Optimal Measurements for Quantum Fidelity between Gaussian States

Changhun Oh, Changhyoup Lee, Leonardo Banchi, Su-Yong Lee, Carsten Rockstuhl, and Hyunseok Jeong

1 Center for Macroscopic Quantum Control, Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea
2 Institute of Theoretical Solid State Physics, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany
3 QOLS, Blackett Laboratory, Imperial College London, London SW7 2AZ, United Kingdom
4 School of Computational Sciences, Korea Institute for Advanced Study, Hoegi-ro 85, Dongdaemun-gu, Seoul 02455, Korea
5 Institute of Nanotechnology, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany

(Dated: January 11, 2019)

Quantum fidelity is a measure to quantify the closeness of two quantum states. In an operational sense, it is defined as the minimal overlap between the probability distributions of measurement outcomes and the minimum is taken over all possible positive-operator valued measures (POVMs). Quantum fidelity has been investigated in various scientific fields, but the identification of associated optimal measurements has often been overlooked despite its great importance for practical purposes. We find here the optimal POVMs for quantum fidelity between multi-mode Gaussian states in a closed analytical form. Our general finding is specified for selected single-mode Gaussian states of particular interest and we identify three types of optimal measurements: a number-resolving detection, a projection on the eigenbasis of operator $\hat{x}\hat{p} + \hat{p}\hat{x}$, and a quadrature detection, each of which is applied to distinct types of single-mode Gaussian states. We also show the equivalence between optimal measurements for quantum fidelity and those for quantum parameter estimation, enabling one to easily find the optimal measurements for displacement, phase, squeezing, and loss parameter estimations using Gaussian states.

I. INTRODUCTION

Quantification of the similarity of quantum states is of utmost importance in quantum information processing such as quantum error correction and quantum communication [1,2]. There are various measures of the closeness of two quantum states such as trace distance [3], quantum Chernoff bound [6,7], and quantum relative entropy [9]. Among the diverse measures, one of the most common measures is quantum fidelity [8]. Theoretically, it is defined as the minimal overlap of the probability distributions obtained by an optimal positive-operator valued measure (POVM) performed on two states. It has also been widely employed to verify how close actual states are to target states in experiments [10,11], practically assessing quantum information processing protocols such as quantum teleportation [14] [15] and quantum cloning [17,21]. It has been known that the quantum fidelity not only plays a crucial role in quantum parameter estimation [5,22], but also sets a bound for quantum hypothesis testing [23,24] and quantum Chernoff bound [6,7].

In general, quantum fidelity can be measured in two different, but equivalent ways in an experiment: One from the full knowledge of two quantum states, and the other from the probability distributions obtained by an optimal POVM. The first approach is experimentally very demanding due to the requirement of full state tomography, which necessitates a number of measurement

settings and computationally laborious post-processing for high-dimensional states. The second approach, on the other hand, requires one to measure just the probability distributions with an optimally chosen POVM. The latter is thus more preferred and illustrated in Fig. 1. The experimental evaluation of quantum fidelity is straightforwardly attainable as long as the optimal measurement is known and experimentally implementable. One could employ alternative approaches that have been proposed to directly measure quantum fidelity between two quantum states [23,27], but they are not universal to systems and even require an interaction between the states to be involved. Therefore, finding optimal measurements for quantum fidelity offers the simplest way to efficiently measure quantum fidelity.

One useful platform for quantum information processing is continuous variable systems, such as optical fields with indefinite photon numbers [8]. Especially, bosonic Gaussian states are practical resources because they are relatively less demanding to generate and manipulate in

\[ \hat{\rho}_0 \rightarrow \{ \hat{E}_x \} \]

\[ \hat{\rho}_1 \rightarrow \{ \hat{E}_x \} \]

FIG. 1. Quantum fidelity between two states $\hat{\rho}_0$ and $\hat{\rho}_1$ can be measured by the minimal overlap between the probability distributions $p_0(x)$ and $p_1(x)$, where the measurement outcomes $x$ are obtained by an optimally chosen POVM $\{ \hat{E}_x \}$. 

\[ p_0(x) \]

\[ p_1(x) \]
II. OPTIMAL POVM FOR QUANTUM FIDELITY

Let us consider two distinct probability distributions $p_0(x)$ and $p_1(x)$ with possible outcomes $x$. One notable measure of statistical distinguishability of these distributions is the Bhattacharyya coefficient [2, 12, 49],

$$
\left( \sum_x \sqrt{p_0(x)p_1(x)} \right)^2.
$$

This quantity takes the maximum value of 1 if and only if two given probability distributions are equivalent, i.e., $p_0(x) = p_1(x)$ for all possible outcomes $x$. This notion of distinguishability has been extended to quantum regime by minimizing over all possible POVMs $\{E_x\}$ performed to two given states $\hat{\rho}_0$ and $\hat{\rho}_1$ such that

$$
F(\hat{\rho}_0, \hat{\rho}_1) = \min_{\{E_x\}} \left( \sum_x \sqrt{p_0(x)p_1(x)} \right)^2.
$$

Here the probability distributions $p_i(x) = \text{Tr}[\hat{\rho}_i E_x]$ are obtained by performing a given POVM $\{E_x\}$, satisfying $\sum_x E_x = \mathbb{1}$, $E_x \geq 0$, on two states. The quantum fidelity reduces to a simpler form as [8]

$$
F(\hat{\rho}_0, \hat{\rho}_1) = \left( \text{Tr} \sqrt{\hat{\rho}_1^{-1/2} \hat{\rho}_0 \hat{\rho}_1^{-1/2}} \right)^2.
$$

From the definition of quantum fidelity, it is obvious that finding the optimal POVM is crucial to maximally distinguish two given quantum states. It has been found that the optimal measurements have to satisfy

$$
\hat{E}_x^{1/2}(\hat{\rho}_1^{1/2} - \mu_x \hat{\rho}_0^{1/2} \hat{W}^\dagger) = 0, \quad (1)
$$

and

$$
\text{Tr}(\hat{W} \hat{\rho}_0^{1/2} \hat{E}_x \hat{\rho}_1^{1/2}) \in \mathbb{R}, \quad (2)
$$

where $\hat{W}$ is a unitary operator satisfying $\hat{W} \hat{\rho}_0^{1/2} \hat{\rho}_1^{1/2} = \sqrt{\hat{\rho}_1^{-1/2} \hat{\rho}_0 \hat{\rho}_1^{1/2}}$ and $\mu_x$ is a constant [42]. In the case of full-rank states $\hat{\rho}_0$ and $\hat{\rho}_1$, the optimal measurement $\{\hat{E}_x\}$ is unique and consists of projections onto the eigenbasis of a Hermitian operator, written by

$$
\hat{M}(\hat{\rho}_0, \hat{\rho}_1) = \hat{\rho}_1^{-1/2} \sqrt{\hat{\rho}_0 \hat{\rho}_1^{1/2}} \hat{\rho}_1^{-1/2}. \quad (3)
$$

Thus, simplifying the operator $\hat{M}$ to find its eigenbasis is the central task to determine the optimal measurement. We note a simple property of the operator $\hat{M}$,

$$
\hat{M}(\hat{U} \hat{\rho}_0 \hat{U}^\dagger, \hat{U} \hat{\rho}_1 \hat{U}^\dagger) = \hat{U} \hat{M}(\hat{\rho}_0, \hat{\rho}_1) \hat{U}^\dagger, \quad (4)
$$

where $\hat{U}$ is a unitary operator.

III. OPTIMAL MEASUREMENTS FOR MULTI-MODE GAUSSIAN STATES

Let us consider $n$ bosonic modes described by quadrature operators $\hat{Q} \equiv (\hat{x}_1, \hat{p}_1, \hat{x}_2, \hat{p}_2, ..., \hat{x}_n, \hat{p}_n)$ which satisfy the canonical commutation relations [49]

$$
[\hat{Q}_j, \hat{Q}_k] = i\Omega_{jk}, \quad \Omega = \mathbb{1}_n \otimes \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},
$$

where $\mathbb{1}_n$ is the $n \times n$ identity matrix. Transformations of coordinates that preserve the canonical commutation relation can be represented by symplectic transformation matrices $S$ such that $S\Omega S^T = \Omega$.

