Fisher information and quantum estimation

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Abstract

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1 Introduction

2 Fisher information for a non-full rank density matrix

Abstract

We provide a new expression of the quantum Fisher information(QFI) for a general system. Utilizing this expression, the QFI for a non-full rank density matrix is only determined by its support. This expression can bring convenience for a infinite dimensional density matrix with a finite support. Besides, a matrix representation of the QFI is also given.

Quantum metrology is a field that utilizes the character of quantum mechanics to improve the precision of a parameter under detection [1]. For the past few years, this field has drawn a lot of attention and has been developing rapidly [2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17]. Quantum Fisher information(QFI) is a central concept in quantum metrology because it depicts the lower bound on the variance of the estimator $\hat{\theta}$ for the parameter θ due to the Cramér-Rao theorem [18, 19, 20]

$$\mathrm{var}(\hat{\theta}) \geq \frac{1}{\nu F}, \tag{1}$$

where $\mathrm{var}(\cdot)$ is the variance, ν is the number of repeated experiments and F is the QFI. However, the QFI is not just limited in the field of quantum metrology. It has been widely applied in other aspects of quantum physics [21, 22, 103, 24, 25, 26, 27, 28, 95, 30, 31, 32, 33], like quantum information and open quantum systems. Thus, it is necessary and meaningful to study the quantum Fisher information as well as its properties and dynamical behaviors under various circumstances.

Quantum Fisher information is a local quantity, which can be intuitively interpreted as the "velocity" at which the density matrix moves for a given parameter value. This physical interpretation comes from the fact that the QFI is dependent on the parameterized density matrix ρ_θ and its first derivative $\partial_\theta \rho_\theta$. Utilizing the spectral decomposition, when the eigenstates of ρ_θ as projectors, act on ρ_θ and its first derivative, the value is only related to the spectral decomposition within the support, which strongly hints that the QFI may be expressed in the representation of the density matrix's support. To find such an expression is the major motivation of this paper.

In this paper, we provide a new expression of the quantum Fisher information in the representation of the density matrix's support. With this expression, for a non-full rank density matrix, especially for a infinite dimension one, the QFI may be solved in a finite support space without realizing the knowledge out of the support. Recently, it is found [32, 31] that the QFI can be written in the form of the convex roof of variance. To obtain the QFI, one should take the minimum value running over all the possible pure-state ensembles. Utilizing the new expression, we give the condition when the ensemble from the spectral decomposition is the optimal ensemble in which the minimum value attains. Besides, we also provide a matrix representation form of the QFI and give two examples of it.

In the following we consider a N-dimensional system (N can be infinite) with the density operator ρ_θ, which is dependent on the parameter θ. Assume that the spectral decomposition of the density operator is given by

$$\rho_\theta = \sum_{i=1}^{\mathrm{s}} p_i |\psi_i\rangle\langle\psi_i|, \tag{2}$$

where p_i is a eigenvalue and $|\psi_i\rangle$ is a eigenstate. s is the dimension of the support set of ρ_θ, denoted as $\mathrm{supp}(\rho_\theta)$, i.e., $\mathrm{s} = \dim[\mathrm{supp}(\rho_\theta)]$.

For a parameterized quantum state ρ_θ, the quantum Fisher information F is defined as below [19, 20]

$$F := \mathrm{tr}(\rho_\theta L^2), \tag{3}$$

where L is the so-called symmetric logarithmic derivative operator and determined by

$$\partial_\theta \rho_\theta = \frac{1}{2}\left(L\rho_\theta + \rho_\theta L\right). \tag{4}$$

In the eigenbasis of ρ_θ, above equation reads

$$\langle\psi_i|\partial_\theta\rho_\theta|\psi_j\rangle = \frac{1}{2}(p_i + p_j)L_{ij}, \tag{5}$$

where $L_{ij} := \langle\psi_i|L|\psi_j\rangle$. From above equation, one can find that L_{ij} is in principle supported by the full space, but the value of L_{ij} for $i, j > \mathrm{s}$ is arbitrary because above equation is always established for any value of L_{ij} when $i, j > \mathrm{s}$. Nevertheless, the quantum Fisher information is still a determinate quantity because the calculation of it does not use those values of L_{ij} for $i, j > \mathrm{s}$, which we will show below. Thus, one can set $L_{ij} = 0$ for $i, j > \mathrm{s}$ as a matter of convenience.

By substituting Eq. (2) and the normalization relation $\mathbb{I} = \sum_{j=1}^{\mathrm{N}} |\psi_j\rangle\langle\psi_j|$ into Eq. (3), one can obtain the quantum Fisher information as

$$F = \sum_{i=1}^{\mathrm{s}} \sum_{j=1}^{\mathrm{N}} p_i L_{ij} L_{ji}. \tag{6}$$

Here $\mathbb{I}$ is the identity operator. All p_i here is greater than zero because the index $i \leq \mathrm{s}$ and satisfies $\sum_{i=1}^{\mathrm{s}} p_i = 1$. From this equation we see that the randomicity of L_{ij} for $i, j > \mathrm{s}$ does not affect the certainty of the quantum Fisher information. As $p_i > 0$, Eq. (5) can be rewritten into

$$L_{ij} = \frac{2(\partial_\theta\rho_\theta)_{ij}}{p_i + p_j}, \tag{7}$$

where $(\partial_\theta\rho_\theta)_{ij} := \langle\psi_i|\partial_\theta\rho_\theta|\psi_j\rangle$. Utilizing this expression, Eq. (6) can be written in the form

$$F_\theta = \sum_{i=1}^{\mathrm{s}} \sum_{j=1}^{\mathrm{N}} \frac{4p_i}{(p_i + p_j)^2} |(\partial_\theta\rho_\theta)_{ij}|^2, \tag{8}$$

where the Hermiticity of the operator $\partial_\theta\rho_\theta$ was used. Next, from the spectral decomposition of ρ_θ, one can find that

$$(\partial_\theta\rho_\theta)_{ij} = \partial_\theta p_i \delta_{ij} + (p_j - p_i)\langle\psi_i|\partial_\theta\psi_j\rangle, \tag{9}$$

where we have used the equation

$$\langle\psi_i|\partial_\theta\psi_j\rangle = -\langle\partial_\theta\psi_i|\psi_j\rangle, \tag{10}$$

resulted from the orthogonality $\langle\psi_i|\psi_j\rangle = \delta_{ij}$. For $i \in [1,\mathrm{s}]$ and $j \in [\mathrm{s}+1,\mathrm{N}]$, the expression of $(\partial_\theta\rho_\theta)_{ij}$ reduces to $-p_i\langle\psi_i|\partial_\theta\psi_j\rangle$. Substituting Eq. (9) into Eq. (8), we have

$$F_\theta = \sum_{i=1}^{\mathrm{s}} \frac{1}{p_i}(\partial_\theta p_i)^2 + \sum_{i=1}^{\mathrm{s}}\sum_{j=1}^{\mathrm{N}} \frac{4p_i(p_i-p_j)^2}{(p_i+p_j)^2}|\langle\psi_i|\partial_\theta\psi_j\rangle|^2. \tag{11}$$

Furthermore, with the knowledge that $\sum_{j=1}^{\mathrm{N}} = \sum_{j=1}^{\mathrm{s}} + \sum_{j=\mathrm{s}+1}^{\mathrm{N}}$, the second item of above expression can be separated into two parts F_1 and F_2. The first part F_1 reads

$$F_1 = \sum_{i,j=1}^{\mathrm{s}} \frac{4p_i(p_i-p_j)^2}{(p_i+p_j)^2}|\langle\psi_i|\partial_\theta\psi_j\rangle|^2, \tag{12}$$

and the second part F_2 reads

$$F_2 = \sum_{i=1}^{\mathrm{s}}\sum_{j=\mathrm{s}+1}^{\mathrm{N}} 4p_i|\langle\psi_j|\partial_\theta\psi_i\rangle|^2. \tag{13}$$

Based on the normalization relation, it is easy to find that

$$\sum_{j=\mathrm{s}+1}^{\mathrm{N}} |\psi_j\rangle\langle\psi_j| = \mathbb{I} - \sum_{j=1}^{\mathrm{s}} |\psi_j\rangle\langle\psi_j|. \tag{14}$$

Substituting this equation into the expression of F_2, one can obtain

$$F_2 = \sum_{i=1}^{\mathrm{s}} 4p_i\langle\partial_\theta\psi_i|\partial_\theta\psi_i\rangle - \sum_{i,j=1}^{\mathrm{s}} 4p_i|\langle\psi_j|\partial_\theta\psi_i\rangle|^2. \tag{15}$$

Then, the quantum Fisher information can be expressed by

$$\begin{aligned} F_\theta &= \sum_{i=1}^{\mathrm{s}} \frac{1}{p_i}(\partial_\theta p_i)^2 + \sum_{i=1}^{\mathrm{s}} 4p_i\langle\partial_\theta\psi_i|\partial_\theta\psi_i\rangle \\ &\quad - \sum_{i,j=1}^{\mathrm{s}} \frac{8p_ip_j}{p_i+p_j}|\langle\psi_i|\partial_\theta\psi_j\rangle|^2. \end{aligned} \tag{16}$$

From this equation one can find that the quantum Fisher information for a non-full rank density matrix is determined by its support. The information of eigenstates out of the support is not necessary for the calculation of the QFI. This advantage would bring some convenience for the calculation in some cases, especially when N is infinite and s is finite.

According the theory of the classical Fisher information [18, 19, 20], it is natural to treat the first item of Eq. (16) as the classical contribution of quantum Fisher information [103] because $\sum_{i=1}^{\mathrm{s}} \frac{1}{p_i}(\partial_\theta p_i)^2 = 4\sum_{i=1}^{\mathrm{s}} \left(\partial_\theta\sqrt{p_i}\right)^2$. Then the quantum Fisher information for a quantum system can be separated into two parts, the classical contribution and quantum contribution, namely,

$$F_\theta = F_{\mathrm{ct}} + F_{\mathrm{qt}}, \tag{17}$$

where the classical contribution reads

$$F_{\mathrm{ct}}=\sum_{i=1}^{\mathrm{s}}4\left(\partial_\theta\sqrt{p_i}\right)^2, \tag{18}$$

and the quantum contribution reads

$$F_{\mathrm{qt}}=\sum_{i=1}^{\mathrm{s}}4p_i\langle\partial_\theta\psi_i|\partial_\theta\psi_i\rangle-\sum_{i,j=1}^{\mathrm{s}}\frac{8p_ip_j}{p_i+p_j}|\langle\psi_i|\partial_\theta\psi_j\rangle|^2. \tag{19}$$

The separation of the quantum Fisher information is not just in form. From the equations above, one can find that the classical contribution of the quantum Fisher information is a special case of the classical Fisher information. It can be treated as the classical Fisher information obtained through the measurement $\{|\psi_i\rangle\}$ in the eigenspace of ρ_θ: $\mathbb{E}^{\mathrm{N}}$. The eigenspace $\mathbb{E}^{\mathrm{N}}$ is spanned by the basis $\{|\psi_i\rangle\}$, and $\{p_i\}$ is a classical distribution in this space. From Eq. (18), it is not difficult to find that the classical contribution F_{ct} is only related to the derivative of the eigenvalues, which indicates that this part of information is coming from the classical distribution in $\mathbb{E}^{\mathrm{N}}$. Moreover, we find that the classical contribution has the following properties: (1) it vanishes for pure states; (2) it vanishes for the unitary parametrization; (3) it is invariant under unitary transformation of density matrix, no matter the transformation is parameter-dependent or not.

