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Optimal measurements for quantum multi-parameter estimation with general states

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We generalize the approach by Braunstein and Caves [Phys. Rev. Lett. 72, 3439 (1994)] to quantum multi-parameter estimation with general states. We derive a matrix bound of the classical Fisher information matrix due to each measurement operator. The saturation of all these bounds results in the saturation of the matrix Helstrom Cramér-Rao bound. Remarkably, the saturation of the matrix bound is equivalent as the saturation of the scalar bound with respect to any given positive definite weight matrix. Necessary and sufficient conditions are obtained for the optimal measurements that give rise to the Helstrom Cramér-Rao bound associated with a general quantum state. To saturate the Helstrom bound with separable measurements or collective measurement entangling only a small number of identical states, we find it is necessary for the symmetric logarithmic derivatives commute on the support of the state. As an important application of our results, we construct several local optimal measurements for the problem of estimating the three-dimensional separation of two incoherent optical point sources.

I. INTRODUCTION

Metrology [1–3], the science of precision measurements, has found wide applications in various fields of physics and engineering, including interferometry [4–8], atomic clocks [9–11], optical imaging [12–15], and detection of gravitational waves [16]. In classical metrology, the covariance matrix of a maximum likelihood estimator can always asymptotically achieve the classical Cramér-Rao (CR) bound proportional to the inverse of the Classical Fisher Information Matrix (CFIM) [17, 18]. In quantum metrology, the CR bound can be further minimized over all possible quantum measurements to yield the its quantum generalization. However, over the years different quantum generalizations of the CR bound have been developed motivated by the fact that the minimum variance for all the parameters may not be achievable simultaneously in a single measurement. The most stronger bound in the current literature is the Holevo CR bound [19–22]. However, this bound involves a complicated minimization over a set of locally unbiased operators. Other well-known bounds include the Yuen and Lax [23] CR bound which is in terms of the right logarithmic derivatives and the Helstrom CR bound [24, 25]. But the widely used quantum CR bound by quantum physicists perhaps is the one proposed by Helstrom due to its simplicity and intimate connections to the geometric structure of quantum states [26]. Therefore we focus on the saturation of the Helstrom CR bound in this paper. In the Helstrom CR bound, the CFIM is maximized over all POVM measurements to give the Quantum Fisher Information Matrix (QFIM). Throughout this paper, we assume the limit of the large sample size. Therefore the saturation of the Helstrom CR bound, becomes the search for optimal measurements that saturates the QFIM. Braunstein and Caves showed [27] that for single parameter estimation such an optimal measurement always exists. However the QFIM in multi-parameter estimation in general may not be achievable by any quantum measurement even in the asymptotic sense of the large sample size [28].

On the other hand, a general theory of quantum multi-parameter estimation is desired in many practical scenarios, including superresolution [29–39] spurred by the seminal work [12], Hamiltonian estimation [40–43], parameter estimation in interferometry [44–48]. For a pure state, the saturation of the Helstrom CR bound is now fully understood due to the works of Matsumoto [49] and Pezzè et al [45]. However, for a general mixed state, the necessary and sufficient conditions for any positive operator-valued measure (POVM) measurement to saturate the Helstrom CR bound are still uncharted. In this paper, we derive the saturation conditions by generalizing the earlier approach developed by Braunstein and Caves [27] for single parameter estimation to multi-parameter estimation. For the POVM operator corresponding to a zero probability outcome, we find that the saturation of the Helstrom CR bound imposes a constraint which is satisfied automatically in the case of single parameter estimation and therefore does not appear there. It is also found that for the existence of optimal measurements it is necessary to have the symmetric logarithmic derivatives commute on the support of a state. Based on the saturation conditions, we also construct several local optimal measurements in the problem of estimating the three-dimensional separation of two monochromatic, incoherent point sources, which is shown in Fig. 1. We emphasize that the saturation conditions we find may have possible applications not only in the superresolution of

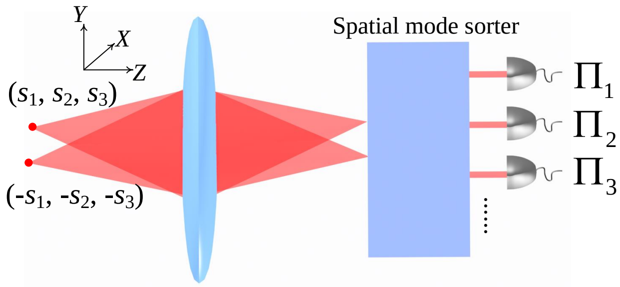

Figure 1. Schematic setup of the estimation of the three-dimensional separation of two point light sources, whose coordinates are denoted as $\pm(s_1,\, s_2,\, s_3)$. Π_k denotes a projector of a measurement, which can be implemented by spatial mode sorters [50–52]. The measurement is performed at the image plane. Alternatively, the measurement can also be performed at the pupil plane, i.e., the Fourier transformed plane of the image plane (not shown).

optical imaging, but also in quantum sensing [5].

This paper is organized as follows: In Sec. II, we define the notations and concepts which is necessary for the subsequent derivations. In Sec. III, we recover the Helstrom CR bound by generalizing the approach of Braunstein and Caves [27] and show that the saturation of the matrix Helstrom CR bound is equivalent as the saturation of the corresponding scalar bound with respect to any given positive definite cost matrix. In Sec. IV, we derive the necessary and sufficient conditions for the optimal measurements that saturate the matrix Helstrom CR bound. In Sec. V, we apply our saturation conditions to the problem of three-dimensional imaging of two optical incoherent point sources. We summarize our findings and discuss several open questions in Sec. VI.

II. PRELIMINARY NOTATIONS AND DEFINITIONS

Before starting our derivations, some notations and definitions are in order for later use: (a) A general probe state is described by the density operator

$$\rho_{\boldsymbol{\lambda}} = \sum_n p_{n\boldsymbol{\lambda}} \left|\psi_{n\boldsymbol{\lambda}}\right\rangle \left\langle\psi_{n\boldsymbol{\lambda}}\right| , \tag{1}$$

where $p_{n\boldsymbol{\lambda}}$'s are *strictly* positive and $|\psi_{n\boldsymbol{\lambda}}\rangle$'s are orthonormal and do not vanish globally for all $\boldsymbol{\lambda}$. We denote the *kernel (null space)* of $\rho_{\boldsymbol{\lambda}}$ at some specific value $\boldsymbol{\lambda}_0$ as

$$\ker(\rho_{\boldsymbol{\lambda}_0}) \equiv \mathrm{span}\{|\psi\rangle : \langle\psi_{n\boldsymbol{\lambda}_0}|\psi\rangle = 0,\, \forall n\}, \tag{2}$$

and the *support* of $\rho_{\boldsymbol{\lambda}}$ at $\boldsymbol{\lambda}_0$ as

$$\mathrm{supp}(\rho_{\boldsymbol{\lambda}_0}) \equiv \mathrm{span}\{|\psi_{n\boldsymbol{\lambda}_0}\rangle\text{'s}\}. \tag{3}$$

For a vector $|\psi\rangle$, its projection on $\ker(\rho_{\boldsymbol{\lambda}})$ is denoted as $|\psi^0\rangle$ and projection on $\mathrm{supp}(\rho_{\boldsymbol{\lambda}})$ is denoted as $|\psi^\perp\rangle$. According to linear algebra there is a unique decomposition $|\psi\rangle = |\psi^0\rangle + |\psi^\perp\rangle$. (b) We use a short hand notation ∂_i as the derivative with respect to the estimation parameter λ_i, for example $\partial_i\rho_{\boldsymbol{\lambda}} \equiv \partial\rho_{\boldsymbol{\lambda}}/\partial\lambda_i$. In addition the projections of $|\partial_i\psi_{\boldsymbol{\lambda}}\rangle$ on the kernel and support of $\rho_{\boldsymbol{\lambda}}$ are denoted as $|\partial_i^0\psi_{\boldsymbol{\lambda}}\rangle$ and $|\partial_i^\perp\psi_{\boldsymbol{\lambda}}\rangle$ respectively, where

$$|\partial_i^0\psi_{\boldsymbol{\lambda}}\rangle \equiv |\partial_i\psi_{\boldsymbol{\lambda}}\rangle - |\partial_i^\perp\psi_{\boldsymbol{\lambda}}\rangle , \tag{4}$$

$$|\partial_i^\perp\psi_{\boldsymbol{\lambda}}\rangle \equiv \sum_n \left|\psi_{n\boldsymbol{\lambda}}\right\rangle \left\langle\psi_{n\boldsymbol{\lambda}}\middle|\partial_i\psi_{\boldsymbol{\lambda}}\right\rangle . \tag{5}$$

(c) The POVM operator is denoted as Π_k with spectral decomposition

$$\Pi_k \equiv \sum_\alpha q_{k\alpha} \left|\pi_{k\alpha}\right\rangle \left\langle\pi_{k\alpha}\right| , \tag{6}$$

where $q_{k\alpha}$'s are strictly positive and $|\pi_{k\alpha}\rangle$'s are orthonormal. If $\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k) = 0$ then Π_k is called a *null* (POVM) operator otherwise it is called a *regular* (POVM) operator. A basis vector $|\pi_{k\alpha}\rangle$ is *null* if $\langle\psi_{n\boldsymbol{\lambda}}|\pi_{k\alpha}\rangle = 0$, $\forall n$ otherwise it is *regular*. We emphasis that null operator will make the CFIM elements ill-defined and therefore some regularization is required when calculating their contributions to the CFIM.

