asymptotically optimal test between two hypotheses, we will construct an estimator M, which achieves the AQHCRK bound to the discrete case of theorem 3 if θ is odd.

M is constructed as follows. First, let Θ' be the set of positive even numbers. Next, let M' be a POVM of the form

$$M(\theta') = \text{diag}(\underbrace{0, \ldots, 0}_{\theta'-2}, I_2, 0, 0, \ldots)$$

where I_2 is the 2×2 identity matrix. We independently apply M' to each sample, and let $\hat{\theta}'_i \in \Theta'$ be the observed value for the ith sample. Let $\hat{\theta}_{\max} = \max\{\hat{\theta}'_1, \ldots, \hat{\theta}'_n\}$. Our next step is the estimation in a submodel $\Theta' = \{\hat{\theta}_{\max}, \hat{\theta}_{\max} - 1\} \subset \Theta$. Let N_n be a POVM given in (15) where $\theta = \hat{\theta}_{\max} - 1$ and $\theta + \delta = \hat{\theta}_{\max}$. Since each $M'(\theta')$ commutes with $\rho_{\hat{\theta}_{\max}-1}$ and $\rho_{\hat{\theta}_{\max}}$, due to [13], M' and N_n commute. Applying such a measurement N_n, the estimate $\hat{\theta}$ of θ is given by

$$\hat{\theta} = \begin{cases} \hat{\theta}_{\max} - 1 & \text{if } \hat{\theta}_{\max} - 1 \in \Theta' \text{ is observed,} \\ \hat{\theta}_{\max} & \text{if } \hat{\theta}_{\max} \in \Theta' \text{ is observed.} \end{cases}$$

The exponent of MSE of this estimator M is given by

$$\liminf_{n\to\infty} \frac{1}{n}\log V_\theta(M) = \begin{cases} -D(\rho_{\theta-1} \| \rho_\theta) = -\log\left(1 + J^{R,1}_{\theta,-1}\right) & \text{if } \theta \text{ is odd,} \\ -D(\rho_{\theta-1} \| \rho_\theta) > -\log\left(1 + J^{R,1}_{\theta,-1}\right) & \text{if } \theta \text{ is even} \end{cases}$$

where

$$D(\rho_{\theta-1} \| \rho_\theta) = \log\frac{\theta}{\theta-1} + \frac{1}{\theta-1}\log\frac{2}{\sqrt{3}}$$

if θ is even.

4.3. Submodels of the Gaussian state model

We consider singular submodels of the Gaussian state model, whose theory [25, 16] is reviewed in the next subsection. In the last subsection of this section, we study a vector-valued submodel of the Gaussian state model, to see the effect of non-commutativity explicitly. Before that, for preparation, we study a submodel of this model, which has scalar-valued parameter.

4.3.1. Gaussian state model. For simplicity, we chose the unit such that $\hbar = 1$. The Gaussian state model is a family of states living in the Fock space, $\mathcal{H} = \text{span}\{|n\rangle; n = 0, 1, 2, \ldots\}$, such that

$$\rho_\theta^G = \int \frac{\mathrm{d}p\,\mathrm{d}q}{2\pi(\sigma^2 - 1/2)} \exp\left(-\frac{(p - \theta^1)^2 + (q - \theta^2)^2}{2(\sigma^2 - 1/2)}\right) |p, q\rangle\langle p, q|,$$

where $|p, q\rangle$ is a coherent state. After some calculations, one would obtain [16]

$$
\begin{aligned}
L_{1,\theta}^S &= \frac{1}{\sigma^2}(P - \theta^1), \qquad L_{2,\theta}^S = \frac{1}{\sigma^2}(Q - \theta^2), \\
L_{1,\theta}^R &= \frac{1}{\sigma^4 - 1/4}\left(\sigma^2(P - \theta^1) + \frac{\sqrt{-1}}{2}(Q - \theta^2)\right), \\
L_{2,\theta}^R &= \frac{1}{\sigma^4 - 1/4}\left(\sigma^2(Q - \theta^2) - \frac{\sqrt{-1}}{2}(P - \theta^1)\right), \\
J_\theta^S &= \frac{1}{\sigma^2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \qquad J_\theta^R = \frac{1}{\sigma^4 - 1/4}\begin{bmatrix} \sigma^2 & -\frac{\sqrt{-1}}{2} \\ \frac{\sqrt{-1}}{2} & \sigma^2 \end{bmatrix}.
\end{aligned}
\tag{18}
$$