In the mean time, with some transformation, Eq. (19) can be rewritten as

$$F_{\mathrm{qt}}=\sum_{i=1}^{\mathrm{s}}p_iF_Q(|\psi_i\rangle)-\sum_{i\neq j}^{\mathrm{s}}\frac{8p_ip_j}{p_i+p_j}|\langle\psi_i|\partial_\theta\psi_j\rangle|^2, \tag{20}$$

where

$$F_Q(|\psi_i\rangle)=4\left(\langle\partial_\theta\psi_i|\partial_\theta\psi_i\rangle-|\langle\psi_i|\partial_\theta\psi_i\rangle|^2\right) \tag{21}$$

is the quantum Fisher information of the eigenstate $|\psi_i\rangle$. From this equation, it is clear that F_{qt} is related to the basis of $\mathbb{E}^{\mathrm{N}}$. In $\mathbb{E}^{\mathrm{N}}$, F_{qt} is determined by the weighted average of all the quantum Fisher information $F_Q(|\psi_i\rangle)$ of the basis vector $|\psi_i\rangle$ and the coupling between these vectors. This manifests that this part of information originates from the quantum structure of space $\mathbb{E}^{\mathrm{N}}$. These are the geometric meanings of the classical and quantum contribution as well as the intrinsic reason for the separation.

We know the classical contribution of the QFI always vanishes for the unitary parametrization. But for a non-unitary parametrization procedure, including the channel estimation [34, 35, 36, 37, 38, 39] and the noise estimation [40, 41], the classical contribution does have an influence on the precision. However, only improving the classical contribution without enhancing the quantum counterpart, the precision is not available to surpass the shot-noise limit, the lower limit for a total classical scenario. The estimation of the decoherence strength [41], in which the classical contribution plays the leading role, is an example of this scenario.

The quantum Fisher information is a local quantity, which can be intuitively interpreted as the "velocity" at which the matrix moves for a given parameter value. In mathematics, this means that the quantum Fisher information depends on the density matrix ρ_θ and its first derivative $\partial_\theta \rho_\theta$. Utilizing the spectral decomposition, there exists items such as $|\psi_i\rangle\langle\partial_\theta\psi_j|$ and $|\partial_\theta\psi_i\rangle\langle\psi_j|$. When these items are traced with the eigenstates out of the support, the values turn out to be zero. This is the intuitive reason that the QFI can be expressed in the representation of the support. If the QFI is related to the higher order derivatives, like the second one $\partial_\theta^2\rho_\theta$, then there would exist the item like $|\partial_\theta\psi_i\rangle\langle\partial_\theta\psi_j|$. As $|\partial_\theta\psi_i\rangle$ is not always orthogonal with $|\psi_j\rangle$, when this item is traced with the projectors out of the support, the value cannot always be zero, then the quantum Fisher information has to be related to the whole Hilbert space, rather than the support only.

For the unitary parametrization $\exp(i\theta H)$, the classical contribution vanishes, and the quantum Fisher information reduces to

$$F_Q = \sum_{i=1}^{\mathrm{s}} p_i F_Q(|\psi_i\rangle) - \sum_{i\neq j}^{\mathrm{s}} \frac{8p_ip_j}{p_i+p_j}|\langle\psi_i|H|\psi_j\rangle|^2. \tag{22}$$

In the mean time, $F_Q(|\psi_i\rangle)$ reduces to the form that is proportional to the variance of operator H on the eigenstates, i.e.,

$$F_Q(|\psi_i\rangle) = 4(\Delta H)^2_{|\psi_i\rangle}, \tag{23}$$

where $(\Delta H)^2_{|\psi_i\rangle} := \langle\psi_i|H^2|\psi_i\rangle - |\langle\psi_i|H|\psi_i\rangle|^2$ is the variance. Recently, Tóth and Petz [32] found that for a rank-2 system the quantum Fisher information can be treated as the convex roof of the variance, then Yu [31] proves that this theorem is also established for a general system, namely,

$$F_\theta = \min_{\{q_k,|\Psi_k\rangle\}} 4\sum_k q_k(\Delta H)^2_{|\Psi_k\rangle}. \tag{24}$$

Here $\{q_k, |\Psi_k\rangle\}$ refers to a set of pure-state ensembles, which satisfies

$$\rho_\theta = \sum_k q_k|\Psi_k\rangle\langle\Psi_k|. \tag{25}$$

One should notice that the ensemble of the eigenvalues and eigenstates $\{p_i, |\psi_i\rangle\}$ is one of these ensembles, but not the only one. Comparing Eq. (22) with Eq. (24), one can find that the condition for the ensemble $\{p_i, |\psi_i\rangle\}$ being the optimal ensemble is that the transition item

$$\langle\psi_i|H|\psi_j\rangle = 0, \text{ for any } i \neq j. \tag{26}$$

For example, in some Mach-Zehnder interferometer, $H = \frac{1}{2i}(a^\dagger b - ab^\dagger)$, where a, b are the annihilation operators of two modes, and $a^\dagger$, $b^\dagger$ are the creation operators respectively. Choosing an appropriate input state, like an even state [33] or a Fock state [30] in one port, the item $\langle\psi_i|H|\psi_j\rangle$ vanishes for any $i \neq j$, then the ensemble $\{p_i, |\psi_i\rangle\}$ is the optimal ensemble and the QFI reduces to $F_\theta = 4\sum_{i=1}^{\mathrm{s}} p_i(\Delta H)^2_{|\psi_i\rangle}$.

This condition can be checked through another way. Based on Ref. [31], we introduce an observable

$$\mathrm{Y} = \sum_{i,j} \frac{2\sqrt{p_ip_j}}{p_i+p_j} H_{ij}|\psi_i\rangle\langle\psi_j|, \tag{27}$$

where $H_{ij}=\langle\psi_i|H|\psi_j\rangle$. Denote the spectral decomposition $\mathrm{Y}=\sum_k \alpha_k|y_k\rangle\langle y_k|$, then the optimal pure state can be constructed as

$$|U_k\rangle=\frac{1}{\sqrt{u_k}}\sum_i U_{ki}\sqrt{p_i}|\psi_i\rangle, \tag{28}$$

with $u_k=\sum_i |U_{ki}|^2 p_i$ and $U_{ki}=\langle\psi_i|y_k\rangle$. When $|U_k\rangle=|\psi_k\rangle$, there must be $|y_k\rangle=|\psi_k\rangle$. As $|y_k\rangle$ is the eigenstate of observable Y, then one can see that the condition for $|y_k\rangle=|\psi_k\rangle$ is that all the off-diagonal elements of observable Y have to vanish, i.e., $H_{ij}=0$ for any $i\neq j$, which coincides with our result.

2.1 Matrix representation

In this section we show a matrix representation of the quantum Fisher information. We consider the classical contribution first. Define a N-dimensional diagonal matrix D with elements $D_{ii}=p_i$, then the classical contribution can be rewritten in the form

$$F_{\mathrm{ct}}=4\mathrm{Tr}\left(\partial_\theta\sqrt{D}\right)^2. \tag{29}$$

This equation is equivalent to Eq. (18) as $p_i=0$ for $i\in[\mathrm{s}+1,\mathrm{N}]$.

Define a N-dimensional matrix $\mathcal{P}$ with the elements $\mathcal{P}_{ij}:=|\langle\psi_i|\partial_\theta\psi_j\rangle|^2$. It is easy to see that the matrix $\mathcal{P}$ is real and symmetric. The symmetry can be proved by using Eq. (10) into the definition above. Denote a constant N-dimensional matrix $\mathcal{I}$ whose elements are 1, i.e., $\mathcal{I}_{ij}=1$ for any i and j, and define a N-dimensional block diagonal matrix $\mathcal{G}$, which is $\mathcal{G}=\mathrm{diag}[\mathcal{H}_{\mathrm{s}\times\mathrm{s}},0_{(\mathrm{N}-\mathrm{s})\times(\mathrm{N}-\mathrm{s})}]$, where $\mathcal{H}_{\mathrm{s}\times\mathrm{s}}$ is a s-dimensional real symmetric matrix. The elements of $\mathcal{H}$ are the harmonic mean values, $\mathcal{H}_{ij}=2p_ip_j/(p_i+p_j)$. With the help of above matrices, as well as the symmetry of $\mathcal{P}$, i.e., $\mathcal{P}_{ij}=\mathcal{P}_{ji}$, the quantum contribution can be written in the form

$$F_{\mathrm{qt}}=4\mathrm{Tr}\left[\left(D\mathcal{I}-\mathcal{G}\right)\mathcal{P}\right]. \tag{30}$$

This is the matrix representation of quantum contribution of the QFI. It is easy to see that the coefficient matrix $D\mathcal{I}-\mathcal{G}$ is traceless.

The matrix $\mathcal{P}$ can be treated as the "transfer" matrix between the vector of the eigenstates $(|\psi_1\rangle,\cdots,|\psi_i\rangle,\cdots,|\psi_{\mathrm{N}}\rangle)^{\mathrm{T}}$ and its derivative vector. For a unitary parametrization, the element of $\mathcal{P}$ reads $\mathcal{P}_{ij}=|\langle\phi_i|H|\phi_j\rangle|^2$. In this case, the diagonal element of $\mathcal{P}$ is the survive probability of the eigenstate $|\phi_i\rangle$ under the evolution H and the non-diagonal element is the transition probability between $|\phi_i\rangle$ and $|\phi_j\rangle$ under H.

Compared with Eqs. (18) and (19), the matrix representation of the quantum Fisher information is related to the entire N-dimensional space. However, the coefficient matrix D, $\mathcal{G}$ and the "transfer" matrix $\mathcal{P}$ are all real and symmetric. For a unitary parametrization, in the matrix representation, one does not need to calculate the average value of H^2, but the transition item $\langle\psi_i|H|\psi_j\rangle$ has to be calculated through the entire space, not only those in the support. In the mean time, using the expression of Eq. (19), one has to calculate the average value of H^2 under the eigenstates, but the transition item needn't to be calculated out of the support. These two representations have their own merits and will bring convenience if being used properly.

In the following we give two examples utilizing this matrix representation. First we apply it in the qubit case. In this case, the parameterized density matrix ρ_θ can be decomposed as $\rho_\theta = \sum_{i=1}^{2} p_i(\theta)|\psi_i(\theta)\rangle\langle\psi_i(\theta)|$. Then the coefficient matrix reads

$$D\mathcal{I} - \mathcal{G} = \begin{pmatrix} 0 & p_1 - 2\det\rho_\theta \\ p_2 - 2\det\rho_\theta & 0 \end{pmatrix}, \tag{31}$$

where the equation $p_1 p_2 = \det\rho_\theta$ has been used. Thus, it is easy to obtain the quantum contribution as

$$F_{\mathrm{qt}} = 4\left(1 - 4\det\rho_\theta\right)\mathcal{P}_{12}, \tag{32}$$

where $\mathcal{P}_{12} = |\langle\psi_1|\partial_\theta\psi_2\rangle|^2$.

When the state is a pure state, for instance $p_1 = 1$ and $p_2 = 0$, there is $\det\rho_\theta = 0$, then the quantum contribution reduces to

$$F_{\mathrm{qt}} = 4\mathcal{P}_{12} = 4|\langle\psi_1|\partial_\theta\psi_2\rangle|^2. \tag{33}$$

This form coincides with the traditional quantum Fisher information form for pure state: $F_Q = \langle\partial_\theta\psi_1|\partial_\theta\psi_1\rangle - |\langle\psi_1|\partial_\theta\psi_1\rangle|^2$, which can be proved by substituting the normalization relation $\mathbb{I} = |\psi_1\rangle\langle\psi_1| + |\psi_2\rangle\langle\psi_2|$ into the item $\langle\partial_\theta\psi_1|\partial_\theta\psi_1\rangle$. The classical contribution can also be obtained in this case, which reads

$$F_{\mathrm{ct}} = \frac{\left(\partial_\theta p_{1,2}\right)^2}{\det\rho_\theta} = \frac{\det\rho_\theta}{1 - 4\det\rho_\theta}\left[\partial_\theta\left(\ln\det\rho_\theta\right)\right]^2 \tag{34}$$

for mixed states and $F_{\mathrm{ct}} = 0$ for pure states. For a unitary parametrization, the quantum contribution reads

$$F_{\mathrm{qt}} = 4\left(1 - 4\det\rho_0\right)|\langle\phi_1|H|\phi_2\rangle|^2, \tag{35}$$

with $|\phi_i\rangle$ a eigenstate of ρ_0. As D is independent of θ, the classical contribution vanishes for both mixed and pure states.