Gaussian states are a special class of continuous variables states. They are defined as the states whose Wigner function is a Gaussian distribution [3, 28–31]. It is known that an arbitrary Gaussian state can be written in the Gibbs-exponential form as [11],

$$
\hat{\rho} = \hat{\rho}_G(G, u) \equiv \exp \left[ -\frac{1}{2} (\hat{Q} - u)^T G(\hat{Q} - u) \right] / Z_V, \quad (5)
$$

where $u = \text{Tr}[\hat{\rho} \hat{Q}]$ is the first moment vector, $G$ is the Gibbs matrix defined as $G = 2i\Omega \coth^{-1}(2V/\Omega)$ with the covariance matrix $V_{jk} = \text{Tr}[\hat{\rho}(\hat{Q}_j - u_j)(\hat{Q}_k - u_k)]/2$, and $Z_V = \text{det}(V + i\Omega/2)$ is a normalization factor which we omit throughout this work for convenience. The Gibbs-exponential form of Eq. [5] makes it easy to deal with the square root of density matrices.

After some algebra (see Appendix A for the detail), we find that the operator $\hat{M}$ takes the exponential form, written up to an unimportant normalization factor as

$$
\hat{M} \propto \hat{D}(u_1) \exp \left[ -\frac{1}{2} \hat{Q}^T G_M \hat{Q} - v_M^T \hat{Q} \right] \hat{D}^\dagger(u_1), \quad (6)
$$
where the matrix $G_M$ is the solution of the equation
\[
e^{i\Omega G_M}e^{\Omega G_1}e^{i\Omega G_M} = e^{i\Omega G_0},
\]
and $\hat{D}(u) = e^{-u^T\Omega Q}$ is the displacement operator, $v_M$ is a real vector, which can be explicitly expressed for particular cases as below. For equal covariance matrices $G_0 = G_1$, Eq. (7) has a trivial solution $G_M = 0$, allowing Eq. (6) to take a simpler form $\hat{M} = e^{v_M^T(Q-u_1)}$ where $v_M = (S^{-1})^T[\vec{\nu}/2]_i \tanh(\nu_i/2)\xi_i |v_0$. The eigenbasis of the operator $\hat{M}$ is thus that of a quadrature operator followed by a unitary operator $\hat{D}(u_1)$, which is also that of a quadrature operator. For $G_0 \neq G_1$, on the other hand, one can write
\[
\hat{M} = \hat{D}(u_1)\hat{\rho}_G [G_M, u_M] \hat{D}^\dagger(u_1)
\]
\[
\propto \hat{D}(u_1)\hat{D}(u_M) \exp \left[-\frac{1}{2}Q^T G_M Q \right] \hat{D}^\dagger(u_M)\hat{D}(u_1),
\]
where $v_M = G_M u_M$. The expression of $u_M$ is provided in Appendix A. Note that $v_M = 0$ for equal displacements ($u_0 = u_1$). When $G_0$ and $G_1$ are diagonalized by the same symplectic matrix $S$, all modes of the states can be completely decoupled to be a product of single-mode states by applying a unitary operation $\hat{U}_S$ corresponding to $S$. We thus investigate single-mode cases more intensively in the following section.

It is known that the Gibbs matrices are singular when symplectic eigenvalues of the covariance matrix are equal to 1/2 \[\text{[11]}\]. The continuity of the above expression enables the singular case to be treated as a limiting case. To this end, we replace the singular symplectic eigenvalues by 1/2 + $\epsilon$ with a small positive $\epsilon$, by which Eq. (7) is well-defined as
\[
e^{i\Omega G_M} = e^{-i\Omega G_1/2} e^{i\Omega G_0/2} e^{i\Omega G_1/2} e^{-i\Omega G_1/2}.
\]
In the limit $\epsilon \to 0$, the unique solution of the above expression gives rise to the optimal measurements. It is worth emphasizing that when rank-deficient states are involved, optimal measurements may not be unique.

IV. OPTIMAL MEASUREMENTS FOR SINGLE-MODE GAUSSIAN STATES

Any single-mode Gaussian state can be written as
\[
\hat{\rho} = \hat{D}(u)\hat{S}(\xi)\hat{\rho}_T \hat{S}^\dagger(\xi)\hat{D}^\dagger(u),
\]
where $\hat{\rho}_T = \sum_{n=0}^\infty \bar{n}^n/(\bar{n} + 1)^{n+1} |n\rangle \langle n|$ is a thermal state with the average number of thermal quanta $\bar{n} = (\coth(\nu/2) - 1)/2$, and $\hat{S}(\xi)$ is a squeezing operator with a squeezing parameter $\xi = re^{i\theta_s} \in \mathbb{C}$. Note that when $\theta_s = 0$, the Gibbs matrix is written as
\[
G = 2\coth^{-1}(2\bar{n} + 1) \begin{pmatrix} e^{2r} & 0 \\ 0 & e^{-2r} \end{pmatrix}.
\]

Let us consider two single-mode Gaussian states $\hat{\rho}_i$ ($i = 0, 1$) characterized by $u_i$ and $G_i$. With introducing a symplectic matrix $S$ that diagonalizes $G_1$ such that $G_1 = (S^{-1})^T D_1 S^{-1}$ with $D_1 = \nu S_2 \text{[11]}$, the two-Gaussian states can be written in a more compact way as
\[
\hat{\rho}_0 = \hat{D}(u_1)\hat{U}_S \hat{\rho}_G [S^T G_0 S, S^{-1}(u_0 - u_1)] \hat{U}_S^\dagger \hat{D}^\dagger(u_1),
\]
\[
\hat{\rho}_1 = \hat{D}(u_1)\hat{U}_S \hat{\rho}_G [D_1, 0] \hat{U}_S^\dagger \hat{D}^\dagger(u_1),
\]
where $\hat{U}_S$ is a unitary operator satisfying $\hat{U}_S Q \hat{U}_S^\dagger = S^{-1} \hat{Q}$. Thus, without loss of generality, the above symplectic transformation simplifies the initial problem of distinguishing between two arbitrary Gaussian states, so that we focus on distinguishing between one squeezed state and a thermal state, up to Gaussian unitary operations $\hat{D}(u_1)$ and $\hat{U}_S$. Furthermore, since thermal states are invariant under rotation, we can further simplify the problem to one between a thermal state and a squeezed state along $\hat{x}$ or $\hat{p}$ direction. In order to do that, we introduce a rotation operator $\hat{U}_O$ and a corresponding orthogonal matrix $O$ defined such that $\hat{U}_O Q \hat{U}_O^\dagger = O^{-1} \hat{Q}$ and $O^T(S^T G_0 S)O = D_0$, so that the two single-mode Gaussian states can be decomposed as
\[
\hat{\rho}_0 = \hat{D}(u_1)\hat{U}_S \hat{U}_O \hat{\rho}_G [D_0, v_0] \hat{U}_O^\dagger \hat{U}_S^\dagger \hat{D}^\dagger(u_1),
\]
\[
\hat{\rho}_1 = \hat{D}(u_1)\hat{U}_S \hat{U}_O \hat{\rho}_G [D_1, 0] \hat{U}_O^\dagger \hat{U}_S^\dagger \hat{D}^\dagger(u_1),
\]
where $v_0 = (SO)^{-1}(u_0 - u_1)$. Since the quantum fidelity is invariant under unitary operations by definition, without loss of generality, the matrix $\hat{M}$ for arbitrary two single-mode states can be expressed by $\hat{M}$ for a general Gaussian state that is squeezed by a squeezing parameter $\bar{\gamma}_0$ along $\hat{x}$ or $\hat{p}$ axis, $\hat{\sigma}_0 \equiv \hat{\rho}_G [D_0, v_0]$, and a thermal state, $\hat{\sigma}_1 \equiv \hat{\rho}_G [D_1, 0]$, under a transformation by $\hat{U} \equiv \hat{D}(u_1)\hat{U}_S \hat{U}_O$. Such simplification enables the matrix $\hat{M}$ to take the form of
\[
\hat{M} = \hat{U} \hat{\sigma}_0^{-1/2} \hat{\sigma}_1^{1/2} \hat{\sigma}_0^{-1/2} \hat{\sigma}_1^{1/2} \hat{U}^\dagger.
\]

Consider the case that $\hat{\rho}_0$ and $\hat{\rho}_1$ are full-rank states, i.e., $n_i \neq 0$. For the states with $G_0 = G_1$, one can easily show that $\hat{M} = e^{\nu_M^T(Q-u_1)}$ where $\nu_M = \tanh(\nu/2)(S^{-1})^T v_0$ and its eigenbasis is that of a quadrature operator, as in the multi-mode case. When $G_0 \neq G_1$, on the other hand, the operator of Eq. (10) can be expressed as
\[
\hat{M} = \hat{U} \hat{D}(u_M) \hat{\rho}_G [G_M, 0] \hat{D}^\dagger(u_M) \hat{U}^\dagger,
\]
for which Eqs. (6) and (8) are taken into account. Here, $G_M$ is obtained by solving Eq. (7) with $G_i$ replaced by $D_i$. Let us now simplify the matrix $\hat{M}$ of Eq. (11) and find its eigenbasis.