The submodels $\{\rho_{(\theta_0^1,\theta^2)}^G; \theta^2 \in \mathbb{R}\}$ and $\{\rho_{(\theta^1,\theta_0^2)}^G; \theta^1 \in \mathbb{R}\}$ are exponential families, and the equality in the SLD QCR inequality,

$$V_\theta(M) \geqslant \sigma^2,$$

is achieved for both models, the former by the spectral decomposition of P, and the latter by the spectral decomposition of Q.

For the model $\{\rho_\theta^G; \theta \in \mathbb{R}^2\}$ with 2-dim parameter, it is known that the equality in the RLD QCR inequality is achieved. Namely, with $G = I$, the RLD and the SLD QCR inequality is given by

$$\text{Sp}\,V_\theta(M) \geqslant 2\sigma^2 + 1, \qquad \text{Sp}\,V_\theta(M) \geqslant 2\sigma^2,$$

respectively. For SLDs, because scalar multiplications of P and Q are not commutative, the achievable bound is larger than the bound by SLD QCR.

If the thermal noise is very large and thus σ is very large, the difference between the SLD QCR and RLD QCR is negligible, meaning that the effect of non-commutativity is relatively negligible.

Letting $|p, q\rangle$ be a coherent state, the optimal estimator is

$$\{|\theta^1, \theta^2\rangle\langle\theta^1, \theta^2|\}.$$

This POVM is often referred to as the optimal simultaneous measurement of P and Q, for this satisfies the relation

$$\int \frac{\mathrm{d}p\,\mathrm{d}q}{2\pi} p|p, q\rangle\langle p, q| = P, \qquad \int \frac{\mathrm{d}p\,\mathrm{d}q}{2\pi} q|p, q\rangle\langle p, q| = Q, \tag{19}$$

and gives the smallest sum of MSEs in all such POVMs.

4.3.2. A singular submodel with scalar parameter. The model $\{\rho_\theta; \theta \in \mathbb{R}\}$, where

$$\rho_\theta = \begin{cases} \rho_{(0,0)}^G \otimes \rho_{(\theta,0)}^G & (\theta \leqslant 0) \\ \rho_{(\theta,0)}^G \otimes \rho_{(0,0)}^G & (\theta \geqslant 0), \end{cases}$$

has a singularity at $\theta = 0$, and the singular point is differentiable both from the left and the right. In the following, we denote by P_i and Q_i the quadrature operators of the mode i.

The SLD QHCRK inequality for $\theta \neq 0$ coincides with the SLD QCR inequality, and is given by

$$V_\theta(M) \geqslant \sigma^2 \qquad (\theta \neq 0). \tag{20}$$

The equality is achieved by the spectral decomposition of P_2 (resp. P_1) if $\theta < 0$ (resp. $\theta > 0$), in this region of the parameter. However, that neither P_1 nor P_2 is unbiased all over the model.

At the point $\theta = 0$, due to (6) and (18), we have

$$\lim_{\delta \to 0+} L_{\theta,\delta}^{S,t} = \frac{1}{\sigma^2}(t P_1 + (1-t)P_2),$$

and letting $t = \frac{1}{2}$, we obtain the lower bound,

$$V_0(M) \geqslant 2\sigma^2. \tag{21}$$

The estimator given by the spectral decomposition of $P_1 + P_2$ is unbiased at all $\theta \in \Theta$, and achieves the equality in the inequality (21). This estimator, however, does not achieve the lower bound by (20) at $\theta \neq 0$.