Next we give another example. Consider a density matrix with the following form [111]

$$\rho_\theta = \sum_{n=0}^{\infty} Q_n \rho_\theta^{(n)}, \tag{36}$$

where Q_n is a real number and independent of θ. $\rho_\theta^{(n)}$ is a state of n particles in the entire Hilbert space. This form is representative for an optical system taking into account the superselection rules [111]. For a unitary parametrization, the spectral decomposition of ρ_θ reads

$$\rho_\theta = \sum_{n=0}^{\infty}\sum_{i=0}^{n} Q_n q_i^{(n)} |\psi_i^{(n)}\rangle\langle\psi_i^{(n)}|, \tag{37}$$

where $|\psi_i^{(n)}\rangle = e^{-iH\theta}|\phi_i^{(n)}\rangle$. In this case, the classical contribution vanishes. If the transition between the eigenstates in different particle spaces through the Hamiltonian H is forbidden, which is feasible in some cases [43], namely, $\langle\phi_i^{(n)}|H|\phi_j^{(n')}\rangle = 0$ when $n \neq n'$, then the "transfer" matrix $\mathcal{P}$ can be written in a block diagonal form $\mathcal{P} = \sum_{n=0}^{\infty}\mathcal{P}^{(n)}$, where $\mathcal{P}^{(n)}$ is the corresponding "transfer" matrix for fixed n particles. According to the feature of trace operation, only the corresponding block diagonal part of the coefficient matrices D, $\mathcal{I}$ and $\mathcal{G}$ matters in the calculation of the quantum contribution. If we define $D^{(n)}$, $\mathcal{I}^{(n)}$ and $\mathcal{G}^{(n)}$ as the coefficient matrices for fixed n particles, then the block diagonal parts of D, $\mathcal{I}$ and $\mathcal{G}$ can be expressed as $\sum_n Q_n D^{(n)}$, $\sum_n \mathcal{I}^{(n)}$ and $\sum_n Q_n \mathcal{G}^{(n)}$. Thus, the quantum Fisher information reads

$$F_Q = 4\sum_{n=0}^{\infty} Q_n \mathrm{Tr}\left[\left(D^{(n)}\mathcal{I}^{(n)} - \mathcal{G}^{(n)}\right)\mathcal{P}^{(n)}\right]. \tag{38}$$

Also, one can find that the quantum Fisher information $F^{(n)}$ in the subspace of fixed n particles can be written as

$$F_Q^{(n)} = 4\mathrm{Tr}\left[\left(D^{(n)}\mathcal{I}^{(n)} - \mathcal{G}^{(n)}\right)\mathcal{P}^{(n)}\right]. \tag{39}$$

Thus, one can write the total quantum Fisher information in the form

$$F_Q = \sum_{n=0}^{\infty} Q_n F_Q^{(n)}. \tag{40}$$

This total quantum Fisher information is the weighted average of all the quantum Fisher information for fixed n particles. This form of the QFI has been widely used in the optical interferometry devices when no external global phase reference is present [44].

More generally, taking into account the transition between the eigenstates in different particle subspaces, $\mathcal{P}$ can still be separated into blocks according to the particle number. Denote the sub-block in the upper and lower triangular of $\mathcal{P}$ between n and n' particle subspaces as $\mathcal{P}^{(nn')}$ and $\mathcal{P}^{(n'n)}$, respectively. The diagonal block $\mathcal{P}^{(n)}$ is the same as above. Then, $\mathcal{P}$ can be expressed in the form $\mathcal{P} = \sum_n \mathcal{P}^{(n)} + \sum_{n\neq n'}\mathcal{P}^{(nn')}$, so as $\mathcal{I}$ and $\mathcal{G}$. Here all the elements of $\mathcal{P}^{(nn')}$ is non-negative based on the property of $\mathcal{P}$. Thus, the total quantum Fisher information can be written as

$$F_Q = \sum_n Q_n F_Q^{(n)} + \sum_{n\neq n'} 4\mathrm{Tr}\left[C^{(nn')}\mathcal{P}^{(n'n)}\right], \tag{41}$$

where $C^{(nn')} = Q_n D^{(n)}\mathcal{I}^{(nn')} - \mathcal{G}^{(nn')}$.

From this equation one can find that when all the elements of $C^{(nn')}$ is non-negative, the transition between the eigenstates in different particle subspaces, i.e., the second item of Eq. (41), can enhance the total QFI. Apart from this condition, the effect has to be discussed case by case.

2.2 Conclusion

In this paper, we provide a new analytic expression of the quantum Fisher information. For a non-full rank density matrix, this new expression is only determined by the support of the density matrix. With this new expression, the QFI for some infinite systems can be solved in a finite support space. This would bring significant advantage during the calculation in some scenarios. Besides, we also provide a matrix representation form of the quantum Fisher information and give two examples

3 Fidelity susceptibility and quantum Fisher information for density operators with arbitrary ranks

abstract

Taking into account the density matrices with non-full ranks, we show that the fidelity susceptibility is determined by the support of the density matrix. Combining with the corresponding expression of the quantum Fisher information, we rigorously prove that the fidelity susceptibility is proportional to the quantum Fisher information. As this proof can be naturally extended to the full rank case, this proportional relation is generally established for density matrices with arbitrary ranks. Furthermore, we give an analytical expression of the quantum Fisher information matrix, and show that the quantum Fisher information matrix can also be represented in the density matrix's support.

3.1 Introduction

Quantum Fisher information (QFI) is the central concept in quantum metrology [45, 46, 47, 48, 49, 50, 51, 53, 54, 55, 52, 56]. It depicts the theoretical bound for the variance of an estimator [93, 94]

$$\mathrm{Var}(\hat{\theta}) \geq \frac{1}{F}. \tag{42}$$

Here $\hat{\theta}$ is the estimator for the parameter θ, $\mathrm{Var}(\cdot)$ describes the variance, and F is the so-called quantum Fisher information. A related concept widely used in quantum physics is fidelity, which was first introduced by Uhlmann in 1976 [59]. For a parameterized state $\rho(\theta)$ and its neighbor state in parameter space $\rho(\theta+\delta\theta)$, where $\delta\theta$ is a small change of θ, the fidelity is defined as

$$f(\theta, \theta+\delta\theta) := \mathrm{Tr}\sqrt{\sqrt{\rho(\theta)}\rho(\theta+\delta\theta)\sqrt{\rho(\theta)}}. \tag{43}$$

The form of fidelity is not unique, several alternative forms of fidelity have been proposed and discussed [60, 61, 62]. However, the Uhlmann fidelity is the most well-used form because it has a natural relation with Bures distance. The fidelity only refers to the Uhlmann fidelity in this paper. The fidelity in Eq. (43) reveals the distinguishability between state $\rho(\theta)$ and state $\rho(\theta+\delta\theta)$. It depends on the small change parameter $\delta\theta$. To avoid this dependence, the concept of fidelity susceptibility (FS) is introduced [63]. It is generally believed that the first-order term of $\delta\theta$ in fidelity is zero [64, 65], thus FS is determined by the second-order term with the definition

$$\chi_f := -\frac{\partial^2 f(\theta, \theta+\delta\theta)}{\partial(\delta\theta)^2}. \tag{44}$$

FS is a more effective tool than fidelity itself in quantum physics, especially in detecting the quantum phase transitions [63, 66, 67].

Interestingly, the above two seemingly irrelevant concepts are in fact closely related to each other. Generally, people vaguely believe that for a given state, the first-order term in fidelity equals to zero and the expression of FS is proportional to that of QFI [64, 65, 68, 69]. This is certainly inarguable for the cases with pure states or full-rank density matrices [64, 65]. However, for density matrices with non-full ranks, a clear and rigorous proof is still lacking. In this work, we will resolve this problem.

Recently, we have obtained the expression of the QFI for a non-full rank density matrix, which is determined by the support of the density matrix [70]. This makes us wonder that if the FS can be written in a similar way and still proportional to the QFI, just like the cases with pure states or full-rank density matrices. In this paper, we give a detailed calculation of the fidelity for a non-full rank density matrix. We find that its first-order term still equals to zero and FS is also determined by the support of the density matrix. The whole calculation is rigorous and the expression of FS is proportional to that of QFI. Our proof can be easily extended to the full-rank case. In addition, inspired by this result, we further study the quantum Fisher information matrix (QFIM), which is the counterpart of the QFI for the multiple-parameter estimations. Through the calculation, we find that the QFIM is also determined by the support of the density matrix.

The paper is organized as follows. In Sec. 3.2, for a non-full rank density matrix, we give the detailed calculation of the fidelity. We show that its first-order term also vanishes as the case with full rank. In this way, we get the expression of the FS, which is only determined by the density matrix's support, and proportional to the expression of QFI. In addition, we apply the expression of QFI (or FS) to a non-full rank X state. In Sec. 3.3, we give the calculation of the QFIM and show that like QFI, QFIM is also determined by the support of the density matrix. We also apply this expression to a multiple parametrized X state with non-full rank. Section 3.4 is the conclusion of this work.

3.2 Proportional Relationship between FS and QFI

In the following, we derive the expression of fidelity for a non-full rank density matrix. From which, we find the first-order term of fidelity vanishes. Then we get the expression of the FS, which is determined by the support of the density matrix. With the corresponding expression of the QFI, we prove the proportional relationship between FS and QFI. Although our proof concentrates on the density matrices with non-full ranks, it could be extended to the ones with full ranks as well.

3.2.1 Proof the Proportional Relationship

We will first obtain the expression of FS from the definition of fidelity in Eq. (43). For brevity, we rewrite the expression of fidelity as $f = \mathrm{Tr}\sqrt{\mathcal{M}}$ with $\mathcal{M} := \sqrt{\rho(\theta)}\rho(\theta+\delta\theta)\sqrt{\rho(\theta)}$. We start our calculation by expanding $\rho(\theta+\delta\theta)$ up to the second order of the small change $\delta\theta$ as $\rho(\theta+\delta\theta) = \rho(\theta) + \partial_\theta\rho\delta\theta + \frac{1}{2}\partial_\theta^2\rho\delta^2\theta$ with $\partial_\theta\rho := \partial\rho/\partial\theta$ and $\partial_\theta^2\rho := \partial^2\rho/\partial\theta^2$. Then the matrix $\mathcal{M}$ takes the form

$$\mathcal{M} = \rho^2(\theta) + \mathcal{A}\delta\theta + \frac{1}{2}\mathcal{B}\delta^2\theta. \tag{45}$$

where $\mathcal{A} = \sqrt{\rho(\theta)}\partial_\theta\rho\sqrt{\rho(\theta)}$ and $\mathcal{B} = \sqrt{\rho(\theta)}\partial_\theta^2\rho\sqrt{\rho(\theta)}$. This allows us to assume the square root of $\mathcal{M}$ in the form like

$$\sqrt{\mathcal{M}} = \rho(\theta) + \mathcal{X}\delta\theta + \mathcal{Y}\delta^2\theta, \tag{46}$$

which is also up to the second-order term of $\delta\theta$. As a result, taking square of both sides of Eq. (46), one can find the relations

$$\mathcal{A} = \rho\mathcal{X} + \mathcal{X}\rho, \tag{47}$$

$$\frac{1}{2}\mathcal{B} = \rho\mathcal{Y} + \mathcal{Y}\rho + \mathcal{X}^2. \tag{48}$$

Once the matrices $\mathcal{A}$ and $\mathcal{B}$ are obtained, the information of the matrices $\mathcal{X}$ and $\mathcal{Y}$ will be extracted from these two relationships.