III. RECOVERING THE HELSTROM CR BOUND

The CFIM quantifies the sensitivity of a probability distribution to a small change in $\boldsymbol{\lambda}$ [26]. Its matrix element is defined as [17, 18]

$$F_{ij} = \sum_k \mathcal{F}_{ij}^k, \tag{7}$$

where

$$\mathcal{F}_{ij}^k \equiv \partial_i \mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k)\partial_j \mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k)/\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k). \tag{8}$$

Note that null operators contribute to the CFIM elements terms of the type 0/0, which should be understood in the sense of the multivariate limit. Due to this observation, it is natural to discuss the CFIM element separately for null and regular operators. For both regular and null operators, we prove the following inequality in subsecs III A and III B

$$\sum_{ij} u_i\mathcal{F}_{ij}^k u_j \le \sum_{ij} u_i u_j \mathcal{I}_{ij}^k, \tag{9}$$

where $\boldsymbol{u}$ is an arbitrary, real, and nonzero vector [53], $L_{i\boldsymbol{\lambda}}$ is the Symmetric Logarithmic Derivative (SLD) with respect to parameter λ_i defined as [19, 24, 54]

$$[L_{i\boldsymbol{\lambda}}\rho_{\boldsymbol{\lambda}} + \rho_{\boldsymbol{\lambda}}L_{i\boldsymbol{\lambda}}]/2 = \partial_i\rho_{\boldsymbol{\lambda}}, \tag{10}$$

and

$$\mathcal{I}_{ij}^k \equiv \mathrm{Re}[\mathrm{Tr}(\rho_{\boldsymbol{\lambda}} L_{i\boldsymbol{\lambda}} \Pi_k L_{j\boldsymbol{\lambda}})] \tag{11}$$

is the QFIM element corresponding to a regular or null POVM operator Π_k. Note that Eq. (9) for null operators is not discussed in Ref. [27] since it is automatically saturated in the case of single parameter estimation, as we will see in the next section. It is readily checked that summation over k in Eq. (9) yields the Helstrom CR bound [19, 24, 54]

$$\sum_{ij} u_i F_{ij} u_j \leq \sum_{ij} u_i I_{ij} u_j, \tag{12}$$

where

$$I_{ij} \equiv \mathrm{Re}[\mathrm{Tr}(\rho_{\boldsymbol{\lambda}} L_{i\boldsymbol{\lambda}} L_{j\boldsymbol{\lambda}})]. \tag{13}$$

A. Proof of Eq. (9) for regular POVM operators

Proof. For regular POVM operators, we prove Eq. (9) by generalizing the technique by Braunstein and Caves [27]. The Classical Fisher Information Matrix (QFIM) element corresponding to a regular POVM Π_k is defined as

$$\mathcal{F}_{ij}^k(\boldsymbol{\lambda}) = \partial_i \mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k)\partial_j \mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k)/\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k). \tag{14}$$

Using Eq. (10) and the cyclic property of trace, i.e.,

$$\mathrm{Tr}(L_{i\boldsymbol{\lambda}}\rho_{\boldsymbol{\lambda}}\Pi_k) = \mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k L_{i\boldsymbol{\lambda}}) = [\mathrm{Tr}(\rho_{\boldsymbol{\lambda}} L_{i\boldsymbol{\lambda}}\Pi_k)]^*, \tag{15}$$

we obtain [27, 54]

$$\begin{aligned}\partial_i \mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k) &= \mathrm{Tr}(\partial_i\rho_{\boldsymbol{\lambda}}\Pi_k)\\ &= \frac{1}{2}[\mathrm{Tr}(L_{i\boldsymbol{\lambda}}\rho_{\boldsymbol{\lambda}}\Pi_k) + \mathrm{Tr}(\rho_{\boldsymbol{\lambda}}L_{i\boldsymbol{\lambda}}\Pi_k)]\\ &= \mathrm{Re}[\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k L_{i\boldsymbol{\lambda}})]. \end{aligned}\tag{16}$$

Therefore for a real and nonzero vector $\boldsymbol{u}$, we obtain

$$\begin{aligned}\sum_{ij} u_i \mathcal{F}_{ij}^k u_j &= \frac{[\mathrm{Re}\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k \sum_i u_i L_{i\boldsymbol{\lambda}})]^2}{\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k)}\\ &\leq \frac{\left|\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k \sum_i u_i L_{i\boldsymbol{\lambda}})\right|^2}{\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k)}\\ &\leq \sum_{ij} u_i u_j \mathrm{Tr}(\rho_{\boldsymbol{\lambda}} L_{i\boldsymbol{\lambda}}\Pi_k L_{j\boldsymbol{\lambda}})\\ &= \frac{1}{2}\sum_{ij} u_i u_j\,[\mathrm{Tr}(\rho_{\boldsymbol{\lambda}} L_{i\boldsymbol{\lambda}}\Pi_k L_{j\boldsymbol{\lambda}})\\ &+\mathrm{Tr}(\rho_{\boldsymbol{\lambda}} L_{j\boldsymbol{\lambda}}\Pi_k L_{i\boldsymbol{\lambda}})]\\ &= \sum_{ij} u_i u_j \mathrm{Re}[\mathrm{Tr}(\rho_{\boldsymbol{\lambda}} L_{i\boldsymbol{\lambda}}\Pi_k L_{j\boldsymbol{\lambda}})], \end{aligned}\tag{17}$$

we have in the second inequality applied the Cauchy-Swartz inequality $\left|\mathrm{Tr}(A^\dagger B)\right|^2 \leq \mathrm{Tr}(A^\dagger A)\mathrm{Tr}(B^\dagger B)$, with $A \equiv \sqrt{\Pi_k}\sqrt{\rho_{\boldsymbol{\lambda}}}$ and $B \equiv \sum_i \sqrt{\Pi_k} u_i L_{i\boldsymbol{\lambda}}\sqrt{\rho_{\boldsymbol{\lambda}}}$. Due to the fact $u_i u_j$ is symmetric in indices i, j, we have symmetrized $\mathrm{Tr}(\rho_{\boldsymbol{\lambda}} L_{i\boldsymbol{\lambda}}\Pi_k L_{j\boldsymbol{\lambda}})$ in the second last equality to obtain the last equality. □

B. Proof of Eq. (9) for null POVM operators

Before we start the proof, let us first prove an observation that will be useful later.

Lemma 1. *A measurement operator Π_k is null if and only if $\forall n$, $|\psi_{n\boldsymbol{\lambda}}\rangle$ lies in the kernel of Π_k, i.e.,*

$$\Pi_k |\psi_{n\boldsymbol{\lambda}}\rangle = 0 \tag{18}$$

Proof. The lemma is a consequence of the semi-positive definiteness of $\rho_{\boldsymbol{\lambda}}$ and Π_k. To see this, let us note a null measurement operator satisfies,

$$\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k) = \sum_n p_{n\boldsymbol{\lambda}} \langle\psi_{n\boldsymbol{\lambda}}|\Pi_k|\psi_{n\boldsymbol{\lambda}}\rangle = 0 \tag{19}$$

Since $\rho_{\boldsymbol{\lambda}}$ is positive-definite on its support, we conclude $p_{n\boldsymbol{\lambda}}$'s are strictly positive, as we defined in Sec. II. Therefore Eq. (19) becomes

$$\langle\psi_{n\boldsymbol{\lambda}}|\Pi_k|\psi_{n\boldsymbol{\lambda}}\rangle = 0 \tag{20}$$

On the other hand, we may decompose $|\psi_{n\boldsymbol{\lambda}}\rangle$ into components that lie in the support and kernel of Π_k. Then, since Π_k is positive definite on its support, Eq. (20) is equivalent as the fact that $|\psi_{n\boldsymbol{\lambda}}\rangle$ completely lies in the kernel of Π_k.

□

Now let us prove Eq. (9) for the case of null measurement operators.

Proof. Introducing short hand notation

$$g_{ij}^k(\boldsymbol{\lambda}') \equiv \mathrm{Tr}(\partial_i\rho_{\boldsymbol{\lambda}'}\Pi_k)\mathrm{Tr}(\partial_j\rho_{\boldsymbol{\lambda}'}\Pi_k), \tag{21}$$

$$h^k(\boldsymbol{\lambda}') \equiv \mathrm{Tr}(\rho_{\boldsymbol{\lambda}'}\Pi_k), \tag{22}$$

the CFIM element $\mathcal{F}_{ij}^k$ corresponding to a null projector Π_k defined in the main text can be rewritten as

$$\mathcal{F}_{ij}^k(\boldsymbol{\lambda}) \equiv \lim_{\boldsymbol{\lambda}'\to\boldsymbol{\lambda}} \frac{g_{ij}^k(\boldsymbol{\lambda}')}{h^k(\boldsymbol{\lambda}')}. \tag{23}$$

Since the right hand side of Eq. (23) is of the type 0/0, we need to Taylor expand both the numerator and denominator, which will involve the derivatives of $\rho_{\boldsymbol{\lambda}}$. It is straightforward to show that the first order derivatives of $g_{ij}^k(\boldsymbol{\lambda}')$ and $h^k(\boldsymbol{\lambda}')$ vanish at $\boldsymbol{\lambda}$, i.e.,

$$\partial_p g_{ij}^k(\boldsymbol{\lambda}) = \mathrm{Tr}(\partial_p\partial_i\rho_{\boldsymbol{\lambda}}\Pi_k)\cancel{\mathrm{Tr}(\partial_j\rho_{\boldsymbol{\lambda}}\Pi_k)} \tag{24}$$

$$+\cancel{\mathrm{Tr}(\partial_i\rho_{\boldsymbol{\lambda}}\Pi_k)}\mathrm{Tr}(\partial_p\partial_j\rho_{\boldsymbol{\lambda}}\Pi_k) = 0, \tag{25}$$

$$\partial_p h^k(\boldsymbol{\lambda}) = \mathrm{Tr}(\partial_p \rho_{\boldsymbol{\lambda}} \Pi_k) = 0, \tag{26}$$

due to Lemma 1. Therefore we need to expand $g_{ij}^k(\boldsymbol{\lambda}')$ and $h^k(\boldsymbol{\lambda}')$ to the second order in $\delta\boldsymbol{\lambda} \equiv \boldsymbol{\lambda}' - \boldsymbol{\lambda}$ and calculate their second derivatives at $\boldsymbol{\lambda}$, i.e.,

$$\partial_p \partial_q g_{ij}^k(\boldsymbol{\lambda}) = \mathrm{Tr}(\partial_p \partial_i \rho_{\boldsymbol{\lambda}} \Pi_k)\mathrm{Tr}(\partial_q \partial_j \rho_{\boldsymbol{\lambda}} \Pi_k) + \mathrm{Tr}(\partial_q \partial_i \rho_{\boldsymbol{\lambda}} \Pi_k)\mathrm{Tr}(\partial_p \partial_j \rho_{\boldsymbol{\lambda}} \Pi_k), \tag{27}$$

$$\partial_p \partial_q h^k(\boldsymbol{\lambda}) = \mathrm{Tr}(\partial_p \partial_q \rho_{\boldsymbol{\lambda}} \Pi_k). \tag{28}$$

If we define

$$T_{ij}^k \equiv \frac{1}{2}\mathrm{Tr}(\partial_i \partial_j \rho_{\boldsymbol{\lambda}} \Pi_k), \tag{29}$$