We conjecture, however, that this estimator is optimal, and that the lower bound (21) is a lower bound all over the model. Indeed, we can improve the lower bound (20) as follows. Almost in parallel with theorem 2, we have the following Koike-type inequality:

$$V_\theta(M) \geqslant (1\ 1) \begin{pmatrix} \operatorname{Tr} \rho_\theta L_{\theta,\delta_1}^{R,1}\left(L_{\theta,\delta_1}^{R,1}\right)^\dagger & \operatorname{Tr} \rho_\theta L_{\theta,\delta_1}^{R,1}\left(L_{\theta,\delta_2}^{R,1}\right)^\dagger \\ \operatorname{Tr} \rho_\theta L_{\theta,\delta_2}^{R,1}\left(L_{\theta,\delta_1}^{R,1}\right)^\dagger & \operatorname{Tr} \rho_\theta L_{\theta,\delta_2}^{R,1}\left(L_{\theta,\delta_2}^{R,1}\right)^\dagger \end{pmatrix}^{-1} \begin{pmatrix} 1 \\ 1 \end{pmatrix}. \tag{22}$$

Let us choose infinitesimally small δ_2, or take the limit $\delta_2 \to 0$. Then, the right-hand side is

$$\frac{1}{J} + \frac{(\delta_1)^2}{e^{J((\theta)^2 + (\delta_1)^2)} - 1 - (\theta)^2 J}, \tag{23}$$

with J being the $(1, 1)$-component of J_θ^R for the model $\{\rho_\theta^G; \theta \in \mathbb{R}^2\}$, which is given in equations (18).

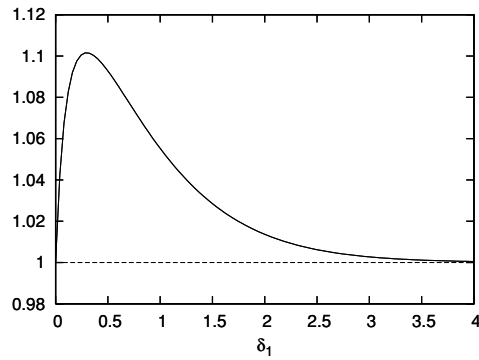The detail of the calculation is omitted, but the key is the following equality:

$$\operatorname{Tr} \rho_0^{G-1} \rho_{(x,y)}^G \rho_{(z,w)}^G = \exp(J(xz + yw) - A(xw - yz)), \tag{24}$$

with A being the $(1, 2)$-component of J_θ^R for the model $\{\rho_\theta^G; \theta \in \mathbb{R}^2\}$, which is given in the equations (18). The rough derivation of equation (24) will be given in section 5.

Let us chose δ_1 to be very small, or take the limit $\delta_1 \to 0$, and consider the case where $\frac{(\theta)^2}{\sigma^2} \ll 1$ and $\frac{1}{\sigma^2} \ll 1$. Then, the bound (23) is very close to the bound (21), which we conjecture is the tight bound all over the model. At least, as in figure 1, the new lower bound improves the bound by the SLD QHCRK inequality with $\delta \to 0$ in some cases.

4.3.3. A singular model with the vector-valued parameter. The model $\{\rho_\theta; \theta \in \mathbb{R}\}$, where

$$\rho_\theta = \begin{cases} \rho_{(0,0)}^G \otimes \rho_{(\theta^1,\theta^2)}^G & (\theta^1 \leqslant 0, \theta^2 \leqslant 0) \\ \rho_{(\theta^1,0)}^G \otimes \rho_{(0,\theta^2)}^G & (\theta^1 \geqslant 0, \theta^2 \leqslant 0) \\ \rho_{(0,\theta^2)}^G \otimes \rho_{(\theta^1,0)}^G & (\theta^1 \leqslant 0, \theta^2 \geqslant 0) \\ \rho_{(\theta^1,\theta^2)}^G \otimes \rho_{(0,0)}^G & (\theta^1 \geqslant 0, \theta^2 \geqslant 0), \end{cases}$$

Figure 1. A Koike-type lower bound is plotted against δ_1, when $\sigma = 1$ and $\theta = 1$. With optimal δ_1, the new equality improves the SLD QHCRK inequality with $\delta \to 0$, which equals 1 ($= \sigma^2$).

has a singular point at $\theta = 0$, and the singular point is differentiable both from the left and the right. The parameter space Θ is broken down into the following three parts according to types of singularity.

(1) $\theta^1 \neq 0$ and $\theta^2 \neq 0$: differentiable.
(2) $\theta^1 \neq 0$ or $\theta^2 \neq 0$: differentiable with respect to θ^1 or θ^2.
(3) $\theta^1 = 0$ and $\theta^2 = 0$: undifferentiable with respect to θ^1 and θ^2.