The effect of the first moments $u_0$ and $u_1$ is contained in the displacement vector $u_M$ whose full expression is shown in Appendix A. The crucial step to obtain the
optimal measurements is thus the diagonalization of the operator \( \hat{\rho}_G[M,0] \). From the form of \( \hat{\rho}_G[M,0] \), one can see that the eigenbasis of \( \hat{M} \) is classified by the signs of the eigenvalues, \( d_1 \) and \( d_2 \), of \( G_M \).

(i) If the signs of eigenvalues of \( G_M \) are the same \((d_1d_2 > 0)\), i.e., \( G_M \) is positive-definite or negative-definite, the eigenbasis of \( \hat{M} \) is that of the number operator \( \hat{n}_0 = (\hat{x}^2 + \hat{p}^2 - 1)/2 \) followed by Gaussian unitary operations including \( \hat{U} \) and a squeezing operation that makes the magnitude of eigenvalues same.

(ii) If the signs of eigenvalues are different \((d_1d_2 < 0)\), the eigenbasis of \( \hat{M} \) is that of \( \hat{x}\hat{p} + \hat{p}\hat{x} \) followed by Gaussian unitary operations.

(iii) If only one of the eigenvalues is zero \((d_1d_2 = 0)\), but \( d_1 + d_2 \neq 0 \), the eigenbasis of \( \hat{M} \) is that of a quadrature operator along a certain direction.

In summary, once the signs of the eigenvalues of \( G_M \) are known, the optimal measurement can be determined by the above classification. It can also be represented as a function of \( \bar{n}_0 \) and \( \bar{r}_0 \) for a given \( \bar{n}_1 \), as shown in Fig. 2, where the regions are distinguished by the spectrum of the matrix \( G_M \) (see Appendix B to get the spectrum).

It is worth discussing special cases, when each type is optimal. First, consider the case that \( \bar{n}_0 = \bar{n}_1 \) and \( \bar{r}_0 \) is also a thermal state, so that \( D_0 = \text{diag}(g_0, g_0) \), and \( G_0 \) and \( G_1 \) are diagonalized by the same symplectic transformation. In this case, Eq. (7) leads to \( \hat{\rho}_G[M,0] = \text{exp} \left( -\frac{1}{2}(g_1 - g_0)\hat{Q}^\dagger\hat{Q} \right) \), and the eigenbasis of \( \hat{M} \) is the number basis followed by \( \hat{U} \) and \( \hat{D}(u_M) \). Hence, type-(i) is optimal. This result can also be inferred by the fact that the same unitary operation diagonalizes both states into thermal states, and their eigenbasis is the number state. Second, consider the case when \( \bar{n}_0 = \bar{n}_1 \) and \( D_0 \) has distinct eigenvalues, i.e., \( \bar{\sigma}_0 \) is a squeezed state. It renders the signs of \( d_1 \) and \( d_2 \) being different regardless of \( \bar{r}_0 \) and \( \bar{n}_0 = \bar{n}_1 \), i.e., type-(ii) is optimal. Third, consider the case that either of \( d_1 \) or \( d_2 \) is zero. When \( d_2 = 0 \), Eq. (7) has a solution only when

\[
e^{2r} = \frac{n_0(n_0 + 1)(2n_1 + 1)}{n_1(n_1 + 1)(2n_0 + 1)},
\]

and the operator \( \hat{M} \) is simply written as \( \hat{M} = UD(u_M) \exp \left[ -\frac{1}{2} \hat{x}^2 \right] D^\dagger(u_M)U \). Thus, type-(iii) with the quadrature measurement of \( \hat{x} \) is optimal, reproducing the same results in Ref. 33. Similarly, when \( d_1 = 0 \), Eq. (7) has a solution only when

\[
e^{2r} = \frac{n_1(n_1 + 1)(2n_0 + 1)}{n_0(n_0 + 1)(2n_1 + 1)}.
\]

and type-(iii) with the quadrature measurement of \( \hat{p} \) is optimal.

Now consider the case of rank-deficient Gaussian states. Since all rank-deficient Gaussian states are a pure state and the inverse of a pure state does not exist, \( \hat{M} \) of Eq. (7) needs to be treated with care. Assuming \( \hat{\rho}_1 \) is a pure state without loss of generality, one can write the operator \( \hat{M} \) of Eq. (5) with projecting \( \hat{\rho}_0 \) and \( \hat{\rho}_1 \) into the support of \( \hat{\rho}_1 \), where the inverse can be defined, as

\[
\hat{M} = \hat{\rho}_1^{-1/2} \sqrt{\hat{\rho}_1^{1/2} \hat{\Pi}_1 \hat{\rho}_0 \hat{\Pi}_1^{1/2} \hat{\rho}_1^{-1/2}},
\]

where \( \hat{\Pi}_1 \) is the projector onto the support of \( \hat{\rho}_1 \). For \( \hat{\rho}_1 = |\psi_1\rangle \langle \psi_1 | \) and consequently \( \hat{\Pi}_1 = |\psi_1\rangle \langle \psi_1 | \), it is therefore clear that \( \hat{M} \propto |\psi_1\rangle \langle \psi_1 | \). The same result can also be derived by considering pure states as a limiting case of zero-temperature (see Appendix C for the detail). Thus, an optimal POVM set is \( \{|\psi_1\rangle \langle \psi_1 |, 1 - |\psi_1\rangle \langle \psi_1 | \} \), and can be implemented by applying the Gaussian unitary transformation \( S(\xi_1)D(\alpha_1) \) that transforms \( \hat{\rho}_1 \) to a vacuum state followed by performing on/off detection. It is worth emphasizing again that the optimal measurement offered by the operator \( \hat{M} \) when pure states are involved is not unique, so that the suggested setup is merely one of the optimal measurements, all satisfying the conditions of Eqs. (1) and (2).

V. OPTIMAL POVM FOR QUANTUM FISHER INFORMATION

Quantum parameter estimation is an informational task to estimate an unknown parameter \( \theta \) of interest by using quantum systems [5]. In a standard scenario of quantum parameter estimation, \( N \) independent copies of quantum states that contain information about the unknown parameter are measured by a POVM, and the estimation is performed by manipulating the measurement data. The ultimate precision bound of the estimation
is governed by quantum Cramér-Rao inequality, stating that the mean square error of any unbiased estimator is lower-bounded by the inverse of quantum Fisher information multiplied by the number of copies $N$. Thus, quantum Fisher information is the most crucial quantity which determines the ultimate precision of estimation [22], which is written as

$$H(\theta) = \text{Tr}[\dot{\rho}_\theta \hat{L}_\theta^2],$$

where $\hat{L}_\theta$ is the symmetric logarithmic derivative (SLD) operator satisfying $\partial \rho / \partial \theta = \dot{\rho}_\theta \hat{L}_\theta + \hat{L}_\theta \dot{\rho}_\theta$.

The quantum Fisher information $H(\theta)$ can be written in terms of quantum fidelity $F(\rho_\theta, \rho_{\theta+d\theta})$ as

$$H(\theta) = 4[1 - F(\rho_\theta, \rho_{\theta+d\theta})].$$

It implies that quantum parameter estimation is related to distinguishing two infinitesimally close states $\rho_\theta$ and $\rho_{\theta+d\theta}$. Indeed, similar to the quantum fidelity, quantum Fisher information is defined as the maximal classical information multiplied by the number of copies over all possible POVMs, and the optimal POVM $\{\hat{E}_x\}$ has to satisfy

$$\hat{E}_x^{1/2} (\hat{H}_\theta^{1/2} - \lambda_x \hat{L}_\theta \hat{H}_\theta^{1/2}) = 0,$$

$$\text{Tr}[\hat{E}_x \dot{\rho}_\theta \hat{L}_\theta] \in \mathbb{R}. \quad (15)$$

It is known that the projection onto the eigenbasis of $\hat{L}_\theta$ is the optimal measurement for quantum Fisher information [15]. This means that the SLD operator plays the same role as the operator $\hat{M}$ for quantum fidelity. We prove that the above conditions are indeed equivalent to the conditions of Eqs. [1] and [2], resulting in the relation $\hat{M}(\rho_\theta, \rho_{\theta+d\theta}) \approx 1 + \hat{L}_\theta d\theta/2$ for infinitesimal $d\theta$ (see Appendix D for the proof). This indicates that the optimal POVM for quantum fidelity between $\rho_\theta$ and $\rho_{\theta+d\theta}$ offers the optimal measurement for quantum parameter estimation that reaches the quantum Fisher information.