Substitution of Eq. (29) into Eqs. (27, 28) gives

$$\partial_p \partial_q g_{ij}^k(\boldsymbol{\lambda}) = 4(T_{pi}^k T_{qj}^k + T_{qi}^k T_{pj}^k), \tag{30}$$

$$\partial_p \partial_q h^k(\boldsymbol{\lambda}') = 2T_{pq}^k. \tag{31}$$

Substituting $g_{ij}^k(\boldsymbol{\lambda}') = \sum_{p,q} \partial_p \partial_q g_{ij}^k(\boldsymbol{\lambda}) \delta\lambda_p \delta\lambda_q$ and $h^k(\boldsymbol{\lambda}') = \sum_{p,q} \partial_p \partial_q h^k(\boldsymbol{\lambda}) \delta\lambda_p \delta\lambda_q$ into Eq. (23), with notice of Eqs. (30, 31), we arrive at

$$\mathcal{F}_{ij}^k(\boldsymbol{\lambda}) = \frac{2\sum_{pq}(T_{pi}^k T_{qj}^k + T_{qi}^k T_{pj}^k)\delta\lambda_p \delta\lambda_q}{\sum_{pq} T_{pq}^k \delta\lambda_p \delta\lambda_q}. \tag{32}$$

According to Eq. (10) we find

$$\begin{aligned}
\mathrm{Re}\mathrm{Tr}(\rho_{\boldsymbol{\lambda}} L_{i\boldsymbol{\lambda}} \Pi_k L_{j\boldsymbol{\lambda}}) &= \frac{1}{2}[\mathrm{Tr}(\rho_{\boldsymbol{\lambda}} L_{i\boldsymbol{\lambda}} \Pi_k L_{j\boldsymbol{\lambda}}) + \text{c.c.}] = \frac{1}{2}[\mathrm{Tr}(L_{j\boldsymbol{\lambda}} \rho_{\boldsymbol{\lambda}} L_{i\boldsymbol{\lambda}} \Pi_k) + \mathrm{Tr}(L_{i\boldsymbol{\lambda}} \rho_{\boldsymbol{\lambda}} L_{j\boldsymbol{\lambda}} \Pi_k)] \\
&= \mathrm{Tr}(L_{j\boldsymbol{\lambda}} \partial_i \rho_{\boldsymbol{\lambda}} \Pi_k) + \mathrm{Tr}(\partial_i \rho_{\boldsymbol{\lambda}} L_{j\boldsymbol{\lambda}} \Pi_k) - \frac{1}{2}\cancel{\mathrm{Tr}(L_{j\boldsymbol{\lambda}} L_{i\boldsymbol{\lambda}} \rho_{\boldsymbol{\lambda}} \Pi_k)} - \frac{1}{2}\cancel{\mathrm{Tr}(L_{i\boldsymbol{\lambda}} L_{j\boldsymbol{\lambda}} \rho_{\boldsymbol{\lambda}} \Pi_k)} \\
&= \mathrm{Tr}(\partial_i (L_{j\boldsymbol{\lambda}} \rho_{\boldsymbol{\lambda}}) \Pi_k) + \mathrm{Tr}(\partial_i (\rho_{\boldsymbol{\lambda}} L_{j\boldsymbol{\lambda}}) \Pi_k) - \cancel{\mathrm{Tr}(\partial_i L_{j\boldsymbol{\lambda}} \rho_{\boldsymbol{\lambda}} \Pi_k)} - \cancel{\mathrm{Tr}(\rho_{\boldsymbol{\lambda}} \partial_i L_{j\boldsymbol{\lambda}} \Pi_k)} \\
&= \mathrm{Tr}(\partial_i (L_{j\boldsymbol{\lambda}} \rho_{\boldsymbol{\lambda}} + \rho_{\boldsymbol{\lambda}} L_{j\boldsymbol{\lambda}}) \Pi_k) = 2\mathrm{Tr}(\partial_i \partial_j \rho_{\boldsymbol{\lambda}} \Pi_k),
\end{aligned} \tag{33}$$

where the cancellations of the terms are due to Lemma 1. In view of Eq. (29), we arrive at

$$T_{ij}^k = \frac{1}{4}\mathrm{Re}\mathrm{Tr}(\rho_{\boldsymbol{\lambda}} L_{i\boldsymbol{\lambda}} \Pi_k L_{j\boldsymbol{\lambda}}) = \frac{1}{4}\mathcal{I}_{ij}^k. \tag{34}$$

We first derive the following inequality for later use. For real and non-zero $\delta\boldsymbol{\lambda}$ and $\boldsymbol{u}$, we obtain

$$\begin{aligned}
(\sum_{ij} \delta\lambda_i T_{ij}^k u_j)^2 &= \frac{1}{16}(\mathrm{Re}[\sum_{ij} \delta\lambda_i \mathrm{Tr}(\rho_{\boldsymbol{\lambda}} L_{i\boldsymbol{\lambda}} \Pi_k L_{j\boldsymbol{\lambda}}) u_j])^2 \\
&\leq \frac{1}{16}\big|\sum_{ij} \delta\lambda_i \mathrm{Tr}(\rho_{\boldsymbol{\lambda}} L_{i\boldsymbol{\lambda}} \Pi_k L_{j\boldsymbol{\lambda}}) u_j\big|^2 \\
&= \frac{1}{16}\big|\mathrm{Tr}(\sum_i \delta\lambda_i \sqrt{\rho_{\boldsymbol{\lambda}}} L_{i\boldsymbol{\lambda}} \sqrt{\Pi_k} \sum_j u_j \sqrt{\Pi_k} L_{j\boldsymbol{\lambda}} \sqrt{\rho_{\boldsymbol{\lambda}}})\big|^2 \\
&\leq \frac{1}{16}\left[\sum_{ij} \delta\lambda_i \delta\lambda_j \mathrm{Tr}(\sqrt{\rho_{\boldsymbol{\lambda}}} L_{i\boldsymbol{\lambda}} \sqrt{\Pi_k} \sqrt{\Pi_k} L_{j\boldsymbol{\lambda}} \sqrt{\rho_{\boldsymbol{\lambda}}})\right]\left[\sum_{ij} u_i u_j \mathrm{Tr}(\sqrt{\rho_{\boldsymbol{\lambda}}} L_{i\lambda} \sqrt{\Pi_k} \sqrt{\Pi_k} L_{j\boldsymbol{\lambda}} \sqrt{\rho_{\boldsymbol{\lambda}}})\right] \\
&= \left(\sum_{ij} T_{ij}^k \delta\lambda_i \delta\lambda_j\right)\left(\sum_{ij} T_{ij}^k u_i u_j\right)
\end{aligned} \tag{35}$$

where we have used the Cauchy-Swartz inequality $\left|\mathrm{Tr}(A^\dagger B)\right|^2 \leq \mathrm{Tr}(A^\dagger A)\mathrm{Tr}(B^\dagger B)$, with $A \equiv \sum_i \delta\lambda_i \sqrt{\Pi_k} L_{i\boldsymbol{\lambda}} \sqrt{\rho_{\boldsymbol{\lambda}}}$ and $B \equiv \sum_i \sqrt{\Pi_k} u_i L_{i\boldsymbol{\lambda}} \sqrt{\rho_{\boldsymbol{\lambda}}}$ in the second inequality and performed symmetrization to obtain the last equality. Note that the denominator of

Eq. (32) can be rewritten as, upon substitution of Eq. (34),

$$\sum_{pq} T^k_{pq}\delta\lambda_p\delta\lambda_q = \mathrm{ReTr}[\rho_{\boldsymbol\lambda}\delta\Lambda\Pi_k\delta\Lambda] = \mathrm{Tr}[\sqrt{\Pi_k}\delta\Lambda\rho_{\boldsymbol\lambda}(\sqrt{\Pi_k}\delta\Lambda)^\dagger] \geq 0, \quad (36)$$

where $\delta\Lambda \equiv \sum_p L_{p\boldsymbol\lambda}\delta\lambda_p$. Therefore for any $\delta\boldsymbol\lambda$ the denominator of Eq. (32) is non-negative. With these observations, next we find

$$\begin{aligned}\sum_{ij} u_i\mathcal{F}^k_{ij}u_j &= \frac{4\sum_{ij}u_iu_j\sum_{pq}T^k_{pi}T^k_{qj}\delta\lambda_p\delta\lambda_q}{\sum_{pq}T^k_{pq}\delta\lambda_p\delta\lambda_q} \\ &= \frac{4(\sum_{pi}\delta\lambda_pT^k_{pi}u_i)^2}{\sum_{pq}T^k_{pq}\delta\lambda_p\delta\lambda_q} \\ &\leq \frac{4(\sum_{pq}T^k_{pq}\delta\lambda_p\delta\lambda_q)\sum_{ij}u_iu_jT^k_{ij}}{\sum_{pq}T^k_{pq}\delta\lambda_p\delta\lambda_q} \\ &= \sum_{ij}u_iu_j\mathcal{I}^k_{ij}, \end{aligned} \quad (37)$$

where we have used Eq. (35) in the inequality to get the upper bound. □

C. Equivalence between the saturations of the scalar and matrix Helstrom CR bounds

Remarkably, based on the following Lemma, the saturation of the matrix bound (12) is equivalent as the saturation of the corresponding scalar bound with respect to any given positive definite weight matrix, which has been used in previous papers [46, 47].

Lemma 2. *Given two positive semi-definite matrices A, B and a positive definite weight matrix G called weight matrix, if $A \preccurlyeq B$, i.e., $B - A$ is positive semi-definite, then the following statements are equivalent*

(i) $\exists$ a positive definite weight matrix G_0 such that $Tr(G_0A) = Tr(G_0B)$

(ii) $A = B$

(iii) $\forall$positive definite weight matrix G, $Tr(GA) = Tr(GB)$ holds

(iv) $\exists$ a positive definite weight matrix G_0 such that $Tr(G_0A^{-1}) = Tr(G_0B^{-1})$

(v) $\forall$positive definite matrix G, $Tr(GA^{-1}) = Tr(GB^{-1})$ holds

Proof. We notice that once the (i) $\Longleftrightarrow$ (ii) is justified, proof of the equivalence between any statements becomes straightforward. To prove (i) $\Longleftrightarrow$ (ii), it is sufficient to show that (i) $\Longrightarrow$ (ii) as the opposite direction is trivial. Condition (i) implies that $\mathrm{Tr}[G_0(B-A)] = 0$. Now moving to the basis that diagonalizes the matrix $B - A$, i.e., $B - A = U^\dagger DU$, where D is diagonal, we find

$$\mathrm{Tr}[G_0(B-A)] = \mathrm{Tr}(U^\dagger G_0UD) = \sum\nolimits_n \tilde{G}_{0nn}D_{nn} = 0 \quad (38)$$

where $\tilde{G}_0 \equiv U^\dagger G_0U$ is representation of G_0 in the basis that diagonalizes $B - A$. Since $A \preceq B$, $B - A$ is also semi-positive definite and therefore $D_{nn} \geq 0$. On the other hand G_0 is positive definite, which indicates diagonal matrix element of its representation in every basis is positive. Then we know $\tilde{G}_{0nn} > 0$. The only way to satisfy Eq. (38) is $D_{nn} = 0$ for all n. Therefore we conclude that $A = B$. □

In Lemma 2, if we take A as the CFIM and B as the QFIM, we immediately conclude that the saturation of the matrix Helstrom bound is equivalent as the scalar bound with respect to any given positive definite weight matrix.