In the case of (1), QHCRK inequalities for $\theta \neq 0$ coincide with their differentiable versions (QCRs). Namely, in the region $\{\theta; \theta^1 \leqslant 0, \theta^2 \leqslant 0\}$ the bound by the RLD QHCRK inequality

$$\text{Sp } V_\theta(M) \geqslant 2\sigma^2 + 1 \tag{25}$$

is achieved by the estimator $\{|\theta^1, \theta^2\rangle\langle\theta^1, \theta^2| \otimes I\}$, where $|\theta^1, \theta^2\rangle$ is a coherent state. The similar holds for the region $\{\theta; \theta^1 \geqslant 0, \theta^2 \geqslant 0\}$. In the region $\{\theta; \theta^1 \leqslant 0, \theta^2 \geqslant 0\}$ the bound by the SLD QHCRK inequality

$$\text{Sp } V_\theta(M) \geqslant 2\sigma^2$$

is achieved by the simultaneous spectral decomposition of $P_2 \otimes Q_1$. The similar holds for the region $\{\theta; \theta^1 \geqslant 0, \theta^2 \geqslant 0\}$. However, none of those 'locally optimal' estimators is unbiased all over the model.

Next, we consider the case of (2). Namely, we consider the region $\{\theta; \theta^1 \leqslant 0, \theta^2 = 0\}$. (Other regions in this case are essentially the same.) If $\theta^1 \leqslant 0$ and $\theta^2 = 0$, due to (6) and (18), we can compute $\lim_{\delta \to 0+} L_{i,\theta,\delta}^{S,t_i} \lim_{\delta \to 0+} L_{i,\theta,\delta}^{R,t_i}$ $(i = 1, 2)$, explicitly, and the RLD and the SLD QHCRK inequalities are obtained as

$$\text{Sp } V_\theta(M) \geqslant \frac{\left(\sigma^4 - \frac{1}{4}\right)}{\sigma^4\left(2t_2^2 - 2t_2 + 1\right) - \frac{(1-t_2)^2}{4}}\left\{2\sigma^2\left(t_2^2 - t_2 + 1\right) + 1 - t_2\right\},$$

$$\text{Sp } V_\theta(M) \geqslant \frac{\sigma^2}{2t_2^2 - 2t_2 + 1} + \sigma^2,$$

respectively.

Now, our concern is the value of t_2 which gives the largest lower bound (see figure 2). If σ is very large (thus the effect of non-commutativity is negligible), then the right-hand side of the RLD QHCRK is almost the same as the right-hand side of the SLD QHCRK, and gives the largest lower bound at $t_2 = 1/2$. On the other hand, let us consider the opposite extreme
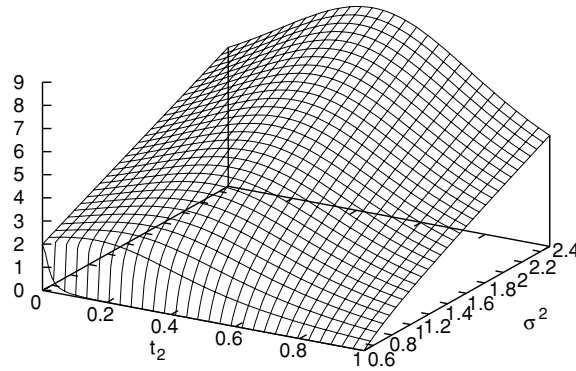
Figure 2. The lower bound by the QHCRK inequality is plotted against t_2 and σ^2. When $\sigma^2 = \frac{1}{2}$ (no thermal noise), the largest lower bond is given by $t_2 = 0$. As σ^2 tends to larger values, the peak moves towards $t_2 = \frac{1}{2}$.

case where the noise is purely quantum, that is, the Gaussian states are coherent states. This case is obtained by letting $\sigma^2 = 1/2$. If and only if $t_2 = 0$, the right-hand side of the RLD QHCRK gives the non-trivial lower bound,

$$\mathrm{Sp} V_\theta(M) \geqslant 2.$$

(If $t_2 \neq 0$, the right-hand side of the inequality vanishes.)

To sum up, the value of t_2 which gives the best bound is dependent on the non-commutativity inherent in the model.