Especially for Gaussian states, since the matrix $G_M$ and the vector $v_M$ are infinitesimal for $\rho_\theta$ and $\rho_{\theta+d\theta}$ and thus

$$\hat{M}(\rho_\theta, \rho_{\theta+d\theta}) \approx 1 - \hat{D}(u_\theta) (\hat{Q}^T G_M \hat{Q} - v_M^T \hat{Q}) \hat{D}^T(u_\theta),$$

the SLD operator is simply written as

$$\hat{L}_\theta d\theta = -\hat{D}(u_\theta) (\hat{Q}^T G_M \hat{Q} - 2v_M^T \hat{Q}) \hat{D}^T(u_\theta) + \nu,$$

where $\nu = \text{Tr}[\hat{D}^T(u_\theta) \dot{\rho}_\theta \hat{D}(u_\theta) \hat{Q}^T G_M \hat{Q}]$ can be determined from $\text{Tr}[\dot{\rho}_\theta \hat{L}_\theta] = 0$. Taking an infinitesimal limit in Eq. [7], one can show that the optimal measurement (for an infinitesimal $d\theta$) is the solution of

$$4V_\theta G_M V_\theta + \Omega G_M \Omega + 2d\theta \frac{\partial V_\theta}{\partial \theta} = 0,$$

and is formally written in a basis-independent form as

$$G_M = i\Omega \sum_{m=0}^{\infty} W_\theta^{-m-1} \frac{\partial W_\theta}{\partial \theta} W_\theta^{-m-1} d\theta. \quad (18)$$

and $v_M = V_\theta^{-1} (\partial u_\theta / \partial \theta) d\theta/2$. Here $u_\theta$ and $V_\theta$ are the first moment vector and the covariance matrix of $\dot{\theta}$, respectively, and $W_\theta = -2V_\theta^{1/2}$. The derivation of $G_M$ and $v_M$ is provided in Appendix E. The relation of $\hat{M}$ and the SLD operator $\hat{L}_\theta$ and the expression of $G_M$ and $v_M$ enable to find SLD operators directly from the operator $\hat{M}$. Finally, from the SLD operator one can easily derive the expression of the quantum Fisher information:

$$H(\theta) = -\text{Tr} \left[ \frac{\partial V_\theta}{\partial \theta} G_M + \frac{\partial u_\theta}{\partial \theta} V_\theta^{-1} \frac{\partial u_\theta}{\partial \theta} \right]. \quad (19)$$

The derivation is provided in Appendix D. As a remark, note that the expressions of $G_M$, $v_M$ and quantum Fisher information are equivalent to those found in Refs. [31] and [50] but our derivation based on quantum fidelity is significantly simpler and straightforward. Furthermore, by replacing a single-parameter $\theta$ by a multi-parameter $\theta$ and defining the SLD operators $\hat{L}_\theta$, by $\partial \rho_\theta / \partial \theta_i = \dot{\rho}_\theta \hat{L}_{\theta_i} + \hat{L}_{\theta_i} \dot{\rho}_\theta$, the expression of quantum Fisher information matrix $H_{ij}(\theta) = \text{Tr}[\dot{\rho}_\theta \hat{L}_{\theta_i} \hat{L}_{\theta_j}]$ can be easily derived by using a similar method [51, 52].

In the following subsections, we find optimal measurements for displacement, phase, squeezing, and loss parameter estimation in relation to our results for quantum fidelity.

### A. Displacement parameter estimation

For a single-mode Gaussian probe state $\hat{\rho}$, the displacement operation $\hat{D}(\alpha)$ only changes the first moment while keeping the second moments fixed:

$$u \rightarrow u + (\alpha, 0)^T, \quad V \rightarrow V,$$

where $\alpha \in \mathbb{R}$ is assumed without loss of generality. Therefore, the first moment vectors and the covariance matrices of $\rho_\alpha$ and $\rho_{\alpha+d\alpha}$ are related as

$$u_{\alpha+d\alpha} = u_\alpha + (d\alpha, 0)^T, \quad V_{\alpha+d\alpha} = V_\alpha,$$

respectively. Since the covariance matrix is invariant, one can immediately see that the optimal measurement for quantum fidelity between $\rho_\alpha$ and $\rho_{\alpha+d\alpha}$ is type-(iii), so that the optimal measurement for estimation of the displacement parameter $\alpha$ is also type-(iii). Explicitly, using the expression of $v_M$, one can easily obtain the SLD operator and quantum Fisher information:

$$\hat{L}_\alpha = \hat{D}(u_\alpha) [V_{\alpha}^{-1}]_{11} \hat{D}^T(u_\alpha) = [V_{\alpha}^{-1}]_{11} (\hat{x} - u_\alpha),$$

$$H(\alpha) = [V_{\alpha}^{-1}]_{11}. \quad$$

### B. Phase parameter estimation

Let us consider a single-mode Gaussian probe state $\hat{\rho}$ that undergoes a phase shifter $\hat{R}(\theta)$ with a phase parameter $\theta$ to be estimated. Since the displacement operation...
performed to the probe state does not change the type of optimal measurement, we focus on only the state with zero-mean for simplicity, i.e.,

\[ \hat{\rho} \to \hat{\rho}_0 = \hat{R}(\theta) \hat{S}(\xi) \hat{\rho}_T \hat{S}^\dagger(\xi) \hat{R}^\dagger(\theta), \]

where \( \hat{R}(\theta) = e^{-i\theta \hat{Q}^\dagger \hat{Q}/2} \) is a rotation operator. The relevant states under investigation are \( \hat{\rho}_0 \) and \( \hat{\rho}_{0+\delta} \), but the full expressions with an arbitrary angle \( \theta \) get involved without altering the type of optimal measurement. We thus consider the states \( \hat{\rho}_0 \) and \( \hat{\rho}_{0+\delta} \) at \( \theta = 0 \), and assume \( \hat{\rho}_0 \) to be the \( p \)-squeezed thermal state and \( \hat{\rho}_{0+\delta} = \lim_{\delta \to 0} \hat{\rho}_0 \) is a rotated squeezed thermal state without loss of generality. Let us proceed with \( \hat{\rho}_0 \) and \( \hat{\rho}_0 \) first, and then take the limit \( \theta \to 0 \) at the end. The covariance matrices of \( \hat{\rho}_0 \) and \( \hat{\rho}_0 \) are respectively written as

\[
V_0 \propto \begin{pmatrix}
 e^{2r} & 0 \\
 0 & e^{-2r}
\end{pmatrix},
\]

\[
V_\theta \propto \begin{pmatrix}
 \cosh 2r + \cos 2\theta \sinh 2r & \sinh 2r \sin 2\theta \\
 \sinh 2r \sin 2\theta & \cosh 2r - \cos 2\theta \sinh 2r
\end{pmatrix},
\]

where the proportionality becomes an equality when adding a pre-factor of \( (2n + 1)/2 \). Since the average numbers of thermal quanta are the same between the above two states, one may immediately infer that the optimal measurement is type-(ii). Let us see if this is indeed the case. For the states \( \hat{\rho}_0 \) and \( \hat{\rho}_0 \), it can be shown that

\[ G_M = A \begin{pmatrix}
 -\sin \theta & \cos \theta \\
 \cos \theta & \sin \theta
\end{pmatrix}, \]

where a constant \( A \) is given such that \( \cos A = (4n^2 + 4n + 2)/(4n^2 + 2n + 1)(4n^2 + 6n + 3) + (2n + 1)^2 \cos 2\theta + 2(2n + 1)^2 \cosh 2r \sin 2\theta \) \( 1/2 \). The matrix \( G_M \) satisfies Eq. \[[10],\] and indicates that the optimal measurement for quantum fidelity between \( \hat{\rho}_0 \) and \( \hat{\rho}_0 \) is type-(iii). To apply this to quantum Fisher information, we take the limit \( \theta \to 0 \), resulting in

\[ G_M = \frac{(2n + 1) \sinh 2r}{2n^2 + 2n + 1} \begin{pmatrix}
 0 & 1 \\
 1 & 0
\end{pmatrix}. \]

Hence,

\[ \hat{M} = 1 - \frac{(2n + 1) \sinh 2r}{2(2n^2 + 2n + 1)} d\theta (\hat{x}\hat{p} + \hat{p}\hat{x}) = 1 + \hat{L}_\theta d\theta/2, \]

(20)

where \( \hat{L}_\theta \) is the SLD operator in phase estimation \[10]. This reveals that the operators \( \hat{M} \) and \( \hat{L}_\theta \) have the common eigenbasis. It is now clear that the optimal measurement for phase parameter estimation is type-(ii), as also recently found via the SLD operator in Ref. \[10\]. Also note that while the above result is derived by an explicit optimal measurement for quantum fidelity, the same result can be easily derived by using Eq. \[18\].