IV. SATURATION OF THE HELSTROM CR BOUND AND THE PARTIAL COMMUTATIVITY CONDITION

The physical implications of $\mathcal{F}^k_{ij}$ and $\mathcal{I}^k_{ij}$ are very important in understanding the saturation of the Helstrom CR bound: from Eq. (9), we see that for each POVM operator Π_k, either regular or null, the corresponding QFIM $\mathcal{I}^k$ is a matrix bound for the corresponding CFIM $\mathcal{F}^k$. The saturation of the Helstrom CR bound requires the saturation of all these matrix bounds. Following this idea, we can derive the saturation conditions for the Helstrom CR bound by saturating Eq. (9) for regular and null POVM operators respectively.

A. Saturation conditions for general POVMs

Theorem 1. *The matrix bound of the CFIM due to a regular operator Π_k is saturated at $\boldsymbol\lambda$, if and only if*

$$\Pi_kL_{i\boldsymbol\lambda}|\psi_{n\boldsymbol\lambda}\rangle = \xi^k_i\Pi_k|\psi_{n\boldsymbol\lambda}\rangle,\ \forall i,\ k,\ n \quad (39)$$

where ξ^k_i is real and independent of n.

Proof. The saturation of the first inequality of Eq. (17) requires that $\mathrm{Tr}(\rho_{\boldsymbol\lambda}\Pi_k\sum_i u_iL_{i\boldsymbol\lambda})$ must be real for any arbitrary real and nonzero vector $\boldsymbol{u}$. Therefore $\mathrm{Tr}(\rho_{\boldsymbol\lambda}\Pi_kL_{i\boldsymbol\lambda})$ must be real for each i. The saturation of the second inequality of Eq. (17) requires that $\sqrt{\Pi_k}\sqrt{\rho_{\boldsymbol\lambda}}$ must be proportional to $\sqrt{\Pi_k}\sum_i u_iL_{i\boldsymbol\lambda}\sqrt{\rho_{\boldsymbol\lambda}}$ for any arbitrary, non-zero and real $\boldsymbol{u}$. Thus $\sqrt{\Pi_k}\sqrt{\rho_{\boldsymbol\lambda}}$ must be proportional to $\sqrt{\Pi_k}L_{i\boldsymbol\lambda}\sqrt{\rho_{\boldsymbol\lambda}}$ for each i, i.e.,

$$\xi^k_i\sqrt{\Pi_k}\sqrt{\rho_{\boldsymbol\lambda}} = \sqrt{\Pi_k}L_{i\boldsymbol\lambda}\sqrt{\rho_{\boldsymbol\lambda}},\ \forall i. \quad (40)$$

Eq. (40) can be rewritten as

$$\sqrt{\Pi_k}(L_{i\boldsymbol\lambda} - \xi^k_i)\sqrt{\rho_{\boldsymbol\lambda}} = 0,\ \forall i. \quad (41)$$

Since $\rho_{\boldsymbol\lambda}$ and $\sqrt{\rho_{\boldsymbol\lambda}}$ has the same kernel, Eq. (41) is equivalent as $\sqrt{\Pi_k}(L_{i\boldsymbol\lambda} - \xi^k_i)\rho_{\boldsymbol\lambda} = 0$, which is equivalent to

$$\Pi_kL_{i\boldsymbol\lambda}\rho_{\boldsymbol\lambda} = \xi^k_i\Pi_k\rho_{\boldsymbol\lambda} \quad (42)$$

due to the same reason. With the spectral decomposition $\rho_{\boldsymbol{\lambda}} = \sum_n p_{n\boldsymbol{\lambda}} |\psi_{n\boldsymbol{\lambda}}\rangle\langle\psi_{n\boldsymbol{\lambda}}|$, we arrive at Eq. (39). The proportionality constant ξ_i^k can be found by taking the trace inner product with $\sqrt{\Pi_k}\sqrt{\rho_{\boldsymbol{\lambda}}}$ on both sides of Eq. (40), i.e.,

$$\xi_i^k = \mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k L_{i\boldsymbol{\lambda}})/\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k),\ \forall i. \tag{43}$$

Therefore, the condition of $\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k L_{i\boldsymbol{\lambda}})$ being real is equivalent to that ξ_i^k is real, which concludes the proof. □

Theorem 2. *The matrix bound of the CFIM due to a null operator* Π_k *is saturated at* $\boldsymbol{\lambda}$*, if and only if*

$$\Pi_k L_{i\boldsymbol{\lambda}}|\psi_{n\boldsymbol{\lambda}}\rangle = \eta_{ij}^k \Pi_k L_{j\boldsymbol{\lambda}}|\psi_{n\boldsymbol{\lambda}}\rangle,\ \forall i,\, j,\, k,\, n \tag{44}$$

where the η_{ij}^k *is real and independent of* n.

Proof. Since the saturation of Eq. (37) is equivalent as the saturation of the two inequalities in Eq. (35), we will work with Eq. (35) subsequently. The saturation of the first inequality in Eq. (35) requires $\sum_{ij}\delta\lambda_i \mathrm{Tr}(\rho_{\boldsymbol{\lambda}}L_{i\boldsymbol{\lambda}}\Pi_k L_{j\boldsymbol{\lambda}})u_j$ is real for any $\delta\boldsymbol{\lambda}$, $\boldsymbol{u}$. This indicates that $\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}L_{i\boldsymbol{\lambda}}\Pi_k L_{j\boldsymbol{\lambda}})$ must be real for any pair i, j. The saturation of the second inequality in Eq. (35) requires $\sum_i \delta\lambda_i\sqrt{\Pi_k}L_{i\boldsymbol{\lambda}}\sqrt{\rho_{\boldsymbol{\lambda}}}$ be proportional to $\sum_j u_j\sqrt{\Pi_k}L_{j\boldsymbol{\lambda}}\sqrt{\rho_{\boldsymbol{\lambda}}}$ for any $\delta\boldsymbol{\lambda}$, $\boldsymbol{u}$. Thus $\sqrt{\Pi_k}L_{i\boldsymbol{\lambda}}\sqrt{\rho_{\boldsymbol{\lambda}}}$ must be proportional to $\sqrt{\Pi_k}L_{j\boldsymbol{\lambda}}\sqrt{\rho_{\boldsymbol{\lambda}}}$ for each pair $(i,\, j)$, i.e.,

$$\sqrt{\Pi_k}L_{i\boldsymbol{\lambda}}\sqrt{\rho_{\boldsymbol{\lambda}}} = \eta_{ij}^k\sqrt{\Pi_k}L_{j\boldsymbol{\lambda}}\sqrt{\rho_{\boldsymbol{\lambda}}},\ \forall i,\, j,\, k. \tag{45}$$

Since $\rho_{\boldsymbol{\lambda}}$ and $\sqrt{\rho_{\boldsymbol{\lambda}}}$ has the same kernel, Eq. (45) is equivalent as $\sqrt{\Pi_k}(L_{i\boldsymbol{\lambda}} - \eta_{ij}^k L_{j\boldsymbol{\lambda}})\rho_{\boldsymbol{\lambda}} = 0$, which is equivalent to

$$\Pi_k L_{i\boldsymbol{\lambda}}\rho_{\boldsymbol{\lambda}} = \eta_{ij}^k \Pi_k L_{j\boldsymbol{\lambda}}\rho_{\boldsymbol{\lambda}} \tag{46}$$

due to the same reason. With the spectral decomposition $\rho_{\boldsymbol{\lambda}} = \sum_n p_{n\boldsymbol{\lambda}}|\psi_{n\boldsymbol{\lambda}}\rangle\langle\psi_{n\boldsymbol{\lambda}}|$, we arrive at Eq. (44). The proportionality constant η_{ij}^k can be found by taking the trace inner product with $\sqrt{\Pi_k}L_{j\boldsymbol{\lambda}}\sqrt{\rho_{\boldsymbol{\lambda}}}$ on both sides of Eq. (40), i.e.,

$$\eta_{ij}^k = \frac{\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}L_{j\boldsymbol{\lambda}}\Pi_k L_{i\boldsymbol{\lambda}})}{\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}L_{j\boldsymbol{\lambda}}\Pi_k L_{j\boldsymbol{\lambda}})} \tag{47}$$

Since $\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}L_{j\boldsymbol{\lambda}}\Pi_k L_{j\boldsymbol{\lambda}})$ is real, the condition that $\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}L_{i\boldsymbol{\lambda}}\Pi_k L_{j\boldsymbol{\lambda}})$ must be real is equivalent to that η_{ij}^k must be real, which concludes the proof. □

B. The partial commutativity condition

Up to now Theorems 1-2 focus on the exact saturation of the QFIM. For limited experimental situations, where only separable measurements or collective measurements that involve only a small number of states are experimentally implementable, the CFIM scales exactly linearly with the number of identical states. As a result, the QFIM can only be saturated exactly. We show in the following theorem that saturating the QFIM *exactly* the following theorem must hold.