Consequently, the expression of fidelity could be achieved from Eq. (46) as

$$f = 1 + \mathrm{Tr}(\mathcal{X})\delta\theta + \mathrm{Tr}(\mathcal{Y})\delta^2\theta. \tag{49}$$

Here $\mathrm{Tr}(\mathcal{X})$ and $\mathrm{Tr}(\mathcal{Y})$ are the first and second order terms of the fidelity, respectively. It is generally believed that the first-order term disappears in fidelity, i.e., $\mathrm{Tr}(\mathcal{X}) = 0$. However, this conclusion is only well established for pure states or full rank density matrices [64, 65]. Below we will show that it also holds for density matrices with non-full ranks. This provides a precondition to get the expression of FS, which is determined by the second-term of fidelity

$$\chi_f = -2\mathrm{Tr}\mathcal{Y}. \tag{50}$$

Up to this point, the density matrix $\rho(\theta)$ is still arbitrary, which could be either full rank or non-full rank. Next, to explicitly see the expression of fidelity for non-full rank density matrices, we denote the spectral decomposition of $\rho(\theta)$ as

$$\rho(\theta) = \sum_{i=1}^{M} \lambda_i(\theta)|\psi_i(\theta)\rangle\langle\psi_i(\theta)|. \tag{51}$$

Here $\lambda_i(\theta)$ and $|\psi_i(\theta)\rangle$ are the ith eigenvalue and eigenstate of the density matrix, respectively. M is the rank of the density matrix $\rho(\theta)$, which equals to the dimension of the support of $\rho(\theta)$. We also denote the total dimension of the density matrix as N, which implies that $M \leq N$. In the following, we will use λ_i, $|\psi_i\rangle$ instead of $\lambda_i(\theta)$ and $|\psi_i(\theta)\rangle$ for convenience.

It is known that for the density matrix with rank $M = 1$ (pure state) or $M = N$ (full-rank), the first order term of fidelity $\mathrm{Tr}\mathcal{X} = 0$ [64, 65]. This is a precondition to get the expression of the well-known expression of FS, determined by the second order of fidelity [64, 65]. However, if one straightforwardly substitutes Eq. (51) into Eq. (47) to get the value of $\mathrm{Tr}(\mathcal{X})$, one can find the fact that $\langle\psi_i|\mathcal{X}|\psi_j\rangle$ is arbitrary for $i > M$ and $j > M$, which will result in the arbitrariness of the value of $\mathrm{Tr}(\mathcal{X})$. That is, $\mathrm{Tr}(\mathcal{X})$ may become undeterminable for density matrices with non-full ranks. This may bring a different expression of fidelity susceptibility. In fact, this is not true. Below we will show how to avoid this nondeterminacy.

First, we discuss the structure of $\mathcal{A}$ and $\mathcal{B}$. Substituting Eq. (51) into $\mathcal{A}$ and $\mathcal{B}$, and denote $\langle\psi_i|\mathcal{O}|\psi_j\rangle = \mathcal{O}_{ij}$, one find that

$$\begin{aligned}
\mathcal{A}_{ij} &= \left[\sqrt{\rho(\theta)}\partial_\theta\rho\sqrt{\rho(\theta)}\right]_{ij} = \sqrt{\lambda_i\lambda_j}\left(\partial_\theta\rho\right)_{ij}, \\
\mathcal{B}_{ij} &= [\sqrt{\rho(\theta)}\partial_\theta^2\rho\sqrt{\rho(\theta)}]_{ij} = \sqrt{\lambda_i\lambda_j}\left(\partial_\theta^2\rho\right)_{ij}.
\end{aligned} \tag{52}$$

Here the first and second derivatives of the density matrix are

$$(\partial_\theta\rho)_{ij} = \lambda_i\partial_\theta\lambda_i\delta_{ij} + \sqrt{\lambda_i\lambda_j}\,(\lambda_i - \lambda_j)\,\langle\partial_\theta\psi_i|\psi_j\rangle, \tag{53}$$

$$\begin{aligned}\left(\partial_\theta^2\rho\right)_{ij} &= \partial_\theta^2\lambda_i\delta_{ij} + 2\,(\partial_\theta\lambda_i - \partial_\theta\lambda_j)\,\langle\partial_\theta\psi_i|\psi_j\rangle \\ &\quad +\lambda_j\langle\psi_i|\partial_\theta^2\psi_j\rangle + \lambda_i\langle\partial_\theta^2\psi_i|\psi_j\rangle + \sum_k 2\lambda_k\langle\psi_i|\partial_\theta\psi_k\rangle\langle\partial_\theta\psi_k|\psi_j\rangle,\end{aligned} \tag{54}$$

with δ_{ij} the Kronecker delta function. From these expressions, one find that when $i > M$ or $j > M$, $(\partial_\theta\rho)_{ij} = (\partial_\theta{}^2\rho)_{ij} = 0$. That is, both the matrices $[\partial_\theta\rho]$ and $[\partial_\theta^2\rho]$ are block diagonal with the support dimension of M, as well as the density matrix ρ. Thus the matrices $\mathcal{A}$ and $\mathcal{B}$ are also block-diagonal ones, with the elements within the support ($i \leq M$ and $j \leq M$) are nonzero. As a result, denoting the M-dimensional non-zero block of ρ^2, $\mathcal{A}$ and $\mathcal{B}$ as ρ_s^2, $\mathcal{A}_s$ and $\mathcal{B}_s$, we have

$$\mathcal{M} = \begin{pmatrix} \rho_s^2 + \mathcal{A}_s\delta\theta + \frac{1}{2}\mathcal{B}_s\delta^2\theta & 0_{(N-M)\times M} \\ 0_{M\times(N-M)} & 0_{(N-M)\times(N-M)} \end{pmatrix}. \tag{55}$$

Since the square root operation on a block diagonal matrix can be manipulated on each block separately, the square root of $\mathcal{M}$ becomes

$$\sqrt{\mathcal{M}} = \begin{pmatrix} \sqrt{\rho_s^2 + \mathcal{A}_s\delta\theta + \frac{1}{2}\mathcal{B}_s\delta^2\theta} & 0_{(N-M)\times M} \\ 0_{M\times(N-M)} & 0_{(N-M)\times(N-M)} \end{pmatrix}. \tag{56}$$

Comparing the above equation with Eq. (46), one can find that the matrix $\mathcal{X}$ and $\mathcal{Y}$ must be block-diagonal matrices, of which only the elements within the support are nonzero. Therefore, according to Eqs. (46) and (47), one gets the matrix $\mathcal{X}$ as

$$\mathcal{X}_{ij} = \begin{cases} \frac{1}{2}\partial_\theta\lambda_i\delta_{ij} + \frac{\sqrt{\lambda_i\lambda_j}(\lambda_i-\lambda_j)}{\lambda_i+\lambda_j}\langle\partial_\theta\psi_i|\psi_j\rangle, & i,j \in [1, M]; \\ 0, & \text{others}. \end{cases} \tag{57}$$

Then it is easily found that

$$\mathrm{Tr}(\mathcal{X}) = \frac{1}{2}\sum_{i=1}^{M}\partial_\theta\lambda_i = \frac{1}{2}\partial_\theta\mathrm{Tr}\rho = 0. \tag{58}$$

Namely, the first order expansion of fidelity vanishes. In this way, the problem of the nondeterminacy of $\mathrm{Tr}(\mathcal{X})$ is settled. This guarantees that the definition of FS is determined by the second order of fidelity, as shown in Eq. (50).

Next, to obtain the second order of fidelity, one should know the explicit form of the diagonal elements of $\mathcal{Y}$. From Eq. (54), it is easy to get the diagonal elements of $\mathcal{B}$

$$\mathcal{B}_{ii} = \lambda_i\partial_\theta^2\lambda_i - 2\lambda_i^2\langle\partial_\theta\psi_i|\partial_\theta\psi_i\rangle + \sum_k 2\lambda_i\lambda_k|\langle\psi_i|\partial_\theta\psi_k\rangle|^2. \tag{59}$$

where the identity $\langle\partial_\theta^2\psi_i|\psi_i\rangle + \langle\psi_i|\partial_\theta^2\psi_i\rangle = -2\langle\partial_\theta\psi_i|\partial_\theta\psi_i\rangle$ has been used. Then according to the relation (48) and the expressions (57) and (59), one can obtain the diagonal element of $\mathcal{Y}$ within the support as

$$\mathcal{Y}_{ii} = \frac{1}{4}\partial_\theta^2\lambda_i - \frac{1}{8\lambda_i}\left(\partial_\theta\lambda_i\right)^2 - \frac{1}{2}\lambda_i\langle\partial_\theta\psi_i|\partial_\theta\psi_i\rangle + \sum_{k=1}^{M}\frac{2\lambda_i\lambda_k^2}{(\lambda_i+\lambda_k)^2}|\langle\psi_i|\partial_\theta\psi_k\rangle|^2. \tag{60}$$

Considering the fact that $\sum_{i=1}^{M}\frac{1}{4}\partial_\theta^2\lambda_i = \frac{1}{4}\partial_\theta^2\mathrm{Tr}\rho = 0$ and

$$\sum_{i,k=1}^{M}\frac{2\lambda_i\lambda_k^2}{(\lambda_i+\lambda_k)^2}|\langle\psi_i|\partial_\theta\psi_k\rangle|^2 = \sum_{i,k=1}^{M}\frac{\lambda_i\lambda_k}{\lambda_i+\lambda_k}|\langle\psi_i|\partial_\theta\psi_k\rangle|^2, \tag{61}$$

the FS is finally obtained from (50) as

$$\chi_f = -2\mathrm{Tr}\mathcal{Y} \;\; = \;\; \frac{1}{4}F, \tag{62}$$

where F is exactly the expression of QFI for a non-full rank density matrix [70]

$$F \;\; = \;\; \sum_{i=1}^{M}\frac{\left(\partial_\theta\lambda_i\right)^2}{\lambda_i} + \sum_{i=1}^{M}4\lambda_i\langle\partial_\theta\psi_i|\partial_\theta\psi_i\rangle - \sum_{i,k=1}^{M}\frac{8\lambda_i\lambda_k}{\lambda_i+\lambda_k}|\langle\psi_i|\partial_\theta\psi_k\rangle|^2. \tag{63}$$

From this result one can find that for non-full rank density matrices, the proportional relation between QFI and fidelity susceptibility is still valid. One should notice that the calculation above also covers the full rank case when choosing $M = N$. Therefore, we can reach the final conclusion that fidelity susceptibility is proportional to the quantum Fisher information for a general density matrix.

3.2.2 Application to X states

To see how to calculate the QFI or FS, we take the X state as an example, which is defined as [71, 72, 73, 74, 75]

$$\rho_X = \begin{pmatrix} a & 0 & 0 & w^* \\ 0 & b & z^* & 0 \\ 0 & z & c & 0 \\ w & 0 & 0 & d \end{pmatrix}. \tag{64}$$

This type of states include maximally entangled Bell states and Werner states. The properties of this state have been widely discussed [71, 72, 73, 74, 75]. Here we set $z = z^* = \sqrt{bc}$. Then the four eigenvalues of (64) become

$$\lambda_1 = b + c, \quad \lambda_2 = 0, \quad \lambda_\pm = \frac{1}{2}\left[a + d \pm \sqrt{\Delta}\right], \tag{65}$$

where $\Delta = (a-d)^2 + 4|w|^2$. Obviously, the dimension of the support is $M = 3$. In addition, the eigenstates corresponding to λ_1 and $\lambda_\pm$ are

$$|\psi_1\rangle = \epsilon_1\left(0, \sqrt{\frac{b}{c}}, 1, 0\right)^{\mathrm{T}}, \quad |\psi_\pm\rangle = \epsilon_\pm\left(\frac{a-d\pm\sqrt{\Delta}}{2w}, 0, 0, 1\right)^{\mathrm{T}}, \tag{66}$$

where $\epsilon_1=\sqrt{c/(b+c)}$ and $\epsilon_\pm=\frac{\sqrt{2}|w|}{\sqrt{\Delta\pm(a-d)\sqrt{\Delta}}}$.