C. Squeezing parameter estimation

We consider squeezing parameter estimation with an arbitrary Gaussian state as a probe state,

\[ \hat{\rho} \to \hat{\rho}_c = \hat{S}(\xi) \hat{D}(u) \hat{S}(\xi) \hat{\rho}_T \hat{S}^\dagger(\xi) \hat{D}^\dagger(u) \hat{S}^\dagger(\xi), \]

where we assume \( \xi = s \in \mathbb{R} \) for simplicity. It corresponds to the case when we estimate the strength of squeezing parameter along the \( \hat{p} \) axis. Since that \( \hat{\rho}_c \) and \( \hat{\rho}_{c+\delta} \) have different squeezing parameters under the same average number of thermal quanta, just like the case of phase estimation, the optimal measurement is type-(ii). Indeed, one can derive the SLD operator using Eq. \[18\],

\[
\hat{L}_\theta = \frac{2n + 1}{2n^2 + 2n + 1} \hat{D}(u) \hat{Q}^\dagger \\
\times \text{diag}(-e^{2s}(\cosh 2r + \cos \theta_s \sin 2r)),
\]

\[ e^{-2s}(\cosh 2r - \cos \theta_s \sin 2r) \hat{Q} \hat{D}^\dagger(u) + \nu, \]

which is clearly type-(ii) because the signs of eigenvalues of \( G_M \) are different. Quantum Fisher information can also be easily obtained

\[ H(s) = \frac{(2n + 1)^2}{2n^2 + 2n + 1} (e^{-4s}(\cosh 2r - \cos \theta_s \sin 2r)^2 + e^{4s}(\cosh 2r + \cos \theta_s \sin 2r)^2). \]

D. Loss parameter estimation

Consider a single-mode Gaussian probe state \( \hat{\rho} \) that undergoes a phase-insensitive loss channel, and the dynamics of the state is described by the quantum master equation as

\[
\frac{d\hat{\rho}}{dt} = \gamma \hat{a}^{\dagger} \hat{a} \hat{\rho} - \hat{\rho} \hat{a}^{\dagger} \hat{a}, \quad (21)
\]

where \( \hat{a} = (\hat{x} + i\hat{p})/\sqrt{2} \) is the annihilation operator and \( \gamma \) is the loss rate to be estimated. The solution of the above differential equation for a single-mode Gaussian probe state can be given in terms of the first moment vector and the covariance matrix as \[28\].

\[ u_0 \to u_t = e^{-\gamma t/2} u_0, \]

\[ V_0 \to V_t = e^{-\gamma t} V_0 (1 + (1 - e^{-\gamma t})\mathbb{1}_2)/2. \]

Note that the dynamics of the covariance matrix does not change the symplectic transformation diagonalizing the covariance matrix. It is thus clear that the optimal parameter for quantum fidelity between \( \hat{\rho}_c \) and \( \hat{\rho}_{c+\delta} \) is type-(i), so the optimal measurement for loss parameter estimation is also type-(i). Specifically, one can easily obtain that

\[ G_M = A \text{diag}(\sin^4 \phi - e^{-2r} \cos^4 \phi, \sin^4 \phi - e^{-2r} \cos^4 \phi) t d\gamma, \]

\[ H(\gamma) = \frac{\cos^2 \phi (1 - 2 \sin^2 \phi \cos^2 \phi) \sin^2 r}{\sin^2 \phi (1 + 2 \sin^2 \phi \cos^2 \phi \sin^2 r)} t^2. \]
where we have defined $\cos^2 \phi = e^{-\gamma t}$ and $A = 4/(\sin^2 \phi (-2 \sinh^2 \phi \cos \phi + \cosh 2\phi + 7))$ and zero-mean input states are assumed for simplicity. The matrix $G_M$ is obviously negative-definite; thus it corresponds to type-(i). This reproduces the result in Refs. 45 and 47. The optimality of type-(i) holds also for other phase-insensitive loss parameter estimations as long as the symplectic matrix that diagonalizes the covariance matrix does not change.

VI. CONCLUSIONS

We have found the optimal POVMs for quantum fidelity between two multi-mode Gaussian states in a closed analytical form. The full generality of our result has allowed us to further elaborate on the case of single-mode Gaussian states in depth. We have demonstrated that there exist only three different types of optimal measurements, along with Gaussian operations including a unitary operation $U$ that transforms $\hat{\rho}_0$ and $\hat{\rho}_1$ to squeezed states along either $\hat{x}$ or $\hat{p}$ and a thermal state, respectively, and $D(u_M)$ that arises due to the difference in displacements. The number counting measurement is optimal when the covariance matrices of the states are diagonalized by the same symplectic matrix. While the projection onto the eigenbasis of $\hat{x} + \hat{p}$ is optimal when the number of thermal quanta of two quantum states is the same. Optimality of quadrature measurement holds for two cases: when the covariance matrices are the same or when two Gaussian states satisfy the conditions of Eqs. (12) and (13). We have also applied our results to various parameter estimation scenarios in Gaussian metrology. We have proven the equivalence between the optimal measurement for quantum fidelity and that for quantum Fisher information, enabling to readily derive optimal measurements for quantum parameter estimation. We expect our approach to pave the way to further investigate the quantum parameter estimation.

While the number resolving detection and the quadrature measurement are experimentally feasible with current technology, the measurement setup projecting onto the eigenbasis of the POVM $\hat{x} + \hat{p}$ is not yet known. We hope that an appropriate measurement setup will be constructed in the near future in response to the significance arising from this work and the recent study for phase estimation [46]. We also leave further classification of optimal measurements for multi-mode Gaussian states as future work, which can be made straightforwardly from our results at the expense of increased complexity.

ACKNOWLEDGMENTS

C.O. and H.J. are supported by a National Research Foundation of Korea grant funded by the Korea government (MSIP) (No. 2010-0018295) and by the KIST Institutional Program (No. 2E27800-18-P043). L.B. was supported by the UK EPSRC grant EP/K034480/1. S.-Y.L. is supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (No. 2018R1D1A1B07048633).

APPENDIX

Appendix A: Simplification of the operator $\hat{M}$

Here, we simplify the operator $\hat{M} = \hat{p}_1^{-1/2} \sqrt{\hat{p}_1^{-1/2} \hat{p}_0 \hat{p}_1^{-1/2}}$ with $\hat{\rho}_0 = e^{-(q-u)^T G_0 (q-u)/2}$ and $\hat{\rho}_1 = e^{-\hat{Q}^T \hat{G}_1 \hat{Q}}$. Note that $e^{i \mu \hat{Q}} e^{-\hat{Q}^T \hat{G}_1 \hat{Q}/2} \propto e^{-(\hat{Q}-u)^T G_1 (\hat{Q}-u)/2}$ with $u = (e^{-i \Omega G_1} - 1)^{-1} \mu$, which is frequently used in this section. Simplifying $\hat{\rho}_0$ in the following way,

$$\hat{\rho}_0 = e^{i \mu_0 \hat{Q}} e^{-\hat{Q}^T \hat{G}_0 \hat{Q}} e^{-(\hat{Q}-u_0)^T G_1 (\hat{Q}-u_0)/2} \propto e^{i \mu_0 \hat{Q}} e^{-\hat{Q}^T \hat{G}_0 \hat{Q}} e^{\hat{Q}^T \hat{G}_1 \hat{Q}/2},$$

with $l_0 = (e^{-i \Omega G_0} - 1) u_0$, one can have

$$\hat{K} = \hat{p}_1^{-1/2} \hat{p}_0 \hat{p}_1^{-1/2} \propto e^{-\hat{Q}^T \hat{G}_1 \hat{Q}} e^{i \mu_0 \hat{Q}} e^{-\hat{Q}^T \hat{G}_0 \hat{Q}} e^{\hat{Q}^T \hat{G}_1 \hat{Q}/2}.$$

Bringing all the displacement operators to the left side, one can further simplify the matrix $\hat{K}$ as

$$\hat{K} \propto e^{i \mu \hat{Q}} e^{\hat{Q}^T \hat{G}_K \hat{Q}/2},$$

where $k = e^{-i \Omega G_1/2} l_0$ and

$$e^{-\hat{Q}^T \hat{G}_K \hat{Q}} = e^{-\hat{Q}^T \hat{G}_1 \hat{Q}} e^{-\hat{Q}^T \hat{G}_0 \hat{Q}} e^{-\hat{Q}^T \hat{G}_1 \hat{Q}/2}.$$