Theorem 3. *(The partial commutativity condition) To exactly saturate the QFIM, it is necessary to have the SLD must commute on the support of* $\rho_{\boldsymbol{\lambda}}$*, i.e.,* $\langle\psi_{m\boldsymbol{\lambda}}|[L_{i\boldsymbol{\lambda}},\, L_{j\boldsymbol{\lambda}}]|\psi_{n\boldsymbol{\lambda}}\rangle = 0,\ \forall n,\, m.$

Proof. If Π_k is regular, according to Eq. (39), we obtain

$$\begin{aligned}\langle\psi_{m\boldsymbol{\lambda}}|L_{i\boldsymbol{\lambda}}\Pi_k L_{j\boldsymbol{\lambda}}|\psi_{n\boldsymbol{\lambda}}\rangle &= \xi_j^k\langle\psi_{m\boldsymbol{\lambda}}|L_{i\boldsymbol{\lambda}}\Pi_k|\psi_{n\boldsymbol{\lambda}}\rangle \\ &= \xi_i^k\xi_j^k\langle\psi_{m\boldsymbol{\lambda}}|\Pi_k|\psi_{n\boldsymbol{\lambda}}\rangle \\ &= \langle\psi_{m\boldsymbol{\lambda}}|L_{j\boldsymbol{\lambda}}\Pi_k L_{i\boldsymbol{\lambda}}|\psi_{n\boldsymbol{\lambda}}\rangle\end{aligned} \tag{48}$$

If Π_k is null, according to Eq. (44), we obtain

$$\begin{aligned}\langle\psi_{m\boldsymbol{\lambda}}|L_{i\boldsymbol{\lambda}}\Pi_k L_{j\boldsymbol{\lambda}}|\psi_{n\boldsymbol{\lambda}}\rangle &= \eta_{ij}^k\langle\psi_{m\boldsymbol{\lambda}}|L_{j\boldsymbol{\lambda}}\Pi_k L_{j\boldsymbol{\lambda}}|\psi_{n\boldsymbol{\lambda}}\rangle \\ &= \langle\psi_{m\boldsymbol{\lambda}}|L_{j\boldsymbol{\lambda}}\eta^{ijk}\Pi_k L_{j\boldsymbol{\lambda}}|\psi_{n\boldsymbol{\lambda}}\rangle \\ &= \langle\psi_{m\boldsymbol{\lambda}}|L_{j\boldsymbol{\lambda}}\Pi_k L_{i\boldsymbol{\lambda}}|\psi_{n\boldsymbol{\lambda}}\rangle\end{aligned} \tag{49}$$

Thus we can see that the optimal measurement mediates the commutativity between $L_{i\boldsymbol{\lambda}}$ and $L_{j\boldsymbol{\lambda}}$ on the support of $\rho_{\boldsymbol{\lambda}}$, i.e., for any m and n,

$$\begin{aligned}\langle\psi_{m\boldsymbol{\lambda}}|[L_{i\boldsymbol{\lambda}},\, L_{j\boldsymbol{\lambda}}]|\psi_{n\boldsymbol{\lambda}}\rangle &= \sum_k\langle\psi_{m\boldsymbol{\lambda}}|L_{i\boldsymbol{\lambda}}\Pi_k L_{j\boldsymbol{\lambda}}|\psi_{n\boldsymbol{\lambda}}\rangle \\ &\quad - \sum_k\langle\psi_{m\boldsymbol{\lambda}}|L_{j\boldsymbol{\lambda}}\Pi_k L_{i\boldsymbol{\lambda}}|\psi_{n\boldsymbol{\lambda}}\rangle = 0\end{aligned} \tag{50}$$

□

The partial commutativity condition reduces to the weak commutativity condition [49] for pure states and the full commutativity condition for full rank states. While the sufficiency of the partial commutativity to saturate the bound has been proved to be true in the case of pure states [45, 49] and is trivially true in the case of the full rank states, whether it is still true in the general case is beyond the scope of the current work.

When collective measurements that entangle a large number of states are allowed, where the CFIM has the sublinear corrections in general besides the linear term with respect to the number of identical copies, asymptotic saturation becomes relevant. However, we emphasize that our Theorems 1-2 should be asymptotically satisfied if QFIM is asymptotically saturated. Ref. [46] concludes that if all possible measurements are allowed to perform on the large number of states, the weak commutativity condition $\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}[L_{i\boldsymbol{\lambda}},\, L_{j\boldsymbol{\lambda}}]) = 0$ is necessary and sufficient for the saturation of the Helstrom bound. However, the precise connection between our formalism here and Ref. [46] is still an open question.

C. Alternative saturation conditions

When one deals with specific problems, e.g., the problem of superresolution of two incoherent optical point sources in Sec. V, it is useful to consider the spectral decomposition of the POVM operator. Combining with the matrix representation of $L_{i\boldsymbol{\lambda}}$ given in Appendix A, Theorems 1, 2 can be alternatively rewritten as follows:

Theorem 4. *The matrix bound of the CFIM due to a regular operator $\Pi_k = \sum_\alpha q_{k\alpha} |\pi_{k\alpha}\rangle \langle \pi_{k\alpha}|$ is saturated at $\boldsymbol{\lambda}$, if and only if*

$$\langle \psi_{n\boldsymbol{\lambda}} | L^{\perp}_{i\boldsymbol{\lambda}} | \pi_{k\alpha}\rangle + 2 \langle \partial^0_i \psi_{n\boldsymbol{\lambda}} | \pi_{k\alpha}\rangle = \xi^k_i \langle \psi_{n\boldsymbol{\lambda}} | \pi_{k\alpha}\rangle \;\; \forall i,\, n,\, \alpha, \tag{51}$$

where ξ^k_i is real and independent of n and α, and $L^{\perp}_{i\boldsymbol{\lambda}}$ defined as Eq. (A8) denotes the projection of $L_{i\boldsymbol{\lambda}}$ onto supp($\rho_{\boldsymbol{\lambda}}$).

Proof. For a regular POVM operator Π_k with a spectral decomposition $\Pi_k = \sum_\alpha q_{k\alpha} |\pi_{k\alpha}\rangle \langle \pi_{k\alpha}|$ where $q_{k\alpha}$ is strictly positive, Eq. (39) becomes

$$\sum_\alpha q_{k\alpha} |\pi_{k\alpha}\rangle \langle \pi_{k\alpha}| L_{i\boldsymbol{\lambda}} |\psi_{n\boldsymbol{\lambda}}\rangle = \sum_\alpha q_{k\alpha} \xi^k_i |\pi_{k\alpha}\rangle \langle \pi_{k\alpha} | \psi_{n\boldsymbol{\lambda}}\rangle ,\; \forall i,\, n. \tag{52}$$

Since $|\pi_{k\alpha}\rangle$'s are linearly independent, the above equation is equivalent to

$$\langle \pi_{k\alpha} | L_{i\boldsymbol{\lambda}} | \psi_{n\boldsymbol{\lambda}}\rangle = \xi^k_i \langle \pi_{k\alpha} | \psi_{n\boldsymbol{\lambda}}\rangle ,\; \forall i,\, \alpha,\, n. \tag{53}$$

with ξ^k_i being real and independent of n. According to Eq. (A11), we have

$$\langle \psi_{n\boldsymbol{\lambda}} | L_{i\boldsymbol{\lambda}} | \pi_{k\alpha}\rangle = \langle \psi_{n\boldsymbol{\lambda}} | L^{\perp}_{i\boldsymbol{\lambda}} | \pi_{k\alpha}\rangle + 2 \langle \partial^0_i \psi_{n\boldsymbol{\lambda}} | \pi_{k\alpha}\rangle \tag{54}$$

which concludes the proof. □

Theorem 5. *The matrix bound of the CFIM due to a null operator $\Pi_k = \sum_\alpha q_{k\alpha} |\pi_{k\alpha}\rangle \langle \pi_{k\alpha}|$ is saturated at $\boldsymbol{\lambda}$, if and only if*

$$\langle \partial_i \tilde{\psi}_{n\boldsymbol{\lambda}} | \pi_{k\alpha}\rangle = \eta^k_{ij} \langle \partial_j \tilde{\psi}_{n\boldsymbol{\lambda}} | \pi_{k\alpha}\rangle \; \forall i,\, j,\, n, \alpha, \tag{55}$$

where $|\tilde{\psi}_{n\boldsymbol{\lambda}}\rangle$ is not necessarily normalized and η^k_{ij} is real and independent of n and α.

Proof. For a null POVM operator $\Pi_k = \sum_\alpha q_{k\alpha} |\pi_{k\alpha}\rangle \langle \pi_{k\alpha}|$, according to Eq. (A11), Eq. (44) becomes

$$\sum_\alpha q_{k\alpha} |\pi_{k\alpha}\rangle \langle \pi_{k\alpha} | L_{i\boldsymbol{\lambda}} | \psi_{n\boldsymbol{\lambda}}\rangle = \sum_\alpha \eta^k_{ij} q_{k\alpha} |\pi_{k\alpha}\rangle \langle \pi_{k\alpha} | L_{j\boldsymbol{\lambda}} | \psi_{n\boldsymbol{\lambda}}\rangle \tag{56}$$

Since $|\pi_{k\alpha}\rangle$'s are linearly independent, the above equation is equivalent to

$$\langle \pi_{k\alpha} | L_{i\boldsymbol{\lambda}} | \psi_{n\boldsymbol{\lambda}}\rangle = \eta^k_{ij} \langle \pi_{k\alpha} | L_{j\boldsymbol{\lambda}} | \psi_{n\boldsymbol{\lambda}}\rangle ,\; \forall i,\, \alpha,\, n. \tag{57}$$

with η^k_{ij} being real and independent of n. Since Π_k is null, $\langle \pi_{k\alpha} | \psi_{n\boldsymbol{\lambda}}\rangle = 0$, $\forall n,\, \alpha$. Therefore, according to Eq. (A11), we have

$$\langle \psi_{n\boldsymbol{\lambda}} | L_{i\boldsymbol{\lambda}} | \pi_{k\alpha}\rangle = 2 \langle \partial^0_i \psi_{n\boldsymbol{\lambda}} | \pi_{k\alpha}\rangle . \tag{58}$$

Therefore according to Eq. (56), we arrive at

$$\langle \partial^0_i \psi_{n\boldsymbol{\lambda}} | \pi_{k\alpha}\rangle = \eta^k_{ij} \langle \partial^0_j \psi_{n\boldsymbol{\lambda}} | \pi_{k\alpha}\rangle \tag{59}$$

For a null operator $\Pi_k = \sum_\alpha q_{k\alpha} |\pi_{k\alpha}\rangle \langle \pi_{k\alpha}|$, due to Lemma 1, we have $\langle \psi_{n\boldsymbol{\lambda}} | \pi_{k\alpha}\rangle = 0$, $\forall n, \alpha$. This implies

$$\langle \partial^0_i \psi_{n\boldsymbol{\lambda}} | \pi_{k\alpha}\rangle = \langle \partial_i \psi_{n\boldsymbol{\lambda}} | \pi_{k\alpha}\rangle \tag{60}$$

$$\langle \partial_i \tilde{\psi}_{n\boldsymbol{\lambda}} | \pi_{k\alpha}\rangle = \langle \partial_i \psi_{n\boldsymbol{\lambda}} | \pi_{k\alpha}\rangle \langle \tilde{\psi}_{n\boldsymbol{\lambda}} | \tilde{\psi}_{n\boldsymbol{\lambda}}\rangle , \tag{61}$$

where $|\tilde{\psi}_{n\boldsymbol{\lambda}}\rangle$ is an unnormalized state. Upon substituting the above two equations into Eq. (59), one can conclude the proof easily. □

We emphasize that at the critical point of the change of the rank of $\rho_{\boldsymbol{\lambda}}$, where there exists $|\tilde{\psi}_{n\boldsymbol{\lambda}}\rangle$ that locally vanishes at $\boldsymbol{\lambda}$ and therefore $|\psi_{n\boldsymbol{\lambda}}\rangle$ is not well-defined. While Eq. (55) is still valid in this case, Eq. (51) should be understood in the sense of taking the limit $\boldsymbol{\lambda}' \to \boldsymbol{\lambda}$ on both sides. We will illustrate this issue in the example of superresolution subsequently, but will not delve into rigorous mathematical discussion on the removable discontinuity of the QFIM at the critical point [55, 56]. Note that $\eta^k_{ii} = 1$, thus for a null projector in single parameter estimation Eq. (55) is satisfied automatically. Moreover, $\eta^k_{ij} = 1/\eta^k_{ji}$. Thus in order to check whether a null projector satisfies Theorem 5, one only needs to verify whether the upper or lower (excluding the diagonal) matrix elements of η^k are real and independent of n and α.