Finally, the case of (3) is analysed. Due to (6) and (18), $\lim_{\delta \to 0+} L_{i,\theta,\delta}^{R,t_i}$ $(i = 1, 2)$ are computed explicitly. Letting $t_1 = t_2 = 1/2$, we have the following RLD QHCRK inequality,

$$\mathrm{Sp} V_\theta(M) \geqslant 4\sigma^2 + 2. \tag{26}$$

This choice of the parameters t_1, t_2 is optimal, for the unbiased estimator which is constructed below achieves this lower bound.

Let

$$P_{1*} = \frac{P_1 + P_2}{\sqrt{2}}, \qquad Q_{1*} = \frac{Q_1 + Q_2}{\sqrt{2}}, \qquad P_{2*} = \frac{P_1 - P_2}{\sqrt{2}}, \qquad Q_{2*} = \frac{Q_1 - Q_2}{\sqrt{2}}.$$

Then, P_{i*}, Q_{i*} satisfies the canonical commutation relation, and P_{i*}, Q_{j*} $(i \neq j)$ commutes. Consider the new split of the system into the modes 1^* and 2^*, introduce a new coherent state $|p, q\rangle^*$ with respect to P_{1*} and Q_{1*}, and define an estimator

$$\{|\theta^1/\sqrt{2}, \theta^2/\sqrt{2}\rangle^{**}\langle\theta^1/\sqrt{2}, \theta^2/\sqrt{2}| \otimes I\}.$$

Observing that the expectations of $P_1 + P_2$ and $Q_1 + Q_2$ coincide with θ^1 and θ^2 respectively, the unbiasedness of the estimator is checked by using (19). A straightforward calculation shows that this estimator achieves the lower bound implied by (26).

This estimator is optimal at $\theta = 0$, and unbiased all over the model. We conjecture that the lower bound at other points of the model is improved to show the optimality of this estimator.

In fact, for example, the lower bound (25) is improved by using the RLD QHCRK inequality with a finite δ. Let $\theta^1 < 0, \theta^2 < 0$, and $\delta_1 = -\theta^1 + t, \delta_2 = -\theta^2 + s$, for $s > 0, t > 0$. Then, due to (24), the RLD QHCRK inequality is calculated as

$$\mathrm{Sp} V_\theta(M) \geqslant \frac{a + d + 2|c|}{ad - b^2 - c^2}.$$
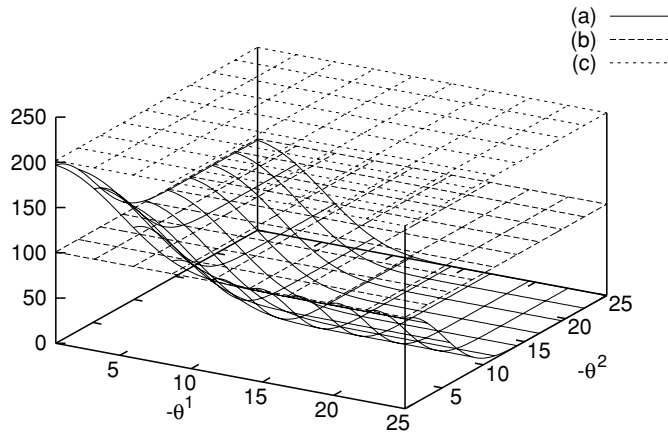
Figure 3. RLD QHCRK bound with $\delta^i = 2\theta^i$ (*a*), and with $\delta^i \to 0$ (*b*), are plotted against $\theta (\theta^i < 0)$. (*c*) is the conjectured lower bound (and is the RLD QHCRK bound at $\theta = 0$). (*a*) is above (*b*) in some region, and is very close to (*c*) around the origin.

Here, letting J and A be the $(1,1)$- and the $(1,2)$-components of the J_θ^R for the model $\{\rho_\theta^G; \theta \in \mathbb{R}^2\}$, respectively,

$$a = \frac{e^{J((\theta^1)^2+(t)^2)} - 1}{(\theta^1+t)^2}, \qquad d = \frac{e^{J((\theta^2)^2+(s)^2)} - 1}{(\theta^2+s)^2}, \qquad b + \sqrt{-1}c = e^{-A(ts+\theta^1\theta^2))} - 1.$$

When $\frac{1}{\sigma^2} \ll 1$ and $\frac{(\theta^i)^2}{\sigma^2} \ll 1$ ($i = 1, 2$), letting $t = \theta^1$ and $s = \theta^2$, the bound is nearly $4\sigma^2$, and is close to (26), which is conjectured to be a lower bound all over the model.