Defining $u_K$ as $(e^{-i \Omega G_1} - 1) u_K \equiv k$, the operator $\hat{K}$ takes a Gibbs-exponential form, written as

$$\hat{K} \propto e^{-(\hat{Q}-u_K)^T G_K (\hat{Q}-u_K)/2},$$

where $u_K$ is a real vector. The operator $\hat{M} = \hat{p}_1^{-1/2} \sqrt{K} \hat{p}_1^{-1/2}$ can thus be written as

$$\hat{M} \propto e^{\hat{Q}^T \hat{G}_1 \hat{Q}} e^{i \mu \hat{Q}} e^{\hat{Q}^T \hat{G}_0 \hat{Q}} e^{\hat{Q}^T \hat{G}_1 \hat{Q}/2},$$

where $l_1 = (e^{-i \Omega G_1/2} - 1) u_K$. Again, we bring all the displacement operators to the left side,

$$\hat{\hat{M}} \propto e^{i \mu \hat{Q}} e^{\hat{Q}^T \hat{G}_M \hat{Q}/2},$$

where $m = e^{i \Omega G_1/2} l_1$ and

$$e^{\hat{Q}^T \hat{G}_M \hat{Q}} = e^{\hat{Q}^T \hat{G}_1 \hat{Q}} e^{\hat{Q}^T \hat{G}_0 \hat{Q}} e^{\hat{Q}^T \hat{G}_1 \hat{Q}/2}.$$

When $G_M = 0$, corresponding to the case that $G_0 = G_1$, we obtain $\hat{\hat{M}} \propto e^{i \mu \hat{Q}}$, where $m = \ldots$
\( e^{i\Omega G_1/2} \) is a pure imaginary vector. Especially if \( G_0 = G_1 = \oplus_{n=1}^{\infty} \nu_4 \), \( m = -i[\oplus_{n=1}^{\infty} \tanh(\nu_i/2)] \Omega \nu_0 \). If \( G_0 = G_1 \) are not diagonal, we introduce a symplectic transformation that diagonalizes the Gibbs matrices, \( G_0 = G_1 = (S^{-1})^T D S^{-1} \), equivalently, \( e^{-Q^T G_0 Q/2} = \hat{U}_S e^{-Q^T D Q/2} \hat{U}_S^\dagger \) where \( \hat{U}_S Q \hat{U}_S^\dagger = S^{-1} \hat{Q} \). As a consequence,

\[
\hat{M} \propto \hat{U}_S e^{i[\oplus_{n=1}^{\infty} \tanh(\nu_i/2)] \Omega \nu_0} \hat{U}_S^\dagger = e^{i[\oplus_{n=1}^{\infty} \tanh(\nu_i/2)] \Omega \nu_0} S^{-1} \hat{Q},
\]

where we have used Eq. (4).

When \( G_M \neq 0 \), we can conclude that the matrix \( \hat{M} \) can be always written in the Gibbs-exponential form,

\[
\hat{M} \propto e^{-(\hat{Q} - u_M)^T G_M (\hat{Q} - u_M)/2},
\]

where \( u_M = (e^{-iG_M} - I)^{-1} m \).

Therefore, we can rewrite \( \hat{M} \) as

\[
\hat{M} \propto \exp \left[ -\frac{1}{2} \hat{Q}^T G_M \hat{Q} - v_M^T \hat{Q} \right].
\]

Here, \( v_M = 0 \) if \( \nu_0 = 0 \), \( v_M = G_M u_M \) if \( G_M \neq G_1 \), and \( G_M = 0 \) and \( v_M = im \) if \( G_0 = G_1 \). From Eqs. (A1) and (A2), it is clear that \( G_M \) is the solution of

\[
e^{i\Omega G_M} e^{i\Omega G_1} e^{i\Omega G} = e^{i\Omega G_0}.
\]

The vector \( u_M \) is written as

\[
u_M = \left( e^{-i\Omega G_M} - I \right)^{-1} e^{i\Omega G_1/2} \left( e^{-i\Omega G_K/2} - 1 \right) \times \left( e^{-i\Omega G_K} - I \right)^{-1} e^{-i\Omega G_1/2} \left( e^{-i\Omega G_0} - I \right) \nu_0.
\]

Appendix B: Full equation for \( d_1 \) and \( d_2 \).

We simplify Eq. (7) for the single-mode case, replacing \( G_0 \) by \( D_0 = \text{diag} (d_1, d_2) \) and \( G_1 \) by \( D_1 = 2 \coth(2\nu_1 + 1) \).

Expanding the matrices by Pauli matrices and using

\[
\cos g_1 = \frac{2\bar{n}_1 + 1}{2\bar{n}_1 (\bar{n} + 1)}, \quad \sinh g_1 = \frac{\bar{n}_1^2 + 2\bar{n}_1 + 1}{2\bar{n}_1 (\bar{n} + 1)},
\]

the left hand side of Eq. (7) is written as

\[
L_0 \hat{1}_2 + L_1 \hat{\sigma}_x + L_2 \hat{\sigma}_y,
\]

where

\[
L_0 = (d_1 + d_2)^2 \frac{2\bar{n}_1 + 1}{2\bar{n}_1 (\bar{n} + 1)} \operatorname{sinh} 2\sqrt{d_1 d_2}, \quad L_1 = -i (d_1 - d_2) \left( \frac{2\bar{n}_1^2 + 2\bar{n}_1 + 1}{2\bar{n}_1 (\bar{n} + 1)} - \frac{2\bar{n}_1 + 1}{4d_1 d_2} \right), \quad L_2 = \frac{2\bar{n}_1^2 + 2\bar{n}_1 + 1}{2\bar{n}_1 (\bar{n} + 1)} \left( \frac{d_1 + d_2}{2\bar{n}_1 (\bar{n} + 1)} \right)^2 \operatorname{sinh} 2\sqrt{d_1 d_2}.
\]

Appendix C: Pure state limit

Consider a single-mode state with a diagonal covariance matrix of

\[
V = \begin{pmatrix}
\frac{1}{2} + \epsilon & 0 \\
0 & \frac{1}{2} + \epsilon
\end{pmatrix}.
\]

Such state is pure in the limit of \( \epsilon \to 0 \). The analysis can be trivially extended to a non-diagonal case by adding a squeezing operation \( SVS^T \). One can find that

\[
e^{i\Omega G} = \frac{W - \hat{1}}{W + \hat{1}} = \left( \frac{1}{\epsilon} + 1 \right) P + \epsilon Q + O(\epsilon^2), \quad e^{-i\Omega G} = \frac{W + \hat{1}}{W - \hat{1}} = \left( \frac{1}{\epsilon} + 1 \right) Q + \epsilon P + O(\epsilon^2).
\]
where $W = -2Vi\Omega$ and

$$P = \frac{1}{2} \begin{pmatrix} 1 - i & i \\ i & 1 \end{pmatrix}, \quad Q = \mathbb{1} - P.$$  

Note $P^2 = P$ and $Q^2 = Q$, so they are projection operators. The Gibbs matrix of the operator $M$ satisfies

$$e^{i\Omega G_1} = e^{-i\Omega G_M} e^{i\Omega G_0} e^{-i\Omega G_M}.$$  \hspace{1cm} (C3) 

In the limit of that $G_1$ corresponds to the pure state $|\psi_1\rangle \langle \psi_1|$, we use Eqs. (C1) to write $e^{i\Omega G_1} \approx \frac{P}{e}$. Then a possible solution for $e^{-i\Omega G_M}$ is $e^{-i\Omega G_M} \approx \alpha P$ because the above equation becomes $\alpha^2 P e^{i\Omega G_0} P = e^{i\Omega G_1} \approx \frac{P}{e}$, which is approximately true for some $\alpha$. Indeed, for any state $\rho_0$ with non-zero overlap with $\hat{\rho}_1$, it is $P e^{i\Omega G_1} P \propto P$. Therefore, $e^{-i\Omega G_M} \propto P \propto e^{i\Omega G_1}$, namely $M \propto 1 - |\psi_1\rangle \langle \psi_1|$, where all approximations in the above equations refer to corrections that disappear in the limit of $\epsilon \to 0$. The operator $M$ implies that the measurement $\{|\psi_1\rangle \langle \psi_1|, 1 - |\psi_1\rangle \langle \psi_1|\}$ is optimal.