D. Recovering the results by Pezzè et al. [45]

Pezzè et al. [45] obtained the necessary and sufficient conditions for a projective measurement consisting of rank one projectors to saturate the Helstrom CR bound for pure states. Here we recover their results through Theorems 4 and 5. For a pure state $\rho_{\boldsymbol{\lambda}} = |\psi_{\boldsymbol{\lambda}}\rangle \langle \psi_{\boldsymbol{\lambda}}|$, the dimension of supp($\rho_{\boldsymbol{\lambda}}$) is one. Therefore ξ^k_i's naturally do not depend on the index n. Furthermore, for a rank one projector, we suppress the subscript α in the basis vector $|\pi_{k\alpha}\rangle$ and observe that ξ^k_i's naturally do not α either. To satisfy Theorem 4, we only require the coefficients ξ^k_i be real. The SLD for a pure state is $L_{i\boldsymbol{\lambda}} = 2(|\partial_i \psi_{\boldsymbol{\lambda}}\rangle \langle \psi_{\boldsymbol{\lambda}}| + |\psi_{\boldsymbol{\lambda}}\rangle \langle \partial_i \psi_{\boldsymbol{\lambda}}|)$ [27, 54], from which we find $L^{\perp}_{i\boldsymbol{\lambda}} = 0$. Multiplying both sides of Eq. (51) by $\langle\pi_k|\psi_{\boldsymbol{\lambda}}\rangle$, the only requirement that ξ^k_i be real gives

$$\mathrm{Im}[\langle\partial^0_i\psi_{\boldsymbol{\lambda}}|\pi_k\rangle\langle\pi_k|\psi_{\boldsymbol{\lambda}}\rangle] = 0. \tag{62}$$

This equation is equivalent as the Eq. (8) in Pezzè et al. [45] and is a generalization of Eq. (29) in Braunstein and Caves [27]. Similarly, taking $|\tilde{\psi}_{n\boldsymbol{\lambda}}\rangle$ as $|\psi_{\boldsymbol{\lambda}}\rangle$ and multiplying both sides of Eq. (55) by $\langle\pi_k|\partial_j\psi_{\boldsymbol{\lambda}}\rangle$, the only requirement that η^k_{ij} be real gives

$$\mathrm{Im}[\langle\partial_i\psi_{\boldsymbol{\lambda}}|\pi_k\rangle\langle\pi_k|\partial_j\psi_{\boldsymbol{\lambda}}\rangle] = 0, \tag{63}$$

which recovers Eq. (7) of Pezzè et al. [45].

V. APPLICATION TO THE THREE-DIMENSIONAL IMAGING OF TWO INCOHERENT OPTICAL POINT SOURCES

Let us now apply the above theorems to estimate the three-dimensional separation of two *incoherent* point sources of monochromatic light. Fig. 1 shows the basic setup of the problem: The longitudinal axis (Z axis) is taken to be the direction of light propagation. We assume the coordinates of the centroid of the two sources is known and chosen as the origin. The coordinates of the two sources are $\pm\boldsymbol{s} \equiv \pm(s_1, s_2, s_3)$ respectively. The transverse coordinates are denoted as $\boldsymbol{s}_\perp \equiv (s_1, s_2)$ and the dimensionless coordinates at the pupil plane are denoted as $\boldsymbol{r} = (x_1, x_2)$ respectively. We consider the one photon mixed state $\rho_{\boldsymbol{s}} = 1/2\,|\Psi_{+\boldsymbol{s}}\rangle\langle\Psi_{+\boldsymbol{s}}| + 1/2\,|\Psi_{-\boldsymbol{s}}\rangle\langle\Psi_{-\boldsymbol{s}}|$, where $|\Psi_{\pm\boldsymbol{s}}\rangle \equiv e^{i\theta_{\pm s}}|\Phi_{\pm\boldsymbol{s}}\rangle$. The pupil function is $\Phi_{\boldsymbol{s}}(\boldsymbol{r}) \equiv \langle\boldsymbol{r}|\Phi_{\boldsymbol{s}}\rangle = \mathcal{A}\mathrm{circ}(r/a)\exp[ik(\boldsymbol{s}_\perp\cdot\boldsymbol{r} - s_3r^2/2)]$ [30, 57] , where the normalization constant $\mathcal{A} = 1/(\sqrt{\pi}a)$, $\mathrm{circ}(r/a)$ is one if $0 \le r \le a$ and vanishes everywhere else, and $r = \sqrt{x_1^2 + x_2^2}$. The overall phase $\theta_{\boldsymbol{s}}$ is chosen such that $\Delta_{\boldsymbol{s}} \equiv e^{2i\theta_{\boldsymbol{s}}}\int d\boldsymbol{r}\Phi^2_{\boldsymbol{s}}(\boldsymbol{r})$ is real. Due to Eq. (B6), we find $\langle\boldsymbol{r}|\Psi_{-\boldsymbol{s}}\rangle \equiv e^{-i\theta_{\boldsymbol{s}}}\Phi_{-\boldsymbol{s}}(\boldsymbol{r})$ and $\langle\Psi_{-\boldsymbol{s}}|\Psi_{+\boldsymbol{s}}\rangle = \Delta_{\boldsymbol{s}}$ is also real. With this observation, we can diagonalize $\rho_{\boldsymbol{s}}$ with the states $|\psi_{1\boldsymbol{s}}\rangle = |\tilde{\psi}_{1\boldsymbol{\lambda}}\rangle/\sqrt{4p_{1\boldsymbol{s}}}$ and $|\psi_{2\boldsymbol{s}}\rangle = |\tilde{\psi}_{2\boldsymbol{s}}\rangle/\sqrt{4p_{2\boldsymbol{s}}}$, where $|\tilde{\psi}_{1\boldsymbol{s}}\rangle = |\Psi_{+\boldsymbol{s}}\rangle + |\Psi_{-\boldsymbol{s}}\rangle$, $|\tilde{\psi}_{2\boldsymbol{s}}\rangle = -\mathrm{i}(|\Psi_{+\boldsymbol{s}}\rangle - |\Psi_{-\boldsymbol{s}}\rangle)$ and the corresponding eigenvalues $p_{1,2\boldsymbol{s}} = (1 \pm \Delta_{\boldsymbol{s}})/2$. The QFIM associated with $\rho_{\boldsymbol{s}}$ has been shown in Ref. [29], which is $I_{ij} = 4\mathrm{Re}[\langle\partial_i\Phi_{\boldsymbol{s}}|\partial_j\Phi_{\boldsymbol{s}}\rangle + \langle\Phi_{\boldsymbol{s}}|\partial_i\Phi_{\boldsymbol{s}}\rangle\langle\Phi_{\boldsymbol{s}}|\partial_j\Phi_{\boldsymbol{s}}\rangle]$. A straightforward calculation shows that the QFIM is diagonal with diagonal matrix elements k^2a^2, k^2a^2 and $k^2a^4/12$. We will focus on the saturation of the QFIM subsequently and construct the corresponding optimal measurements.

Since now we have successfully diagonalized $\rho_{\boldsymbol{s}}$, we can apply Theorems 4-5 to this problem to obtain the necessary and sufficient conditions for optimal measurements. We summarize the results as two corollaries below. The proofs can be found in Appendices B 2 and B 3. Note that our approach to optimal measurements is quite different from the approach of direct calculations by many papers [12, 29, 33, 35], where one needs to calculate the QFIM first and then check whether the CFIM associated with a specific measurement coincides with the QFIM.

Corollary 1. *The matrix bound of CFIM corresponding to a projector $\Pi_k = \sum_\alpha|\pi_{k\alpha}\rangle\langle\pi_{k\alpha}|$ can be saturated locally at in the limit $\boldsymbol{s}\to 0$ [58], if and only if*

$$\langle\partial^0_i\Phi_{\boldsymbol{s}}|\pi_{k\alpha}\rangle\big|_{\boldsymbol{s}=0} = 0\,\forall i,\,\alpha, \tag{64}$$

provided the projector is regular and if and only if

$$\langle\partial_i\Phi_{\boldsymbol{s}}|\pi_{k\alpha}\rangle\big|_{\boldsymbol{s}=0} = \eta^k_{ij}\langle\partial_j\Phi_{\boldsymbol{s}}|\pi_{k\alpha}\rangle\big|_{\boldsymbol{s}=0}\,\forall i,\,j,\,\alpha, \tag{65}$$

provided the projector is null, where ξ^k_i and η^k_{ij} are real and independent of α.

Corollary 2. *On the line $\boldsymbol{s}_\perp = 0$ the matrix bound of CFIM of estimating the transverse separation corresponding to a projector $\Pi_k = \sum_\alpha|\pi_{k\alpha}\rangle\langle\pi_{k\alpha}|$ can be saturated locally, if and only if*

$$\langle\partial_i\tilde{\psi}_{n\boldsymbol{s}}|\pi_{k\alpha}\rangle = \xi^k_i\langle\tilde{\psi}_{n\boldsymbol{s}}|\pi_{k\alpha}\rangle,\ i = 1,\,2,\,\forall n,\,\alpha, \tag{66}$$

provided the projector is regular, and if and only if

$$\langle\partial_i\tilde{\psi}_{n\boldsymbol{s}}|\pi_{k\alpha}\rangle = \eta^k_{ij}\langle\partial_j\tilde{\psi}_{n\boldsymbol{s}}|\pi_{k\alpha}\rangle,\ i,\,j = 1,\,2,\,\forall n,\,\alpha, \tag{67}$$

provided the projector is null, where ξ^k_i and η^k_{ij} are real and independent of n and α.