We consider an estimation of the parameter θ introduced by the following unitary operation

$$U=\exp\left(-i\alpha\sigma_z^\alpha\right), \tag{67}$$

where $\sigma_z^\alpha=\sigma_z\otimes\mathbb{I}$. Here $\mathbb{I}$ is the 2×2 identity matrix and σ_z is a Pauli matrix, which reads $\sigma_z=\mathrm{diag}(1,-1)$. In this case, the QFI reduces to

$$\begin{aligned} F &= 4\lambda_\pm\langle\Delta^2\sigma_z^\alpha\rangle_\pm+4\lambda_1\langle\Delta^2\sigma_z^\alpha\rangle_1 \\ &\quad -\frac{16\lambda_+\lambda_-}{\lambda_++\lambda_-}|\langle\psi_+|\sigma_z^\alpha|\psi_-\rangle|^2-\sum_{i=\pm}\frac{16\lambda_i\lambda_1}{\lambda_i+\lambda_1}|\langle\psi_i|\sigma_z^\alpha|\psi_1\rangle|^2, \end{aligned} \tag{68}$$

where $\langle\Delta^2\sigma_z^\alpha\rangle_i=\langle\psi_i|\left(\sigma_z^\alpha\right)^2|\psi_i\rangle-\langle\psi_i|\sigma_z^\alpha|\psi_i\rangle^2$. It is obvious that QFI is only constituted by the nonzero eigenvalues and the corresponding eigenstates of the density matrix (64), namely, QFI is only determined by the support of (64).

Substituting the values of $\lambda_{\pm,1}$ and $|\psi_{\pm,1}\rangle$ into above expression, the QFI can be finally simplified as

$$F=16\left(\frac{|w|^2}{a+d}+\frac{bc}{b+c}\right). \tag{69}$$

To guarantee the positivity of the density matrix ρ_{X}, it requires that all the diagonal elements of ρ_X are positive and $ad\geq|w|^2$. In the mean time, we know that $b+c\geq 2\sqrt{bc}$ and $a+d\geq 2\sqrt{ad}$, then one can find that

$$F\leq 8\left(|w|+\sqrt{bc}\right). \tag{70}$$

Namely, the maximum QFI is $F_{\max}=8(|\omega|+\sqrt{bc})$, which is satisfied under the condition $a=d=|w|$ and $b=c$. This indicates that by suitably choosing the input state, one could get the maximum QFI, which gives the minimum uncertainty of the unknown parameter α from Eq. (42). One of the optimal X state in this case is the bell state $|\Phi^+\rangle=(|00\rangle+|11\rangle)/\sqrt{2}$. Explicitly, it is

$$|\Phi^+\rangle\langle\Phi^+|=\frac{1}{2}\begin{pmatrix}1&0&0&1\\0&0&0&0\\0&0&0&0\\1&0&0&1\end{pmatrix}. \tag{71}$$

Thus, the maximum value of the QFI is $F_{\max}=4$.

3.3 Extention to QFIM

Quantum Fisher information matrix (QFIM) is the counterpart of QFI in multiple-parameter estimations. Since QFI for a non-full rank density matrix ρ is determined by the support of ρ, then it is reasonable to speculate that QFIM could also be expressed similarly. In the following, we will calculate the specific form of the QFIM for a density matrix with arbitrary rank and show that it is indeed determined by the support of density matrix.

3.3.1 Expression of QFIM

We start from the definition of QFIM, whose elements read [93, 94]

$$\mathcal{F}_{\alpha\beta} = \frac{1}{2}\mathrm{Tr}\left[\rho\left\{L_\alpha, L_\beta\right\}\right], \tag{72}$$

where the symmetric logarithmic derivative (SLD) L_m for the parameter θ_m is determined by

$$\frac{\partial\rho}{\partial\theta_m} = \frac{1}{2}\left(\rho L_m + L_m\rho\right). \tag{73}$$

As the same as the above section, we denote the dimension of the density matrix's support as M, and the total dimension of it is N. And we define $[L_m]_{ij} := \langle\psi_i|L_m|\psi_j\rangle$. From the spectral decomposition of density matrix ρ in (51), one can obtain the mth SLD as

$$[L_m]_{ij} = \begin{cases} \frac{2\delta_{ij}\partial_{\theta_m}\lambda_i}{\lambda_i+\lambda_j} + \frac{2(\lambda_j-\lambda_i)}{\lambda_i+\lambda_j}\langle\psi_i|\partial_{\theta_m}\psi_j\rangle, & i,j\in[1,M]; \\ \text{arbitrary value}, & \text{others}. \end{cases} \tag{74}$$

Here $[L_m]_{ij}$ could be an arbitrary value out of the support of the density matrix. However, this arbitrariness has no influence on the determinacy of QFIM. This is because these random values are not involved in the calculation, which will be shown below.

Based on the definition (72), the elements of QFIM can be expressed by

$$\mathcal{F}_{\alpha\beta} = \frac{1}{2}\sum_{i=1}^{M}\sum_{j=1}^{N}\lambda_i\left([L_\alpha]_{ij}[L_\beta]_{ji} + [L_\beta]_{ij}[L_\alpha]_{ji}\right), \tag{75}$$

where the identity $\sum_{i=1}^{N}|\psi_i\rangle\langle\psi_i| = \mathbb{I}$ has been used. From Eq. (74), one find that when $i\in[1,M]$ and $j\in[1,N]$,

$$[L_\alpha]_{ij}[L_\beta]_{ji} = \frac{4\left(\lambda_i-\lambda_j\right)^2}{\left(\lambda_i+\lambda_j\right)^2}\langle\partial_\alpha\psi_i|\psi_j\rangle\langle\psi_j|\partial_\beta\psi_i\rangle + \frac{4\left(\partial_\alpha\lambda_i\right)\left(\partial_\beta\lambda_j\right)\delta_{ij}}{\left(\lambda_i+\lambda_j\right)^2}, \tag{76}$$

with $\partial_{\alpha,\beta}$ the logogram of $\partial_{\theta_{\alpha,\beta}}$. For a fixed i satisfying $i\le M$, there is

$$\sum_{j=M+1}^{N}[L_\alpha]_{ij}[L_\beta]_{ji} = 4\langle\partial_\alpha\psi_i|\partial_\beta\psi_i\rangle - \sum_{j=1}^{M}4\langle\partial_\alpha\psi_i|\psi_j\rangle\langle\psi_j|\partial_\beta\psi_i\rangle. \tag{77}$$

Then substituting above equation into Eq. (75), one can obtain the final expression of the element of QFIM.

As a result, the QFIM can be splitted into the summation of two parts, i.e.,

$$\mathcal{F}_{\alpha\beta} = F_{\mathrm{ct}} + F_{\mathrm{qt}}, \tag{78}$$

where

$$F_{\mathrm{ct}} = \sum_{i=1}^{M}\frac{(\partial_\alpha\lambda_i)(\partial_\beta\lambda_i)}{\lambda_i} \tag{79}$$

is the classical contribution, which is determined by the eigenvalues of the density matrix, and

$$F_{\mathrm{qt}} = \sum_{i=1}^{M}4\lambda_i\mathrm{Re}(\langle\partial_\alpha\psi_i|\partial_\beta\psi_i\rangle) - \sum_{i,j=1}^{M}\frac{8\lambda_i\lambda_j}{\lambda_i+\lambda_j}\mathrm{Re}(\langle\partial_\alpha\psi_i|\psi_j\rangle\langle\psi_j|\partial_\beta\psi_i\rangle) \tag{80}$$

is the quantum contribution, determined by eigenvalues and eigenstates simultaneously. This division between the classical and quantum contribution is similar to the case of the single-parameter estimations [70, 76].

From Eqs. (79) and (80), one see that there are several properties for QFIM. First, it is a real symmetric matrix, i.e., $\mathcal{F}_{\alpha\beta} \in \mathbb{R}$ and $\mathcal{F}_{\alpha\beta} = \mathcal{F}_{\beta\alpha}$. Second, like the QFI in Sec. 2, the QFIM is determined by the support of the density matrix. Moreover, the diagonal term of QFIM reads

$$\mathcal{F}_{\alpha\alpha} = \sum_{i=1}^{M} \frac{(\partial_\alpha \lambda_i)^2}{\lambda_i} + \sum_{i=1}^{M} 4\lambda_i \langle \partial_\alpha \psi_i | \partial_\alpha \psi_i \rangle - \sum_{i,j=1}^{M} \frac{8\lambda_i \lambda_j}{\lambda_i + \lambda_j} |\langle \partial_\alpha \psi_i | \psi_j \rangle|^2, \tag{81}$$

which is exactly the QFI expression for the single parameter θ_α. In addition, for a pure state $|\psi\rangle\langle\psi|$, the expression of QFIM reduces to the well-known result [93, 94]

$$\mathcal{F}_{\alpha\beta} = 4\mathrm{Re}\left(\langle \partial_\alpha \psi | \partial_\beta \psi \rangle - \langle \partial_\alpha \psi | \psi \rangle \langle \psi | \partial_\beta \psi \rangle\right). \tag{82}$$

3.3.2 Application to X state

We again take the X state (64) as an example. Assume that the parametrization process is described by

$$U_m = \exp\left[-i\left(\alpha\sigma_z^\alpha + \beta\sigma_z^\beta\right)\right], \tag{83}$$

here $\sigma_z^\alpha = \sigma_z \otimes \mathbb{I}$ and $\sigma_z^\beta = \mathbb{I} \otimes \sigma_z$. We set $z = z^* = \sqrt{bc}$. In this case, the element of QFIM are

$$\mathcal{F}_{\alpha\beta} = \sum_{i=\pm,1} 4\lambda_i \mathrm{Re}\left(\langle \psi_i | \sigma_z^\alpha \sigma_z^\beta | \psi_i \rangle\right) - \sum_{i,j=\pm,1} \frac{8\lambda_i\lambda_j}{\lambda_i + \lambda_j} \mathrm{Re}\left(\langle \psi_i | \sigma_z^\alpha | \psi_j \rangle \langle \psi_j | \sigma_z^\beta | \psi_i \rangle\right). \tag{84}$$

As expected, it is only determined by the nonzero eigenvalues and the corresponding eigenstates of the density matrix.

After some calculations, the explicit form of QFIM for X state can be simplified as

$$\mathcal{F} = 16\left[\left(\frac{|w|^2}{a+d} + \frac{bc}{b+c}\right)\mathbb{I} + \left(\frac{|w|^2}{a+d} - \frac{bc}{b+c}\right)\sigma_x\right], \tag{85}$$

Here σ_x is a Pauli matrix. From Eq. (85), one can see that its diagonal element $\mathcal{F}_{\alpha\alpha}$ is exactly the expression of QFI for single-parameter estimation shown in (69).

3.4 Conclusion

In this paper, we study the relationship between the fidelity susceptibility and quantum Fisher information. We give a rigorous proof that the fidelity susceptibility is determined by the support of the density matrices, and it is proportional to the quantum Fisher information. Particularly, this proof is focused on the density matrices with non-full ranks. However, the proof can be easily extended to the full rank case. Then we apply the result to a X state. Furthermore, we show that, similar to the quantum Fisher information, for a non-full rank density matrix, the quantum Fisher information matrix is also determined by the support of the density matrix. We also take the X state as an example to apply this expression.