As is indicated in figure 3, we can observe in some region of the parameter space, the new bound, the RLD QHCRK bound with $\delta^i = 2\theta^i$ ($\theta^i < 0$) improves (25).

5. Proofs

In this section, we give proofs of theorems. First, we prepare a lemma which says that the best unbiased estimator is a projection-valued measure (PVM).

Lemma 1. *Let*

$$T = \int_{\gamma \in g(\Theta)} \gamma M(d\gamma).$$

Then, it holds that

$$\int_{\gamma \in g(\Theta)} \gamma^2 \operatorname{Tr}(\rho_\theta M(d\gamma)) \geqslant \operatorname{Tr}(\rho_\theta T^2).$$

Proof.

$$\int_{\gamma \in g(\Theta)} \gamma^2 \operatorname{Tr}(\rho_\theta M(d\gamma)) - \operatorname{Tr}(\rho_\theta T^2) = \operatorname{Tr}\left(\rho_\theta \int_{\gamma \in g(\Theta)} (\gamma - T)^2 M(d\gamma)\right) \geqslant 0.$$

$\square$

Hence we use an observable T to describe the POVM M in proofs of theorems 1 and 2.

5.1. Proof of theorem 1

Let $T \in \mathcal{L}(\mathcal{H})$ be an operator satisfying $\text{Tr}(\rho_\theta T) = g(\theta)$. By Schwartz's inequality, it holds that

$$\text{Tr}(\rho_\theta(T - g(\theta))^2)\, \text{Tr}(\rho_\theta(L_\theta^S)^2) \geqslant (\text{Tr}(\rho_\theta(T - g(\theta)L_\theta^S)))^2$$
$$= (\text{Tr}((T - g(\theta))(\Delta_\delta \rho_\theta)))^2 = (\Delta_\delta g(\theta))^2. \tag{27}$$

Therefore, (7) holds. In addition,

$$0 \leqslant \text{Tr}(\rho_\theta(L_{\theta,\delta}^S - L_{\theta,\delta}^R)(L_{\theta,\delta}^S - L_{\theta,\delta}^R)^\dagger)$$
$$= \text{Tr}(\rho_\theta(L_{\theta,\delta}^S)^2) - 2\,\text{Tr}(L_{\theta,\delta}^S \Delta_\delta \rho_\theta) + \text{Tr}(\rho_\theta L_{\theta,\delta}^R(L_{\theta,\delta}^R)^\dagger)$$
$$= -\text{Tr}(\rho_\theta(L_{\theta,\delta}^S)^2) + \text{Tr}(\rho_\theta L_{\theta,\delta}^R(L_{\theta,\delta}^R)^\dagger).$$

Hence, (8) holds. The equality in (27) holds if and only if $T - g(\theta) = cL_\theta^S$ for a constant $c \in \mathbb{R}$.

5.2. Proof of theorem 2

Let

$$v = (T - g(\theta), L_{\theta,\delta,1}^S, L_{\theta,\delta,2}^S, \ldots, L_{\theta,\delta,k}^S).$$

Let V be a $(k + 1)$-dimensional $\mathbb{C}$-vector space, Then, v can be regarded as an element of $V \otimes \mathcal{L}(\mathcal{H})$. Let I_V be the identity matrix on V. Let $P = \rho_\theta \otimes I_V$. It holds that

$$0 \leqslant \text{Tr}_\mathcal{H}(Pvv^\dagger) = \begin{pmatrix} V_\theta(M) & {}^t\mathbf{v} \\ \mathbf{v} & K^S \end{pmatrix} (= A, \text{ say}),$$

where $\text{Tr}_\mathcal{H}$ means the partial trace over $\mathcal{H}$. Consequently, we obtain

$$V_\theta(M) - {}^t\mathbf{v}(K^S)^{-1}\mathbf{v} = (1\ {}^t\mathbf{v}(K^S)^{-1})A\begin{pmatrix} 1 \\ (K^S)^{-1}\mathbf{v} \end{pmatrix} \geqslant 0.$$

This implies (9). By a similar argument, (10) is also shown.