**Appendix D: The relation between optimal measurements for quantum fidelity and quantum Fisher information**

Let $\hat{\rho}_0 = \hat{\rho} + d\hat{\rho}$ and $\hat{\rho}_1 = \hat{\rho}$. For simplicity we assume $\hat{\rho}$ is a full-rank state, which implies that $\rho_0$ and $\rho_1$ are full-rank states. Let $\sqrt{\hat{\rho}_1^{1/2} \rho_0 \hat{\rho}_1^{1/2}} = \hat{\rho} + X$ where $X \propto d\hat{\rho}$. Taking the square, we get

$$\rho_0^{1/2} \hat{\rho}_0^{1/2} = \rho_0^{1/2} + \rho_0^{1/2} d\hat{\rho} \hat{\rho}_0^{1/2} = \rho_0^{1/2} + \rho_0^{1/2} X + X \hat{\rho} \hat{\rho}_0^{1/2},$$  

leading to $\rho_0^{1/2} d\hat{\rho} \hat{\rho}_0^{1/2} = \rho_0^{1/2} + X \hat{\rho} \hat{\rho}_0^{1/2}$. For $\hat{\rho} = \sum_k p_k |k\rangle \langle k|$ with $\langle k|l\rangle = \delta_{kl}$, one can show

$$X_{nm} = \sum \frac{p_n p_m}{p_n + p_m} d\rho_{nm}.$$  

When the states are full-rank, the first optimality condition becomes $E_x^{1/2}(1 - \mu_x \hat{\rho}_0^{1/2} \sqrt{\hat{\rho}_1^{1/2} \rho_0 \hat{\rho}_1^{1/2}} \rho_0^{-1/2}) = 0$. In the limit of small $d\hat{\rho}$,

$$\hat{\rho}_0^{1/2} \hat{\rho}_0^{1/2} \rho_0^{1/2} \rho_0^{-1/2} = 1 + \rho_0^{-1/2} X \hat{\rho}_0^{1/2}$$  

$$= 1 + \sum_{n,m} d\rho_{nm} |n\rangle \langle m|$$  

$$= 1 + \hat{L} \theta/2,$$  

where $\hat{L} \theta = 2 \sum_{n,m} d\rho_{nm} (p_n + p_m) |n\rangle \langle m|$ is the SLD operator, so that the condition becomes

$$E_x^{1/2}(1 - \mu_x \hat{\rho}_0^{1/2} \sqrt{\hat{\rho}_1^{1/2} \rho_0 \hat{\rho}_1^{1/2}} \rho_0^{-1/2}) = E_x^{1/2}(1 - \mu_x (1 + \hat{L} \theta/2)) = 0.$$  

This results in

$$\hat{E}_x^{1/2}(1 - \lambda_x \hat{L} \theta) = 0$$  

with a constant $\lambda_x$, which is equivalent to the optimal condition of Eq. (14) for quantum Fisher information.

Now, we turn to the second condition. Eq. (2) can be simplified assuming two quantum states are infinitesimally close:

$$\text{Tr}[U \hat{\rho}_0^{1/2} \hat{E}_x \hat{\rho}_1^{1/2}] = \text{Tr}[\sqrt{\hat{\rho}_1^{1/2} \rho_0 \hat{\rho}_1^{1/2}} \hat{E}_x \hat{\rho}_1^{1/2} \hat{E}_x] = \text{Tr}[(1 + \hat{L} \theta/2) \hat{E}_x \hat{\rho}].$$  

One can immediately see that this is equivalent to Eq. (15).

**Appendix E: Limit of $G_M$ matrix**

Consider the estimation of parameter $\theta$. The matrix $G_M$ is given by the solution of

$$e^{i\Omega G_M} = e^{-i\Omega G_0/2} \sqrt{e^{i\Omega G_0/2} e^{i\Omega G_0 + \theta} e^{i\Omega G_0/2}} e^{-i\Omega G_0/2}.$$  

The operator $G_M$ is infinitesimal, as to the zeroth order the two matrices $G_0$ and $G_0 + \theta$ are equal and $G_M = 0$. Therefore, we write $i\Omega G_M = C \theta$ for some unknown matrix $C$. Similarly we write $i\Omega G_0 = A$ and $i\Omega G_0 + \theta = A + B \theta$ for some matrices $A$ and $B$. From the above equation, $C$ is the solution of

$$\sqrt{e^{i\frac{\theta}{2}} e^{A + B \theta} e^{i\frac{\theta}{2}}} = e^{i\frac{\theta}{2}} e^{C \theta} e^{i\frac{\theta}{2}} \approx e^A + e^{-A} C \theta e^A + O(\theta)^2.$$  

$$e^{A + B \theta} e^{i\frac{\theta}{2}} \approx e^{2A} + e^{-A} C \theta e^A + e^{-A} C \theta e^{-A} + O(\theta)^2.$$  

$$e^{A + B \theta} \approx e^{A + e^{-A}} C \theta e^A + O(\theta)^2.$$  

Using the notation from Ref. [11] we may write $e^{i\Omega G_0} = W_A^{-1} W_B$ and expand the matrices $W_\theta$ as $W_{\theta + \theta}$ as $W_A + W_B \theta$ with $W_\theta = W_A$. Therefore

$$e^{A + B \theta} = e^{i\Omega G_0 + \theta} = 1 - 2 \frac{\theta}{W_A + \theta} + \frac{\theta}{W_A + \theta}$$  

$$= 1 - 2 \frac{\theta}{W_A + \theta} + 2 \frac{\theta^2}{W_A + \theta} + \frac{\theta^2}{W_A + \theta} + O(\theta)^2$$  

$$= e^A + \frac{\theta^2}{2} (e^{-A} - 1) W_B (e^A - 1) + O(\theta)^2$$  

and $C$ is the solution of

$$e^A C + C e^A = \frac{1}{2} (e^{-A} - 1) W_B (e^A - 1),$$  

or using matrix $W$ as

$$(W_\theta + \theta) C (W_\theta - 1) + (W_\theta - 1) C (W_\theta + \theta) = 2 W_B,$$  

namely we get the discrete Lyapunov equation,

$$C - W^{-1} C W_{\theta}^{-1} W_{\theta}^{-1} = W^{-1} \frac{\partial W_\theta}{\partial \theta} W_{\theta}^{-1}. $$
The solution of the Lyapunov equation is

\[ C = \sum_{m=0}^{\infty} W_\theta^{-m-1} \frac{\partial W_\theta}{\partial \theta} W_\theta^{-m-1}, \]

and thus,

\[ G_M = i\Omega \sum_{m=0}^{\infty} W_\theta^{-m-1} \frac{\partial W_\theta}{\partial \theta} W_\theta^{-m-1} d\theta. \]

Especially when \( \partial \tilde{n}_i / \partial \theta = 0 \) and isothermal states, i.e. \( \tilde{n}_i = \bar{n} \) for all \( i \),

\[ C = \sum_{m=0}^{\infty} (-1)^{m+1} W_\theta^{-2m-2} \frac{\partial W_\theta}{\partial \theta} = -\frac{1}{2(2\bar{n}^2 + 2\bar{n} + 1)} \frac{\partial W_\theta}{\partial \theta}, \]

where we have used \( W_\theta^2 = (2\bar{n} + 1)^2 \bar{\rho} \). Thus,

\[ G_M = \frac{1}{2\bar{n}^2 + 2\bar{n} + 1} \frac{\partial V_\theta}{\partial \theta} d\theta. \]

On the other hand, from the definition of \( C \) and \( W_\theta = -2V_\theta i\Omega \), we get that \( G_M \) is the solution of

\[ 4V_\theta G_M V_\theta + \Omega G_M \Omega + 2d\theta \frac{\partial V_\theta}{\partial \theta} = 0. \] (E2)

Writing in the basis in which \( V_\theta \) is symplectically diagonalized, one can recover the previous result [50],

\[ (G_M)_{ij} = \frac{2V_\theta^* \frac{\partial V_\theta^*}{\partial \theta} V_\theta - \Omega \frac{\partial V_\theta^*}{\partial \theta} \Omega / 2}{\lambda_i^* \lambda_j - 1} \]

where \( O^* = SOS^T \), and \( \lambda_i^* \) are the symplectic eigenvalues of \( V_\theta \), and \( S \) is a symplectic matrix that diagonalizes \( V_\theta \). The difference of the factors originate from that of definition of covariance matrices.