4 Quantum Fisher information and symmetric logarithmic derivative via anti-commutators

abstract *Symmetric logarithmic derivative (SLD) is a key quantity to obtain quantum Fisher information (QFI) and to construct the corresponding optimal measurements. Here we develop a method to calculate the SLD and QFI via anti-commutators. This method is originated from the Lyapunov representation and would be very useful for cases that the anti-commutators among the state and its partial derivative exhibits periodic properties. As an application, we discuss a class of states, whose squares linearly depend on the states themselves, and give the corresponding analytical expressions of SLD and QFI. A noisy scenario of this class of states is also considered and discussed. Finally, we readily apply the method to the block-diagonal states and the multi-parameter estimation problems.*

Quantum metrology has been going through a great development in recent years [77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 92, 89, 90, 91]. Quantum Fisher information (QFI) is a crucial concept in quantum metrology as it depicts the lower bound on the variance of an unbiased estimator for the parameter under estimation, according to the quantum Cramér-Rao theorem [93, 94]. The definition of QFI is $F := \langle L^2 \rangle = \mathrm{Tr}(\rho L^2)$ [93, 94], where L is so-called symmetric logarithmic derivative (SLD). Denoting the parameter under estimation as θ, the SLD operator is determined by the equation

$$\partial_\theta \rho = \frac{1}{2}\left(\rho L + L\rho\right). \tag{86}$$

Taking the trace on both sides of this equation, one can see that $\langle L \rangle = 0$. Therefore, the QFI is actually the variance of SLD operator, i.e., $F = \langle \Delta^2 L \rangle$, with $\Delta^2 L := (L - \langle L \rangle)^2$.

The SLD operator is important for two reasons. First, it is obvious that the QFI can be directly obtained when the SLD operator is known. Second, the achievement of quantum Cramér-Rao bound strongly depends on the measurement, namely, it can only be achieved for some optimal measurements. The eigenbasis of SLD operator is such theoretical optimal measurements [95, 96, 97]. Thus, the study of SLD operator could help us to construct or find optimal measurements for the achievement of the highest precision.

The traditional method for the calculation of SLD operator is to expand it in the eigenspace of density matrix. We now denote the spectral decomposition of ρ as $\sum_{i=1}^{M} p_i |\psi_i\rangle\langle\psi_i|$, with p_i, $|\psi_i\rangle$ the ith eigenvalue and eigenstate of ρ, respectively. M is the dimension of ρ's support. When ρ is positive definite (or full rank), M equals to the state's dimension d. In this representation, the element of SLD operator can be expressed by [98, 99, 100]

$$L_{ij} = \frac{2\partial_\theta p_i}{p_i + p_j}\delta_{ij} + \frac{p_i - p_j}{p_i + p_j}\langle \partial_\theta \psi_i | \psi_j \rangle, \tag{87}$$

for any of i, j less than M and L_{ij} can be an arbitrary number for both i, j larger than M. This method to calculate SLD operator is useful when the spectral decomposition of ρ is not difficult to obtain, which is, however, not an easy task generally.

Lyapunov representation is another method to obtain the SLD operator and applied in many scenarios [101, 102, 103]. The definition equation (86) is actually a special form of Lyapunov equation, indicating that SLD operator is a corresponding solution. In this representation, the SLD operator is expressed by [103]

$$L = 2\int_0^{\infty} e^{-\rho s}\left(\partial_\theta \rho\right) e^{-\rho s} ds. \tag{88}$$

One advantage of this representation is that it is basis-independent. Generally, this representation is no easier to obtain than the traditional method. However, similar to the traditional one, Lyapunov representation would be very useful for some scenarios. In this paper, we first review the Lyapunov representation and figure out that Eq. (88) is available for both full and non-full rank density matrices. Then we provide a new basis-independent expression of SLD operator based on the Lyapunov form. The new expression would be extremely useful when the anti-commutator between the density matrix and its partial derivative exhibits periodic properties.

To show the advantage of this method, we apply it in a class of states showing a linear relation with their squares. This class includes all pure and two-level states. We provide simple expressions of SLD operator and corresponding QFI via the given method for this class. Especially, as a special case, general basis-independent expressions of SLD and QFI for *any* two-level state are provided. Noise from the environment are widely exist in reality. The scenario for these states under white noise are considered. Moreover, we also discuss the block diagonal states and the multiparameter estimations.

Lyapunov representation.-As the beginning of this paper, we first review the derivation of Lyapunov representation of SLD operator. Mathematically, Eq. (86) is known as a special form of Lyapunov equation. To solve this equation, one can construct a function $f(s) = e^{-\rho s} L e^{-\rho s}$, which satisfies $f(0) = L$. The partial derivative of $f(s)$ on s is $\partial_s f(s) = -2e^{-\rho s}\left(\partial_\theta \rho\right) e^{-\rho s}$. Integrating both sides of this derivative equation, one can obtain $f(\infty) - f(0) = -2\int_0^\infty e^{-\rho s}(\partial_\theta\rho)e^{-\rho s}ds$. When ρ is full rank, $e^{-\rho s}$ trends to zero for $s \to \infty$, indicating that $f(\infty) = 0$. Thus, the SLD operator can be directly written in the form of Eq. (88). However, when ρ is non-full rank, $f(\infty)$ cannot vanish. Reminding that M and d are the dimensions of the support and ρ respectively, then the limitation of $e^{-\rho s}$ equals to diag$\{0_M, \mathbb{I}_{d-M}\}$ when s trends to positive infinite. Here 0_M is the M-dimensional zero matrix and $\mathbb{I}_{d-M}$ is the $(d-M)$-dimensional identity matrix. Correspondingly, we manually separate the SLD operator into four blocks as

$$L = \begin{pmatrix} A_M & B_{d-M,M} \\ B^\dagger_{d-M,M} & C_{d-M} \end{pmatrix}, \tag{89}$$

where the Hermiticity of L is applied. Utilizing this form, one can see that $f(\infty) = \mathrm{diag}\left\{0_M, C_{d-M}\right\}$. Meanwhile, for the integrand $e^{-\rho s}(\partial_\theta\rho)e^{-\rho s}$, only the elements within the support is nonzero, thus, L has to be in a block diagonal form, i.e., $B_{d-M,M} = 0$. Since the block C_{d-M} cannot be solved by Eq. (86), C_{d-M} is actually undefined here. However, C_{d-M} will not be involved in the calculation of QFI [98, 99], therefore, it will not bring indeterminacy on the final expression of QFI. Based on this reason, we can simply take $C_{d-M} = 0$ for convenience. In this way, the SLD operators for both full and non-full rank density operators can be uniformly expressed in Eq. (88).

A further method.-Defining the anti-commutator ρ^{o} as $\rho^{\mathrm{o}}(\cdot) = \{\rho, \cdot\}$ and noticing the fact that the improper integral $\int_0^\infty$ can also be written as $\lim_{s\to\infty}\int_0^s$, Eq. (88) can be further expressed in the form

$$L=-2\lim_{s\to\infty}\sum_{n=0}^{\infty}\frac{(-s)^{n+1}}{(n+1)!}\left(\rho^{\mathrm{o}}\right)^{n}\partial_\theta\rho. \tag{90}$$

This is a further basis-independent form of SLD. This formula would be very useful when the anti-commutator among ρ and its partial derivative exhibits periodic properties. In some cases, ρ^{o} is the eigen-superoperator of $\partial_\theta\rho$, i.e., $\rho^{\mathrm{o}}\partial_\theta\rho=a\partial_\theta\rho$ with a a real number. When $a>0$, the SLD operator reduces to a very simple form

$$L=\frac{2}{a}\partial_\theta\rho. \tag{91}$$

The simplest case here is the pure states. For a pure state, it is easy to see that $a=1$ as $\rho^2=\rho$. Thus, the SLD operator for pure states is $L=2\partial_\theta\rho$.

Moreover, because of the equality

$$\left(\rho^{\mathrm{o}}\right)^{n}\partial_\theta\rho=\sum_{m=0}^{n}C_n^m\rho^m\left(\partial_\theta\rho\right)\rho^{n-m}, \tag{92}$$

where $C_n^m=n!/[m!(n-m)!]$, the SLD operator in Eq. (90) can also be written in the form

$$L=-2\lim_{s\to\infty}\sum_{n=0}^{\infty}\sum_{m=0}^{n}\frac{(-s)^{n+1}}{(n+1)!}C_n^m\rho^m\left(\partial_\theta\rho\right)\rho^{n-m}. \tag{93}$$

This form of SLD operator could be very useful when $\rho^m\left(\partial_\theta\rho\right)\rho^{n-m}$ are easy to calculate. Especially, when ρ commutes with $\partial_\theta\rho$, above formula reduces to

$$L=\rho^{-1}\partial_\theta\rho=\left(\partial_\theta\rho\right)\rho^{-1}, \tag{94}$$

where the equality $\sum_{m=0}^{n}C_n^m=2^n$ has been applied. The detailed calculation can be found in the supplemental material. Based on this equation, the corresponding QFI reads

$$F=\mathrm{Tr}[\rho^{-1}(\partial_\theta\rho)^2]. \tag{95}$$

Unitary parametrization.-A unitary parametrization process contains a large category of realistic parametrization processes. Recently, an alternative representation of QFI for unitary parametrization processes has been discussed [109, 110]. For a unitary parametrization process, the parametrized state $\rho=U(\theta)\rho_{\mathrm{in}}U^\dagger(\theta)$, with $U(\theta)$ a θ-dependent unitary matrix. The initial state ρ_{in} is θ-independent. A key quantity in this alternative representation is a Hermitian operator $\mathcal{H}=i(\partial_\theta U^\dagger)U$. All the information of parametrization is involved in this basis-independent operator. For a unitary process, the QFI can be expressed by

$$F=\mathrm{Tr}\left(\rho_{\mathrm{in}}L_{\mathrm{eff}}^2\right), \tag{96}$$

where $L_{\mathrm{eff}}=U^\dagger LU$ is the effective SLD operator. In this scenario, it is easy to find that $\rho^m\left(\partial_\theta\rho\right)\rho^{n-m}=iU\rho_{\mathrm{in}}^m\left[\mathcal{H},\rho_{\mathrm{in}}\right]\rho^{n-m}U^\dagger$. Based on Eq. (93), the effective SLD operator can be written as

$$L_{\mathrm{eff}}=-i2\lim_{s\to\infty}\sum_{n=0}^{\infty}\sum_{m=0}^{n}\frac{(-s)^{n+1}}{(n+1)!}C_n^m\rho_{\mathrm{in}}^m\left[\mathcal{H},\rho_{\mathrm{in}}\right]\rho_{\mathrm{in}}^{n-m}. \tag{97}$$

For a pure initial state, as $\rho_{\rm in}[\mathcal{H},\rho_{\rm in}]\rho_{\rm in}=0$, $L_{\rm eff}$ reduces to the known form $L_{\rm eff}=i2[\mathcal{H},\rho_{\rm in}]$ [110]. When the equation $\{\mathcal{H},\rho^2_{\rm in}\}=2\rho_{\rm in}\mathcal{H}\rho_{\rm in}$ is satisfied, $\rho_{\rm in}$ and $[\mathcal{H},\rho_{\rm in}]$ are commutative. Then the effective SLD operator is $L_{\rm eff}=i\left(\mathcal{H}-\rho_{\rm in}\mathcal{H}\rho_{\rm in}^{-1}\right)$.