Based on Corollary 2, we propose the following *recipe* of searching for the optimal measurements: (i) Identify the regular and null basis vectors in a given complete and orthonormal basis $\{|\pi_{k\alpha}\rangle\}$. (ii) For each regular basis vector $|\pi_{k\alpha}\rangle$, calculate the coefficient $\xi^{k\alpha}_i$ defined in Eq. (66) and check whether $\xi^{k\alpha}_i$'s are real for each i and independent of the index n. (iii) Assemble regular basis vectors that have the same coefficient $\xi^{k\alpha}_i$ as a regular projector $\Pi_k = \sum_\alpha|\pi_{k\alpha}\rangle\langle\pi_{k\alpha}|$. (iv) A null basis vector $|\pi_{k\alpha}\rangle$ is *flexible* if $\langle\partial_i\tilde{\psi}_{n\boldsymbol{s}}|\pi_{k\alpha}\rangle = 0$ for all n and i. The rank one projector $\Pi_{k\alpha}$ formed by a flexible basis vector can be added to any of the previous regular projectors or the following null projectors. (v) For a null basis vector that is not flexible, calculate the upper or lower triangular (excluding diagonal) matrix elements $\eta^{k\alpha}_{ij}$ defined in Eq. (67) and check whether they are all real and independent of the index n. If for $n = 1, 2$, both $\langle\partial_i\tilde{\psi}_{n\boldsymbol{s}}|\pi_{k\alpha}\rangle$ and $\langle\partial_j\tilde{\psi}_{n\boldsymbol{s}}|\pi_{k\alpha}\rangle$ vanishes for some i and j, $\eta^{k\alpha}_{ij}$ can be set arbitrarily. (vi) Assemble null basis vectors that have the same η matrix as a null projector $\Pi_k = |\pi_{k\alpha}\rangle\langle\pi_{k\alpha}|$. A similar recipe can also be constructed based on Corollary 1. It is clear from Theorems 4-5 that any partition of a set of optimal projectors is also optimal. However, from the experimental point of view, we would like to minimize the number of projectors for an optimal measurement.

For the case of $\boldsymbol{s} = 0$, we consider the Zernike basis vectors denoted as $|Z^m_n\rangle$ [59], where $|Z^0_0\rangle = |\Phi_{\boldsymbol{s}}\rangle\big|_{\boldsymbol{s}=\boldsymbol{0}}$.

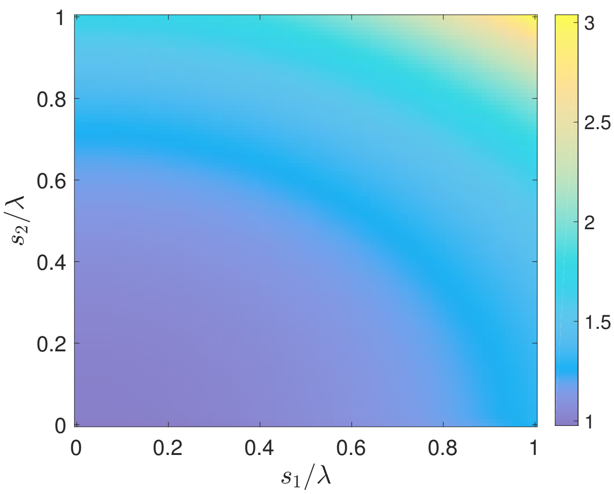

Figure 2. Numerical simulation of the classical Cramér-Rao bound associated with the optimal measurement: $\Pi_1 = \sum_{n=0}^{\infty} |Z_{2n+1}^{1}\rangle \langle Z_{2n+1}^{1}|$, $\Pi_2 = \sum_{n=0}^{\infty} |Z_{2n+1}^{-1}\rangle \langle Z_{2n+1}^{-1}|$ and $\Pi_3 = 1-\Pi_1-\Pi_2$. Note that the QFIM of estimating the transverse separation is diagonal with both diagonal matrix elements k^2a^2. The parameter setting is $a = 0.2$, $\lambda = 1$, $k = 2\pi/\lambda$, $s_3 = 5\lambda$. The plotted quantity is $k^2a^2(F^{-1})_{11}$, where F denotes the CFIM. As we can see, near the origin the quantum Cramér-Rao bound of estimating s_1 is saturated.

Following the recipe above (details can be found in Appendix B 2): (i) $|Z_0^0\rangle$ is the only regular basis vector and the remaining basis vectors are null. (ii) We find $\langle \partial_i^0 \Phi_{\boldsymbol{s}} | Z_0^0\rangle\big|_{\boldsymbol{s}=0} = 0$ for $i = 1, 2, 3$. (iii) Thus we obtain a regular projector $|Z_0^0\rangle\langle Z_0^0|$. (iv) For null basis vectors $|Z_n^m\rangle$ with $(n, m) \neq (1, \pm 1), (2, 0)$, we find $\langle \partial_i \Phi_{\boldsymbol{s}} | Z_n^m\rangle = 0$ for all i. Thus these basis vectors are flexible and can be lumped to the previous regular projector to form a new regular projector Π_1. (v-vi) We then calculate the η matrices corresponding to the null basis vectors $|Z_1^{\pm 1}\rangle$ and $|Z_2^0\rangle$ and find they are all distinct. Therefore we obtain three more null projectors $\Pi_2 = |Z_1^1\rangle\langle Z_1^1|$, $\Pi_3 = |Z_1^{-1}\rangle\langle Z_1^{-1}|$, and $\Pi_4 = |Z_2^0\rangle\langle Z_2^0|$. We conclude that the projectors $\{\Pi_k\}_{k=1}^4$ are the optimal measurement in the limit $\boldsymbol{s} \to 0$.

On the line $\boldsymbol{s}_\perp = 0$, we are interested in estimating the transverse separation and therefore set $i = 1, 2$. After some algebra, it is readily shown that $\tilde{\psi}_{1,2\boldsymbol{s}}(\boldsymbol{r})\big|_{\boldsymbol{s}_\perp=0}$ are even and $\partial_i \tilde{\psi}_{1,2\boldsymbol{s}}(\boldsymbol{r})\big|_{\boldsymbol{s}_\perp=0}$ are odd. We still consider Zernike basis vectors $|Z_n^m\rangle$. Following the previously proposed recipe (details can be found in Appendix B 3: (i) Even basis vectors are either regular or flexible. Odd basis vectors are null and they are also flexible except for $m = \pm 1$. (ii) For regular and even basis vectors $|Z_{2n}^{2m}\rangle$, it is easily calculated that $\xi_i^{(2n,2m)} = 0$ for all i and $|\tilde{\psi}_{1,2\boldsymbol{s}}\rangle$. (iii) Thus we can construct a regular projector as a sum of the rank one projectors formed by all the regular and even basis vectors. (iv) We add all the rank one projectors formed by flexible basis vectors to the previous regular projector to obtain a regular projector $\Pi_1 = 1 - \sum_{n=0}^{\infty} |Z_{2n+1}^{\pm 1}\rangle\langle Z_{2n+1}^{\pm 1}|$. (v) For the remaining null basis vectors, where $m = \pm 1$, we find $\eta_{21}^{(2n+1,\,1)} = 0$ and $\eta_{12}^{(2n+1,\,-1)} = 0$ for $|\psi_{1,\,2\boldsymbol{s}}\rangle$. (vi) Since the set $\{|Z_{2n+1}^{1}\rangle\}$ has the same η matrix and so does the set $\{|Z_{2n+1}^{-1}\rangle\}$, we obtain two null projectors $\Pi_2 = \sum_{n=0}^{\infty} |Z_{2n+1}^{1}\rangle\langle Z_{2n+1}^{1}|$, $\Pi_3 = \sum_{n=0}^{\infty} |Z_{2n+1}^{-1}\rangle\langle Z_{2n+1}^{-1}|$. Note that these optimal projectors are independent of functional form of the radial parts of the Zernike basis functions due to the fact that the radial parts for a fixed angular index m are complete in the radial subspace. In fact, for a state $\langle \boldsymbol{r}|\psi\rangle = \psi(r, \phi)$, one can show that $\langle\psi|\Pi_2|\psi\rangle = 1/\pi \int_0^\infty r dr \left|\int_0^{2\pi} d\phi \psi(r, \phi)\cos\phi\right|^2$ and $\langle\psi|\Pi_3|\psi\rangle = 1/\pi \int_0^\infty r dr \left|\int_0^{2\pi} d\phi \psi(r, \phi)\sin\phi\right|^2$, where one can explicitly see that the probabilities do not depend on the functional form of the radial parts of the basis functions. Furthermore the probability distribution corresponding to such a measurement is insensitive to the small change in the longitudinal separation. Thus one cannot extract any information about s_3 from this measurement. Fig. 2 is the numerical calculation of classical CR bound of estimating s_1 associated with this measurement. As we clearly see from Fig. 2, the Helstrom CR bound of estimating s_1 is saturated near the origin where $\boldsymbol{s}_\perp = 0$. Note that the Helstrom CR bound of estimating s_2 is the same as that of estimating s_1 and hence is omitted here.

On the plane $s_3 = 0$, for the case of $i = 1, 2$, i.e., estimating the transverse separation, following the previous recipe (see Appendix B 4 for details) we find rank one projectors formed by real and parity definite basis functions are optimal on the plane $s_3 = 0$. This result is a generalization of previous one-dimensional transverse estimation [33].

VI. CONCLUSION

We gave the necessary and sufficient conditions for any POVM measurement to give the Helstrom CR bound. Based on these saturation conditions, we predicted several local optimal measurements in the problem of estimating the three-dimensional separation of two incoherent light sources. These predictions are confirmed by numerical simulations.

Based on our results here, many open questions can be further explored, such as searching for a general recipe for the optimal measurement common to all parameters when the partial commutativity condition is satisfied, saturating the QFIM asymptotically due to collective measurements on a large number of identical states, etc. Our work has potential applications in quantum sensing, quantum enhanced imaging, in particular may shed light on investigating the attainability of the Helstrom

CR bound for an initial probe state undergoing noisy dynamics and moment estimation in quantum imaging of finite number of point sources.