The vector \( u_M \) for infinitesimal \( d\theta \) is written as

\[ u_M = (-i\Omega G_M)^{-1} e^{i\Omega G_M/2} (e^{-i\Omega G_M/2} - 1) (e^{-2i\Omega G_M} - 1)^{-1} \times e^{-i\Omega G_M/2} (e^{-i\Omega G_M} - 1) \frac{\partial u_\theta}{\partial \theta} d\theta \]

\[ = G_M^{-1} V_\theta^{-1} \frac{\partial u_\theta}{\partial \theta} d\theta / 2, \]

where we have used \( e^{i\Omega G_M} = \frac{\bar{\rho} - \bar{\rho}^*}{\bar{\rho} + \bar{\rho}^*} \). Thus,

\[ v_M = G_M u_M = V_\theta^{-1} \frac{\partial u_\theta}{\partial \theta} d\theta / 2. \] (E4)

As a final remark, after we calculate \( G_M \) and \( v_M \), the expression of the quantum Fisher information can be derived using Eq. [E2],

\[ H(\theta) = \text{Tr}[\dot{\rho}_\theta \hat{L}_\theta^2], \]

\[ = \text{Tr}[\hat{D}(\hat{u}_\theta)(\hat{Q}^T G_M \hat{Q} - 2v^T_{\hat{M}} \hat{Q} + \nu^2)] / d\theta^2 \]

\[ = \text{Tr}[\dot{\rho}_\theta^0 (Q^T G_M Q^*)] + 4\nu (v^T_{\hat{M}} Q^*) + \nu (Q^T G_M Q) + \nu^2) / d\theta^2 \]

\[ = -\text{Tr} \left[ \frac{\partial V_\theta}{\partial \theta} G_M \right] / (d\theta^2) + \frac{\partial u_\theta}{\partial \theta} V_\theta^{-1} \frac{\partial u_\theta}{\partial \theta}, \]

where \( \dot{\rho}_\theta^0 = \hat{D}(\hat{u}_\theta) \rho_\theta \hat{D}(\hat{u}_\theta) \) is a Gaussian state with a zero-mean and the same covariance matrix of \( \rho_\theta \), and we have used [53]

\[ \text{Tr}[\dot{\rho}_\theta^0 \hat{Q}_n \hat{Q}_m \hat{Q}_k \hat{Q}_l] = \text{Tr}[\dot{\rho}_\theta^0 \hat{Q}_n \hat{Q}_m \text{Tr}[\dot{\rho}_\theta^0 \hat{Q}_l \hat{Q}_k] + \text{Tr}[\dot{\rho}_\theta^0 \hat{Q}_l \hat{Q}_n \text{Tr}[\dot{\rho}_\theta^0 \hat{Q}_m \hat{Q}_k] + \text{Tr}[\dot{\rho}_\theta^0 \hat{Q}_m \hat{Q}_n \text{Tr}[\dot{\rho}_\theta^0 \hat{Q}_k \hat{Q}_l] \text{ and Tr}[\rho_\theta^0 \hat{Q}_n \hat{Q}_m \hat{Q}_k] = V_{nm} + i\Omega_{nm} / 2. \]

Quantum Fisher information matrix for a multi-parameter case can be easily derived with the same method.

[1] M. A. Nielsen and I. L. Chuang, Quantum Computation and Quantum Information (Cambridge University Press, Cambridge, England, 2000).
[2] M. M. Wilde, Quantum Information Theory. Cambridge: Cambridge University Press (2017).
[3] C. Weedbrook, S. Pirandola, R. Garcia-Patron, N. J. Cerf, T. C. Ralph, J. H. Shapiro, and S. Lloyd, Rev. Mod. Phys. 84, 621 (2012).
[4] S. L. Braunstein and P. van Loock, Rev. Mod. Phys. 77, 513 (2005).
[5] C. W. Helstrom, Quantum Detection and Estimation Theory, Mathematics in Science and Engineering Vol. 123 (Academic Press, New York, 1976).
[6] K. M. R. Audenaert, J. Calsamiglia, L. Masanes, R. Munoz-Tapia, A. Acín, E. Bagan, and F. Verstraete, Phys. Rev. Lett. 98, 160501 (2007).
[7] K. M. R. Audenaert, M. Nussbaum, A. Szkoła, and F. Verstraete, Commun. Math. Phys. 279, 251 (2008).
[8] A. Uhlmann, Reports on Mathematical Physics. 9 (2): 273279 (1976).
[9] V. Vedral, Rev. Mod. Phys. 74, 197 (2002).
[10] D. Leibfried, M. D. Barrett, T. Schaetz, J. Britton, J. Chiaverini, W. M. Itano, J. D. Jost, C. Langer, D. J. Wineland, Science 304, 1476 (2004).
[11] C.-Y. Lu, X.-Q. Zhou, O. Gühne, W.-B. Gao, J. Zhang, Z.-S. Yuan, A. Goebel, T. Yang, and J.-W. PAN, Nat. Phys. 3, 91 (2007).
[12] A. Ourjoumtsev, H. Jeong, R. Tualle-Brouri, and P. Grangier, Nature 448, 784 (2007).
[13] C. H. Bennett, G. Brassard, C. Crepard, R. Jozsa, A. Peres, and W. K. Wootters, Phys. Rev. Lett. 70, 1895 (1993).
[14] D. Bouwmeester, J.-W. Pan, K. Mattle, M. Eibl, H. Weinfurter, and A. Zeilinger, Nature (London) 390, 570 (1997).
[15] S. L. Braunstein and H. J. Kimble, Phys. Rev. Lett. 80, 869 (1998).
[16] A. Furusawa et al., Science 282, 706 (1998).
[17] V. Buzek and M. Hillery, Phys. Rev. A 54, 1844 (1996).
[18] G. Lindblad, J. Phys. A 33, 5059 (2000).
[19] N. J. Cerf, A. Ipe, and X. Rottenberg, Phys. Rev. Lett. 85, 1754 (2000).
[20] S. L. Braunstein, N. J. Cerf, S. Iblisdir, P. van Loock, and S. Massar, Phys. Rev. Lett. 86, 4938 (2001).
[21] J. Fiurasek, Phys. Rev. Lett. 86, 4942 (2001).
[22] S. L. Braunstein and C. M. Caves, Phys. Rev. Lett. 72, 3439 (1994).
[23] C. A. Fuchs and J. V. de Graaf, IEEE Trans. Inf. Theory 45, 1216 (1999).
[24] R. Filip, Phys. Rev. A 65, 062320 (2002).
[25] A. K. Ekert, et al., Phys. Rev. Lett. 88, 217901 (2002).
[26] M. Hendrych, M. Dušek, R. Filip, and J. Fiurášek, Phys. Lett. A 310, 95 (2003).
[27] K. Bartkiewicz, K. Lemr, and A. Miranowicz, Phys. Rev. A 88, 052104 (2013).
[28] A. Ferraro, S. Olivares, and M. G. A. Paris, Gaussian States in Quantum Information (Bibliopolis, Berkeley, 2005).
[29] X.-B Wang, T. Hiroshima, A. Tomita, and M. Hayashi, Quantum information with Gaussian states, Phys. Rep. 448, 1 (2007).
[30] G. Adesso, S. Ragy, and A. R. Lee, Continuous variable quantum information: Gaussian states and beyond, Open Syst. Inf. Dyn. 21, 1440001 (2014).
[31] A. Serafini, Quantum Continuous Variables: A Primer of Theoretical Methods (Taylor & Francis, Oxford, 2017).
[32] J. Twamley, J. Phys. A 29, 3723 (1996).
[33] H. Nha and H. J. Carmichael, Phys. Rev. A 71, 032336 (2005).
[34] S. Olivares, M. G. A. Paris, and U. L. Andersen, Phys. Rev. A 73, 062330 (2006).
[35] H. Scutaru, J. Phys. A 31, 3659 (1998).
[36] P. Marian and T. A. Marian, Phys. Rev. A 86, 022340 (2012).
[37] P. Marian, T. A. Marian, and H. Scutaru, Phys. Rev. A 68, 062309 (2003).
[38] P. Marian and T. A. Marian, Phys. Rev. A 77, 062319 (2008).
[39] G. Spedalieri, C. Weedbrook, and S. Pirandola, J. Phys. A 46, 025304 (2013).
[40] Gh.-S. Paraoanu and H. Scutaru, Phys. Rev. A 61, 022306 (2000).
[41] L. Banchi, S. L. Braunstein, and S. Pirandola, Phys. Rev. Lett. 115, 260501 (2015).
[42] C. A. Fuchs and C. M. Caves, Open Systems & Information Dynamics, 3, 345 (1995).
[43] A. Bhattacharyya, Bull, Calcutta Math. Soc. 35, 99, (1943).
[44] R. Balian and E. Brezin, Nuovo Cimento B, 64, 37 (1969).
[45] O. Pinel, P. Jian, N. Treps, C. Fabre, and D. Braun, Phys. Rev. A 88, 040102(R) (2013).
[46] C. Oh, C. Lee, C. Rockstuhl, H. Jeong, J. Kim, H. Nha, S.-Y. Lee, arXiv:1805.08495v2 (2018).
[47] A. Monras and M. G. A. Paris, Phys. Rev. Lett. 98, 160401 (2007).
[48] D. Šafránek and I. Fuentes Phys. Rev. A 94, 062313 (2016).
[49] Arvind, B. Dutta, N. Mukunda, and R. Simon, Pramana, J. Phys. 45, 471 (1995).
[50] Z. Jiang, Phys. Rev. A 89, 032128 (2014).
[51] R. Nichols, P. Liuzzo-Scorpo, P. A. Knott, and G. Adesso, Phys. Rev. A 98, 012114 (2018).
[52] D. Šafránek J. Phys. A: Math. Theor. 52 035304 (2019).
[53] C. W. Gardiner and P. Zoller, Quantum Noise (SpringerVerlag, Berlin, 2004)