Application.-Now we apply Eq. (90) into a class of density operators, which share a common feature as below

$$\rho^2=\alpha\rho-\beta, \tag{98}$$

where α and β are real numbers. In the eigenbasis of ρ, above equation is equivalent to $p_i^2=\alpha p_i-\beta$ for any i, which gives the solution $p_i=[\alpha\pm\sqrt{\alpha^2-4\beta}]/2$. If only one of the solutions is positive, the density matrix is trivially proportional to the identity matrix. Thus, we only consider the situation that both solutions are positive, i.e., $\alpha>0$ and $\beta>0$. Moreover, it is worth to notice that α, β in Eq. (98) can either depends on θ or not. Several well-known states, including all pure and two-level states, satisfy this relation. From Eq. (98), it is easy to see that $\mathcal{P}=\mathrm{Tr}\rho^2=\alpha-\beta$ is the purity of ρ and satisfies $d^{-1}\leq\mathcal{P}\leq 1$ with d the dimension of ρ. From Eq. (90), the SLD operator for this class of states can be expressed by

$$L=\frac{1}{\alpha}\left[2\partial_\theta\rho+\left(\partial_\theta\beta\right)\rho^{-1}-\partial_\theta\alpha\right]. \tag{99}$$

When ρ is non-full rank, i.e., $\det\rho=0$, ρ^{-1} is the inverse matrix of ρ on the support. The detailed derivation of this equation can be found in the supplemental material.

When α, β are both constant numbers independent of θ, the SLD operator reduces to $L=2\partial_\theta\rho/\alpha$. Alternatively, α can be a constant and β is dependent on θ. Under this situation, the SLD operator reduces to $L=\left[2\partial_\theta\rho+(\partial_\theta\beta)\rho^{-1}\right]/\alpha$. A well-known case here is the two-level states, which can be expressed in the Bloch representation $\rho=\left(\mathbb{I}_2+\mathbf{r}\cdot\sigma\right)/2$. Here $\sigma=(\sigma_{\mathbf{x}},\sigma_{\mathbf{y}},\sigma_{\mathbf{z}})^{\mathrm{T}}$ is the vector of Pauli matrices and $\mathbf{r}$ is the Bloch vector. Utilizing this representation, one can immediately find that ρ satisfies Eq. (98) with $\alpha=1$ and $\beta=(1-\mathcal{P})/2$. $\mathcal{P}$ is the purity. Then the SLD operator is

$$L=2\partial_\theta\rho-\frac{1}{2}\left(\partial_\theta\mathcal{P}\right)\rho^{-1}. \tag{100}$$

This is the general basis-independent expression of SLD operator for *any* two-level state. For pure states, it is known that $\mathcal{P}=1$, then L reduces to the known form. For a two-level mixed state, substituting the Bloch representation of ρ and ρ^{-1} into above equation, the entire Bloch representation of SLD operator in Ref. [104] can be reproduced.

Equation (99) is the general expression of SLD operator for all states satisfying Eq. (98). Utilizing this formula, the corresponding basis-independent expression of QFI reads

$$\begin{aligned}F &= \frac{1}{\alpha^2}\Big[2\alpha\mathrm{Tr}\left(\partial_\theta\rho\right)^2+\left(\partial_\theta\beta\right)^2\mathrm{Tr}\rho^{-1} \\ &\quad -\left(2M-1\right)\left(\partial_\theta\alpha\right)\partial_\theta\beta\Big].\end{aligned} \tag{101}$$

For a full rank density matrix, M equals to d. The advantage of this basis-independent expression shows in two aspects. First, during the specific calculation, one can choose a convenient basis, in which $\partial_\theta\rho$ or ρ^{-1} are easy to express or calculate. Second, utilizing a basis-independent formula, the effects of the density matrix on the QFI are more distinct.

The fact that Harmonic mean is less than the Arithmetic mean implies the inequality $\mathrm{Tr}\rho^{-1} \geq M^2$. Meanwhile, it is easy to find $\mathrm{Tr}(\partial_\theta\rho)^2 \geq 0$. Thus, the QFI in Eq. (101) is bounded by the inequality

$$F \geq \frac{1}{\alpha^2}\left[(M\partial_\theta\beta)^2 - (2M-1)\left(\partial_\theta\alpha\right)\partial_\theta\beta\right]. \tag{102}$$

This lower bound only depends on the coefficients and can be used to roughly evaluate the QFI.

For the cases that α and β are both θ-independent, the QFI reduces to $F = 2\mathrm{Tr}(\partial_\theta\rho)^2/\alpha$. When α is a constant and β is dependent on θ, the QFI is in the form

$$F = \frac{1}{\alpha^2}\left[2\alpha\mathrm{Tr}\left(\partial_\theta\rho\right)^2 + \left(\partial_\theta\beta\right)^2\mathrm{Tr}\rho^{-1}\right]. \tag{103}$$

From this equation, the QFI for *any* two-level state can be immediately obtained as

$$F_{\mathrm{q}} = 2\mathrm{Tr}\left(\partial_\theta\rho\right)^2 + \frac{1}{4}\left(\partial_\theta\mathcal{P}\right)^2\mathrm{Tr}\rho^{-1}. \tag{104}$$

This is a general and unified expression for *any* two-level state, including two-level pure states. For any mixed two-level state, the QFI is bound by the inequality $F_{\mathrm{q}} \geq (\partial_\theta\mathcal{P})^2$.

Most quantum states has to face the disturbance from the environment in reality. White noise is very usual in quantum processes. Several quantum metrological problems of states under white noise have been discussed recently [105, 106, 107]. Usually, the white noise is depicted via the depolarizing channel [108]. In this channel, the final state ρ_{f} can be expressed by

$$\rho_{\mathrm{f}} = \eta\rho_{\mathrm{in}} + \frac{1-\eta}{d}\mathbb{I}_d, \tag{105}$$

where ρ_{in} is the initial state and η is the reliability of the channel.

Now consider the situation that the initial state ρ_{in} satisfies Eq. (98), i.e., $\rho_{\mathrm{in}}^2 = \alpha_{\mathrm{in}}\rho_{\mathrm{in}} - \beta_{\mathrm{in}}$. Under this situation, the final state also satisfies Eq. (98) with the coefficients $\alpha = \eta\alpha_{\mathrm{in}} + 2(1-\eta)/d$, and $\beta = \eta^2\beta_{\mathrm{in}} + \eta(1-\eta)\alpha_{\mathrm{in}}/d + (1-\eta)^2/d^2$. In this way, the SLD operator for the final state can be directly obtained by substituting the specific formula of α and β into Eq. (99).

If α_{in} and β_{in} are both θ-independent, so will α and β, the SLD operator then reads

$$L_{\mathrm{f}} = \frac{2d\eta}{d\eta\alpha_{\mathrm{in}} + 2(1-\eta)}\partial_\theta\rho_{\mathrm{in}}. \tag{106}$$

One example for this case is a degenerate mixed state, i.e., $\rho_{\mathrm{in}} = \sum_{i=1}^{N}\frac{1}{N}|\psi_i(\theta)\rangle\langle\psi_i(\theta)|$, where N ($N < d$) is the degeneracy and $\langle\psi_i(\theta)|\psi_j(\theta)\rangle = \delta_{ij}$. It is easy to see that $\rho_{\mathrm{in}}^2 = \rho_{\mathrm{in}}/N$, satisfying Eq. (98). Taking θ as the parameter under estimation, the SLD operator can be directly written as

$$L_{\mathrm{f}} = \frac{d\eta}{d\eta + 2N(1-\eta)}\sum_{i=1}^{d} L_{\mathrm{in},i}, \tag{107}$$

where $L_{\mathrm{in},i} = 2\partial_\theta(|\psi_i\rangle\langle\psi_i|)$ is the SLD operator for $|\psi_i\rangle\langle\psi_i|$. For a pure initial state, i.e., $N = 1$, the SLD operator reduces to the known form discussed in Ref. [107].

Alternatively, the reliability η can also be the parameter under estimation. In this case, it can be checked that ρ_{f} commutes with $\partial_\eta \rho_{\mathrm{f}}$. Thus, for any form of input state ρ_{in}, the SLD operator here is always in the form of Eq. (94), namely, $L = \rho_{\mathrm{f}}^{-1}\partial_\theta \rho_{\mathrm{f}}$.

Extension.-The block diagonal states are widely used and discussed in quantum mechanics. One vivid example is the optical systems taking into account the superselection rules [111]. Generally, a block diagonal state can be written as $\rho = \bigoplus_{i=1}^{n} \rho_i$. Here $\bigoplus$ represents the direct sum. One can check that an available form of SLD operator here is block diagonal, i.e., $L = \bigoplus_{i=1}^{n} L_i$, where L_i is the corresponding SLD operator for ρ_i. Consider the scenario that each block satisfies the equation $\rho_i^2 = \alpha_i \rho_i - \beta_i$. It should be noticed that $\mathrm{Tr}\rho_i < 1$ and the purity for ρ is $\mathcal{P} = \sum_i \alpha_i \mathrm{Tr}\rho_i - \beta_i$. In this scenario, each L_i satisfies Eq. (99). Thus, the entire SLD operator can be expressed by

$$L = \bigoplus_{i=1}^{n} \frac{1}{\alpha_i}\left[2\partial_\theta \rho_i + (\partial_\theta \beta_i)\,\rho_i^{-1} - \partial_\theta \alpha_i\right]. \tag{108}$$

Moreover, if ρ_i is a 2-dimensional block, it can be expanded via the Pauli matrices into $\rho_i = \mu_i \mathbb{I} + \mathbf{r_i}\cdot\sigma$, where $\mu_i = \mathrm{Tr}\rho_i/2$, and $\mathbf{r_i}$ is the Bloch vector for ith block. Then it can be found that ρ_i satisfies Eq. (98) with $\alpha_i = 2\mu_i$ and $\beta_i = 2\mu_i^2 - \mathcal{P}_i/2$. Here $\mathcal{P}_i = \mathrm{Tr}\rho_i^2$. With these coefficients, the SLD operator for ith block reads

$$L_i = \frac{1}{\mu_i}\left(\partial_\theta \rho_i + \xi_i \rho_i^{-1} - \partial_\theta \mu_i\right), \tag{109}$$

where the coefficient $\xi_i = 2\mu_i \partial_\theta \mu_i - \partial_\theta \mathcal{P}_i/4$. If $\det \rho_i = 0$, ξ_i vanishes. One simple example here is all the X states.

Multiparameter estimation.-In multiparameter estimation, the quantum Fisher information matrix $\mathcal{F}$ is also defined via the SLD operators, i.e.,

$$\mathcal{F}_{ij} := \frac{1}{2}\langle\{L_{\theta_i}, L_{\theta_j}\}\rangle, \tag{110}$$

where $L_{\theta_{i(j)}}$ is the SLD operator for parameter $\theta_{i(j)}$. For any state satisfying Eq. (98), $\mathcal{F}_{ij}$ can be expressed by

$$\begin{aligned}\mathcal{F}_{ij} \;=\; & \frac{1}{\alpha^2}\Big[\alpha \mathrm{Tr}\left\{\partial_i \rho, \partial_j \rho\right\} + \partial_i \beta\left(\partial_j \beta\right)\mathrm{Tr}\rho^{-1} \\ & -\left(M - \frac{1}{2}\right)\left(\partial_i \alpha \partial_j \beta + \partial_j \alpha \partial_i \beta\right)\Big].\end{aligned} \tag{111}$$

Here $\partial_{i(j)}$ represents the partial derivative on $\theta_{i(j)}$. Obviously, the diagonal element of $\mathcal{F}$ reduces to the form in Eq. (101). For the cases that α is constant and β is dependent on the parameters, $\mathcal{F}_{ij}$ is in the form

$$\mathcal{F}_{ij} = \frac{1}{\alpha^2}\left[\alpha \mathrm{Tr}\left\{\partial_i \rho, \partial_j \rho\right\} + \partial_i \beta\left(\partial_j \beta\right)\mathrm{Tr}\rho^{-1}\right]. \tag{112}$$

Especially, for a two-level state, this equation reduces to

$$\mathcal{F}_{\mathrm{q},ij} = \mathrm{Tr}\left(\{\partial_i \rho, \partial_j \rho\}\right) + \frac{1}{4}\partial_i \mathcal{P}\left(\partial_j \mathcal{P}\right)\mathrm{Tr}\rho^{-1}. \tag{113}$$

This is the general basis-independent expression of quantum Fisher information matrix for *any* two-level state.