5.3. Proof of theorem 4

In a similar way to (27), Schwartz's inequality implies that

$$c_n^2 V_\theta(M_n) \geqslant \frac{(\Delta_{h/c_n} b(M_n, \theta) + \Delta_{h/c_n} g(\theta))^2}{\text{Tr}(\rho_\theta^n(L_{\theta,h/c_n}^{S,(n)})^2)}$$
$$\geqslant \frac{(\Delta_{h/c_n} b(M_n, \theta) + \Delta_{h/c_n} g(\theta))^2}{\text{Tr}(\rho_\theta^n L_{\theta,h/c_n}^{R,(n)}(L_{\theta,h/c_n}^{R,(n)})^\dagger)} \tag{28}$$

and hence (17) holds as $n \to \infty$.

5.4. Proofs of proposition 3 and theorem 5

Let

$$\langle A, B \rangle_{1,\rho} = \tfrac{1}{2}\,\text{Tr}\,\rho(BA^\dagger + A^\dagger B), \qquad \langle A, B \rangle_{2,\rho} = \tfrac{1}{2}\,\text{Tr}\,\rho(BA^\dagger),$$
$$\vec{X} = (X^1, X^2, \ldots, X^m)^T, \qquad Z_\rho(\vec{X}) = [\langle X^i, X^j \rangle_{2,\rho}].$$

Observe that

$$\text{Re}\, Z_\rho(\vec{X}) = [\langle X^i, X^j \rangle_{1,\rho}].$$

Lemma 2.

$$V_\theta(M) \geqslant Z_\rho(\vec{X}), \qquad\qquad V_\theta(M) \geqslant \operatorname{Re} Z_\rho(\vec{X}).$$

Lemma 3. *Let $\langle \cdot, \cdot \rangle$ be an inner product, and $\vec{X} = (X^1, X^2, \ldots, X^m)^T$, $\vec{L} = (L_1, L_2, \ldots, L_m)^T$, where $X^1, X^2, \ldots, X^m, L_1, L_2, \ldots, L_m$ are members of the vector space of our concern. Denote matrices $[\langle X^i, X^j \rangle]$ and $[\langle L_i, L_j \rangle]$ by $\Gamma_{\vec{X}}$ and $\Gamma_{\vec{L}}$, respectively, and assume $[\langle X^i, L_j \rangle] = \delta^i_j$. Then, $\Gamma^{-1}_{\vec{X}}$ and $\Gamma^{-1}_{\vec{L}}$ exist, and*

$$\Gamma_{\vec{X}} \geqslant \Gamma^{-1}_{\vec{L}}$$

holds.

Lemma 4. *For any positive Hermitian matrix Z, we have*

$$\min_V \operatorname{Sp} GV = \operatorname{Sp} GZ + \operatorname{Spabs} \operatorname{Im} GZ, \tag{29}$$

where V runs over all positive real matrices such that $V \geqslant Z$.

For the proofs of lemmas 2–4, see [16].

Let $\langle \cdot, \cdot \rangle$ be $\langle \cdot, \cdot \rangle_{1,\rho_\theta}$ and let L_i be $L^S_{i,\theta}$ (resp. $L^{S,\mathbf{t}}_{i,\theta,\delta}$) in lemma 3, and combine with lemmas 2 and 4. Noting that $\operatorname{Im} J^S_\theta = 0$ (resp. $\operatorname{Im} J^{S,\mathbf{t}}_{\theta,\delta} = 0$), then we have the first inequality in proposition 3 (resp. the first inequality in theorem 5). Similarly, letting $\langle \cdot, \cdot \rangle$ be $\langle \cdot, \cdot \rangle_{2,\rho_\theta}$ and letting L_i be $L^R_{i,\theta}$ (resp. $L^{R,\mathbf{t}}_{i,\theta,\delta}$) in lemma 3, we have the second inequality in proposition 3 (resp. the second inequality in theorem 5).

5.5. Derivation of equation (24)

Due to $\rho^G_0 = (1-c) \sum_{n=0}^\infty c^{-n} |n\rangle\langle n|$, where $\frac{c^{-1}}{(1-c^{-1})^2} = \sigma^2 - \frac{1}{2}$, we have

$$\operatorname{Tr} \rho^{G-1}_0 \rho^G_{(x,y)} \rho^G_{(z,w)} = (1-c) \int_{\alpha \in \mathbb{C}, \beta \in \mathbb{C}} \frac{\mathrm{d}^2\alpha \, \mathrm{d}^2\beta}{4\pi^2 (\sigma - 1/2)^2}$$

$$\times \exp\left(-\frac{|\alpha - x - \sqrt{-1}y|^2 + |\beta - z - \sqrt{-1}w|^2}{2(\sigma^2 - 1/2)} \right) \sum_{n=0}^\infty c^n \langle n|\alpha \rangle \langle \alpha|\beta \rangle \langle \beta|n \rangle$$

$$= (1-c) \int_{\alpha \in \mathbb{C}, \beta \in \mathbb{C}} \frac{\mathrm{d}^2\alpha \, \mathrm{d}^2\beta}{4\pi^2 (\sigma - 1/2)^2}$$

$$\times \exp\left(-\frac{|\alpha - x - \sqrt{-1}y|^2 + |\beta - z - \sqrt{-1}w|^2}{2(\sigma^2 - 1/2)} \right) \sum_{n=0}^\infty c^n \frac{\alpha^n}{\sqrt{n!}} \exp\left(-\frac{1}{2}|\alpha|^2 \right)$$

$$\times \exp\left(-\frac{|\alpha|^2}{2} + \alpha^*\beta - \frac{|\beta|^2}{2} \right) \frac{\beta^{*n}}{\sqrt{n!}} \exp\left(-\frac{1}{2}|\beta|^2 \right)$$

$$= (1-c) \int_{\alpha \in \mathbb{C}, \beta \in \mathbb{C}} \frac{\mathrm{d}^2\alpha \, \mathrm{d}^2\beta}{4\pi^2 (\sigma - 1/2)^2}$$

$$\times \exp\left(-\frac{|\alpha - x - \sqrt{-1}y|^2 + |\beta - z - \sqrt{-1}w|^2}{2(\sigma^2 - 1/2)} - |\alpha|^2 - |\beta|^2 + \alpha^*\beta \right)$$

$$\times \sum_{n=0}^\infty \frac{(c\alpha\beta^*)^n}{n!}$$

$$= (1 - c) \int_{\alpha \in \mathbb{C}, \beta \in \mathbb{C}} \frac{\mathrm{d}^2 \alpha \, \mathrm{d}^2 \beta}{4\pi^2 (\sigma - 1/2)^2}$$

$$\times \exp\left(-\frac{|\alpha - x - \sqrt{-1}\,y|^2 + |\beta - z - \sqrt{-1}\,w|^2}{2(\sigma^2 - 1/2)} - |\alpha|^2 - |\beta|^2 + \alpha^* \beta + c\alpha\beta^*\right).$$

Repeated application of the formula, $\int \mathrm{e}^{-A(x-B)^2} = \sqrt{\frac{\pi}{A}}$ leads to equation (24).

6. Discussions

We have given the first treatment of quanta singular statistical models. Namely, we proposed two kinds of quantum versions of the HCRK inequality and Koike inequality. One is based on the difference version of SLD, and the other is based on the difference version of RLD. The asymptotic theory based on the RLD QHCRK inequality is also discussed.

We applied those results to some examples. The first example was estimation of entanglement measure, which is very simple but practically of some importance. We constructed an asymptotically optimal estimate in this case. The second example is the estimation of the discrete parameter. It should be stressed that from the viewpoint of conventional state detection theory, the non-asymptotic analysis is very hard, while our approach is technically more tractable. The third example is the estimation of the vector-valued parameter, and here we could observe the effect of non-commutativity.

There are many unsolved problems. Especially, asymptotic theory is far from complete. For example, an asymptotic theory based on SLD QHCRK inequality is desired, for SLD-based lower bounds are better than those based on RLD, if the parameter is scalar. As for the piece-wise differentiable models, we can trivially extend the theory of differentiability by imposing asymptotic unbiasedness instead of $\sqrt{n}$-unbiasedness on the estimator. However, SLD versions of theorems 3 and 4 are very hard to obtain, for we do not have the equivalence of (14). Note that this difficulty is due to non-commutativity, or more specifically, the hardness of calculation of the SLD. Hence, similar problems never arise in classical estimation theory.

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