Conclusion.-In summary, we first reviewed the Lyapunov representation of the SLD operator and showed that this representation is available for both full and non-full rank density matrices. Furthermore, based on the Lyapunov representation, we gave a method for the calculation of SLD operator. This method is particularly useful for those states between whom the anti-commutators and their partial derivatives exhibits periodic properties.

As an application of the given method, we discussed a class of states, which have a linear relation with their squares. The corresponding analytical expressions of the SLD operator and QFI are provided via the method. Especially, we successfully provide the general basis-independent formulas of SLD and QFI for any two-level state. Furthermore, we discussed the white-noisy scenario of these states and extend our discussion to the block diagonal states. For multiparameter estimation, the quantum Fisher information matrix is also analytically given.

The calculation of SLD operator is an important topic in theoretical quantum metrology. We hope this work may draw attention in the community to studying more methods to obtain the SLD operators for various scenarios.

4.0.1 SLD operator for the states commuting with their partial derivative

In the following we give the detailed calculation of the SLD operator for the states commuting with their partial derivative. From the equation

$$L=-2\lim_{s\to\infty}\sum_{n=0}^{\infty}\sum_{m=0}^{n}\frac{(-s)^{n+1}}{(n+1)!}C_n^m\rho^m\left(\partial_\theta\rho\right)\rho^{n-m}, \tag{114}$$

one can see that when ρ commutes with $\partial_\theta\rho$, this equation can be rewritten into

$$L=-\lim_{s\to\infty}\sum_{n=0}^{\infty}\frac{(-2s)^{n+1}}{(n+1)!}\rho^n\left(\partial_\theta\rho\right). \tag{115}$$

Remind that the spectral decomposition of density matrix is in the form

$$\rho=\sum_{i=1}^{M}p_i|\psi_i\rangle\langle\psi_i|, \tag{116}$$

where p_i and $|\psi_i\rangle$ are ith eigenvalue and eigenstate of ρ, respectively. M is the dimension of ρ's support. In this representation, the SLD operator is

$$\begin{aligned}
L &= -\lim_{s\to\infty}\sum_{n=0}^{\infty}\frac{(-2s)^{n+1}}{(n+1)!}\sum_{i=1}^{M}p_i^n|\psi_i\rangle\langle\psi_i|\partial_\theta\rho\\
&= -\sum_{i=1}^{M}\frac{1}{p_i}\lim_{s\to\infty}\left(e^{-2sp_i}-1\right)|\psi_i\rangle\langle\psi_i|\partial_\theta\rho\\
&= \sum_{i=1}^{M}\frac{1}{p_i}|\psi_i\rangle\langle\psi_i|\partial_\theta\rho.
\end{aligned} \tag{117}$$

It is known that $\sum_{i=1}^{M} p_i^{-1}|\psi_i\rangle\langle\psi_i|$ is defined as the inverse matrix of ρ in the support. Thus, the SLD operator can be finally expressed by

$$L = \rho^{-1}\partial_\theta \rho, \tag{118}$$

where ρ^{-1} is the inverse matrix of ρ on the support.

4.0.2 Detailed calculation for the application

1. Calculation of SLD.-In the application, for any state satisfying the equation

$$\rho^2 = \alpha\rho - \beta, \tag{119}$$

one can obtain the following relation

$$\rho^{\circ}\left(\partial_\theta \rho\right) = \alpha \partial_\theta \rho + \left(\partial_\theta \alpha\right)\rho - \partial_\theta \beta. \tag{120}$$

Based on this equation and Eq. (119), the nth order term is in the form

$$\left(\rho^{\circ}\right)^n \partial_\theta \rho = \alpha^n \partial_\theta \rho + \left(\rho\partial_\theta \alpha - \partial_\theta \beta\right)\alpha^{n-1}\sum_{m=0}^{n-1}\left(\frac{2\rho}{\alpha}\right)^m. \tag{121}$$

Submitting this equation into the equation

$$L = -2\lim_{s\to\infty}\sum_{n=0}^{\infty}\frac{(-s)^{n+1}}{(n+1)!}\left(\rho^{\circ}\right)^n \partial_\theta \rho \tag{122}$$

and since $\alpha > 0$, the SLD operator can be expressed by

$$\begin{aligned} L &= \frac{2}{\alpha}\partial_\theta \rho - 2\left(\rho\partial_\theta \alpha - \partial_\theta \beta\right)\times \\ & \lim_{s\to\infty}\sum_{n=0}^{\infty}\frac{(-s)^{n+1}}{(n+1)!}\alpha^{n-1}\sum_{m=0}^{n-1}\left(\frac{2\rho}{\alpha}\right)^m. \end{aligned} \tag{123}$$

Utilizing the spectral decomposition of the density matrix, the term

$$\begin{aligned} & \lim_{s\to\infty}\sum_{n=0}^{\infty}\frac{(-s)^{n+1}}{(n+1)!}\alpha^{n-1}\sum_{m=0}^{n-1}\left(\frac{2\rho}{\alpha}\right)^m \\ = & \lim_{s\to\infty}\sum_{i=1}^{M}\sum_{n=0}^{\infty}\frac{(-s)^{n+1}}{(n+1)!}\alpha^{n-1}\sum_{m=0}^{n-1}\left(\frac{2}{\alpha}\right)^m p_i^m|\psi_i\rangle\langle\psi_i| \\ = & \lim_{s\to\infty}\sum_{i=1}^{M}\frac{\alpha}{\alpha-2p_i}\sum_{n=0}^{\infty}\frac{(-s)^{n+1}}{(n+1)!}\alpha^{n-1}\left[1-\left(\frac{2p_i}{\alpha}\right)^n\right]|\psi_i\rangle\langle\psi_i| \\ = & \lim_{s\to\infty}\sum_{i=1}^{M}\frac{1}{\alpha-2p_i}\left[\frac{1}{\alpha}\left(e^{-s\alpha}-1\right)-\frac{1}{2p_i}\left(e^{-2sp_i}-1\right)\right]|\psi_i\rangle\langle\psi_i|, \end{aligned} \tag{124}$$

where the equality $\sum_{m=0}^{n-1} x^m = (1-x^n)/(1-x)$ has been applied. Since all p_i here are larger than zero, above limitation reduces to the form

$$\frac{1}{2\alpha}\sum_{i=1}^{M} p_i^{-1}|\psi_i\rangle\langle\psi_i| = \frac{1}{2\alpha}\rho^{-1}, \tag{125}$$

where ρ^{-1} is the inverse matrix of ρ on the support. Finally, the SLD operator for any state satisfying Eq. (119) can be expressed by

$$L = \frac{1}{\alpha}\left[2\partial_\theta\rho + (\partial_\theta\beta)\,\rho^{-1} - \partial_\theta\alpha\right]. \tag{126}$$

2. Calculation of QFI.-Based on Eq. (126), the quantum Fisher information $F = \langle L^2\rangle$ can be directly calculated as

$$\begin{aligned} F &= \frac{1}{\alpha^2}\Big[4\langle(\partial_\theta\rho)^2\rangle - 4\,(\partial_\theta\alpha)\,\langle\partial_\theta\rho\rangle \\ &\quad + (\partial_\theta\beta)^2\,\mathrm{Tr}\left(\rho^{-1}\right) - 2M\,(\partial_\theta\alpha)\,(\partial_\theta\beta) + (\partial_\theta\alpha)^2\Big], \end{aligned} \tag{127}$$

where $\langle\{\partial_\theta\rho, \rho^{-1}\}\rangle = 2\mathrm{Tr}(\partial_\theta\rho) = 0$ has been applied. Denoting the purity of ρ as $\mathcal{P}$, i.e., $\mathcal{P} = \mathrm{Tr}\rho^2$, one can see that $\langle\partial_\theta\rho\rangle = \partial_\theta\mathcal{P}/2$, and

$$\langle(\partial_\theta\rho)^2\rangle = \frac{1}{2}\mathrm{Tr}\left[(\rho^{\mathrm{o}}\partial_\theta\rho)\,\partial_\theta\rho\right]. \tag{128}$$

Substituting Eq. (120) into above equation, there is

$$\langle(\partial_\theta\rho)^2\rangle = \frac{1}{2}\alpha\mathrm{Tr}\,(\partial_\theta\rho)^2 + \frac{1}{4}\,(\partial_\theta\alpha)\,(\partial_\theta\mathcal{P}). \tag{129}$$

Therefore, the quantum Fisher information can be expressed by

$$\begin{aligned} F &= \frac{1}{\alpha^2}\Big[2\alpha\mathrm{Tr}\,(\partial_\theta\rho)^2 - (\partial_\theta\alpha)\,(\partial_\theta\mathcal{P}) + (\partial_\theta\alpha)^2 \\ &\quad + (\partial_\theta\beta)^2\,\mathrm{Tr}\left(\rho^{-1}\right) - 2M\,(\partial_\theta\alpha)\,(\partial_\theta\beta)\Big]. \end{aligned} \tag{130}$$

Moreover, since $\mathcal{P} = \alpha - \beta$ here, above equation can finally be written as

$$\begin{aligned} F &= \frac{1}{\alpha^2}\Big[2\alpha\mathrm{Tr}\,(\partial_\theta\rho)^2 + (\partial_\theta\beta)^2\,\mathrm{Tr}\rho^{-1} \\ &\quad - (2M-1)\,(\partial_\theta\alpha)\,(\partial_\theta\beta)\Big]. \end{aligned} \tag{131}$$

3. Calculation of QFI matrix.- For the SLD operators in Eq. (126), the element of quantum Fisher information matrix is

$$\begin{aligned} \mathcal{F}_{ij} &= 2\mathrm{Tr}\left(\rho\,\{\partial_i\rho, \partial_j\rho\}\right) - \partial_j\alpha\partial_i\mathcal{P} - \partial_i\alpha\partial_j\mathcal{P} + \partial_i\alpha\partial_j\alpha \\ &\quad + (\partial_i\beta)\,(\partial_j\beta)\,\mathrm{Tr}\rho^{-1} - M\,(\partial_j\alpha\partial_i\beta + \partial_i\alpha\partial_j\beta). \end{aligned} \tag{132}$$

Since the first term

$$2\mathrm{Tr}\left(\rho\,\{\partial_i\rho, \partial_j\rho\}\right) = \alpha\mathrm{Tr}\,\{\partial_i\rho, \partial_j\rho\} + \frac{1}{2}\,(\partial_i\alpha\partial_j\mathcal{P} + \partial_j\alpha\partial_i\mathcal{P}), \tag{133}$$

and $\partial_i\mathcal{P} = \partial_i\alpha - \partial_i\beta$, $\mathcal{F}_{ij}$ can be simplified as

$$\begin{aligned} \mathcal{F}_{ij} &= \frac{1}{\alpha^2}\Big[\alpha\mathrm{Tr}\,\{\partial_i\rho, \partial_j\rho\} + \partial_i\beta\,(\partial_j\beta)\,\mathrm{Tr}\rho^{-1} \\ &\quad - \left(M - \frac{1}{2}\right)(\partial_i\alpha\partial_j\beta + \partial_j\alpha\partial_i\beta)\Big]. \end{aligned} \tag{134}$$

When $i = j$, above equation reduces to Eq. (131).

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