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Appendix A: The matrix representation of the SLD

We denote the orthonormal basis vectors of the support and the kernel of $\rho_{\boldsymbol{\lambda}}$ as $|\psi_{n\boldsymbol{\lambda}}\rangle$ and $|e_{n\boldsymbol{\lambda}}\rangle$ respectively. Then Eq. (10), the defining equation of the SLD, in the basis formed by $\{|\psi_{n\boldsymbol{\lambda}}\rangle, |e_{n\boldsymbol{\lambda}}\rangle\}$ becomes

$$[L_{i\boldsymbol{\lambda}}]_{mn}\varrho_{n\boldsymbol{\lambda}}+[L_{i\boldsymbol{\lambda}}]_{mn}\varrho_{m\boldsymbol{\lambda}}=2[\partial_i\rho_{\boldsymbol{\lambda}}]_{mn}, \tag{A1}$$

where $[L_{i\boldsymbol{\lambda}}]_{mn}\equiv\langle m|L_{i\boldsymbol{\lambda}}|n\rangle$, $|n\rangle$ is the eigenvector of $\rho_{\boldsymbol{\lambda}}$ which could be either $|\psi_{n\boldsymbol{\lambda}}\rangle$ or $|e_{n\boldsymbol{\lambda}}\rangle$,

$$\begin{aligned}\partial_i\rho_{\boldsymbol{\lambda}}=&\sum_n\partial_i p_{n\boldsymbol{\lambda}}|\psi_{n\boldsymbol{\lambda}}\rangle\langle\psi_{n\boldsymbol{\lambda}}|+\sum_n p_{n\boldsymbol{\lambda}}|\partial_i\psi_{n\boldsymbol{\lambda}}\rangle\langle\psi_{n\boldsymbol{\lambda}}|\\&+\sum_n p_{n\boldsymbol{\lambda}}|\psi_{n\boldsymbol{\lambda}}\rangle\langle\partial_i\psi_{n\boldsymbol{\lambda}}|\end{aligned} \tag{A2}$$

and $\varrho_{n\boldsymbol{\lambda}}$ is the corresponding eigenvalue which could be either the positive eigenvalue $p_{n\boldsymbol{\lambda}}$ or zero. From Eq. (A2), we know that for $|m\rangle=|e_{m\boldsymbol{\lambda}}\rangle$ and $|n\rangle=|e_{n\boldsymbol{\lambda}}\rangle$, where $\varrho_m=\varrho_n=0$,

$$\langle e_{m\boldsymbol{\lambda}}|\partial_i\rho_{\boldsymbol{\lambda}}|e_{n\boldsymbol{\lambda}}\rangle=0,\ \forall m,\,n. \tag{A3}$$

Thus we can choose

$$\langle e_{m\boldsymbol{\lambda}}|L_{i\boldsymbol{\lambda}}|e_{n\boldsymbol{\lambda}}\rangle=0. \tag{A4}$$

Therefore the following choice of the SLD

$$[L_{i\boldsymbol{\lambda}}]_{mn}=\begin{cases}0 & |m\rangle=|e_{m\boldsymbol{\lambda}}\rangle \text{ and } |n\rangle=|e_{n\boldsymbol{\lambda}}\rangle\\ \frac{2[\partial_i\rho_{\boldsymbol{\lambda}}]_{mn}}{\varrho_{m\boldsymbol{\lambda}}+\varrho_{n\boldsymbol{\lambda}}} & \text{else}\end{cases} \tag{A5}$$

can satisfy its matrix definition Eq. (A1). Based on Eqs. (A2, A5), a matrix representation of the SLD,

$$\begin{aligned}L_{i\boldsymbol{\lambda}}=&\sum_n\frac{\partial_i p_{n,\boldsymbol{\lambda}}}{p_{n,\boldsymbol{\lambda}}}|\psi_{n\boldsymbol{\lambda}}\rangle\langle\psi_{n\boldsymbol{\lambda}}|\\&+2\sum_{m,n}\frac{p_{m\boldsymbol{\lambda}}-p_{n\boldsymbol{\lambda}}}{p_{m\boldsymbol{\lambda}}+p_{n\boldsymbol{\lambda}}}\langle\partial_i\psi_{m\boldsymbol{\lambda}}|\psi_{n\boldsymbol{\lambda}}\rangle|\psi_{m\boldsymbol{\lambda}}\rangle\langle\psi_{n\boldsymbol{\lambda}}|\\&+\left[2\sum_{m,n}\langle\partial_i\psi_{n\boldsymbol{\lambda}}|e_{m\boldsymbol{\lambda}}\rangle|\psi_{n\boldsymbol{\lambda}}\rangle\langle e_{m\boldsymbol{\lambda}}|+\text{c.c.}\right],\end{aligned} \tag{A6}$$

can be found [54]. With Eq. (A6), it is straightforward to calculate, for a state $|\psi\rangle=|\psi^0\rangle+|\psi^\perp\rangle$,

$$\begin{aligned}L_{i\boldsymbol{\lambda}}|\psi\rangle=&L^\perp_{i\boldsymbol{\lambda}}|\psi\rangle+2\sum_{m,n}\langle\partial_i\psi_{n\boldsymbol{\lambda}}|e_{m\boldsymbol{\lambda}}\rangle\langle e_{m\boldsymbol{\lambda}}|\psi^0\rangle|\psi_{n\boldsymbol{\lambda}}\rangle\\&+2\sum_{m,n}\langle e_{m\boldsymbol{\lambda}}|\partial_i\psi_{n\boldsymbol{\lambda}}\rangle\langle\psi_{n,\boldsymbol{\lambda}}|\psi^\perp\rangle|e_{m,\boldsymbol{\lambda}}\rangle,\end{aligned} \tag{A7}$$

where

$$\begin{aligned}L^\perp_{i\boldsymbol{\lambda}}\equiv&\sum_n\frac{\partial_i p_{n\boldsymbol{\lambda}}}{p_{n\boldsymbol{\lambda}}}|\psi_{n\boldsymbol{\lambda}}\rangle\langle\psi_{n\boldsymbol{\lambda}}|\\&+2\sum_{m,n}\frac{p_{m\boldsymbol{\lambda}}-p_{n\boldsymbol{\lambda}}}{p_{m\boldsymbol{\lambda}}+p_{n\boldsymbol{\lambda}}}\langle\partial_i\psi_{m\boldsymbol{\lambda}}|\psi_{n\boldsymbol{\lambda}}\rangle|\psi_{m\boldsymbol{\lambda}}\rangle\langle\psi_{n\boldsymbol{\lambda}}|,\end{aligned} \tag{A8}$$

is the projection of the SLD on the subspace $\mathrm{supp}(\rho_{\boldsymbol{\lambda}})$. Upon noting the following identities

$$\langle\partial_i\psi_{n\boldsymbol{\lambda}}|e_{m\boldsymbol{\lambda}}\rangle=\langle\partial_i^0\psi_{n\boldsymbol{\lambda}}|e_{m\boldsymbol{\lambda}}\rangle, \tag{A9}$$

$$\begin{aligned}&\sum_m\langle\partial_i^0\psi_{n\boldsymbol{\lambda}}|e_{m\boldsymbol{\lambda}}\rangle\langle e_{m\boldsymbol{\lambda}}|\psi^0\rangle\\&=\langle\partial_i^0\psi_{n\boldsymbol{\lambda}}|\psi^0\rangle=\langle\partial_i^0\psi_{n\boldsymbol{\lambda}}|\psi\rangle,\end{aligned} \tag{A10}$$

we obtain

$$\langle\psi_{n\boldsymbol{\lambda}}|L_{i\boldsymbol{\lambda}}|\psi\rangle=\langle\psi_{n\boldsymbol{\lambda}}|L^\perp_{i\boldsymbol{\lambda}}|\psi\rangle+2\langle\partial_i^0\psi_{n\boldsymbol{\lambda}}|\psi\rangle. \tag{A11}$$

Appendix B: Details on the example of estimating the separations of two incoherent optical point sources

1. Properties of $|\psi_{1,\,2\boldsymbol{s}}\rangle$

We mention in the main text that $\theta_{\boldsymbol{s}}$ is chosen such that

$$\Delta_{\boldsymbol{s}}\equiv e^{2\mathrm{i}\theta_{\boldsymbol{s}}}\int d\boldsymbol{r}\Phi^2_{\boldsymbol{s}}(\boldsymbol{r}) \tag{B1}$$

is real. Defining

$$\begin{aligned}v_{\boldsymbol{s}}\equiv&\mathrm{Re}[\int d\boldsymbol{r}\Phi^2_{\boldsymbol{s}}(\boldsymbol{r})]\\&=\mathcal{A}^2\int d\boldsymbol{r}\mathrm{circ}(r/a)\cos(2k\boldsymbol{s}_\perp\cdot\boldsymbol{r})\cos(ks_3r^2),\end{aligned} \tag{B2}$$

$$\begin{aligned}w_{\boldsymbol{s}}\equiv&\mathrm{Im}[\int d\boldsymbol{r}\Phi^2_{\boldsymbol{s}}(\boldsymbol{r})]\\&=-\mathcal{A}^2\int d\boldsymbol{r}\mathrm{circ}(r/a)\cos(2k\boldsymbol{s}_\perp\cdot\boldsymbol{r})\sin(ks_3r^2),\end{aligned} \tag{B3}$$

we can express $\theta_{\boldsymbol{s}}$ and $\Delta_{\boldsymbol{s}}$ as

$$\tan 2\theta_{\boldsymbol{s}}=-\frac{w_{\boldsymbol{s}}}{v_{\boldsymbol{s}}}, \tag{B4}$$

$$\Delta_{\boldsymbol{s}} = \sqrt{v_{\boldsymbol{s}}^2 + w_{\boldsymbol{s}}^2}. \tag{B5}$$

As is clear from Eqs. (B2, B3), $v_{\boldsymbol{s}}$ is even in $\boldsymbol{s}$ while $w_{\boldsymbol{s}}$ is odd in $\boldsymbol{s}$. Thus according to Eq. (B4), we know $\theta_{\boldsymbol{s}}$ is odd in $\boldsymbol{s}$, i.e.,

$$\theta_{\boldsymbol{s}} = -\theta_{-\boldsymbol{s}}. \tag{B6}$$

With these observations, the one photon state defined in the main text can be diagonalized by the following state:

$$\begin{aligned}\psi_{1\boldsymbol{s}}(\boldsymbol{r}) &= \frac{1}{\sqrt{2(1+\Delta_{\boldsymbol{s}})}}[\Psi_{+\boldsymbol{s}}(\boldsymbol{r}) + \Psi_{-\boldsymbol{s}}(\boldsymbol{r})] \\ &= \frac{\tilde{\psi}_{1\boldsymbol{s}}(\boldsymbol{r})}{\sqrt{4p_{1\boldsymbol{s}}}},\end{aligned} \tag{B7}$$

$$\begin{aligned}\psi_{2\boldsymbol{s}}(\boldsymbol{r}) &= \frac{-\mathrm{i}}{\sqrt{2(1-\Delta_{\boldsymbol{s}})}}[\Psi_{+\boldsymbol{s}}(\boldsymbol{r}) - \Psi_{-\boldsymbol{s}}(\boldsymbol{r})] \\ &= \frac{\tilde{\psi}_{2\boldsymbol{s}}(\boldsymbol{r})}{\sqrt{4p_{2\boldsymbol{s}}}}\end{aligned} \tag{B8}$$

where

$$\Psi_{\pm\boldsymbol{s}}(\boldsymbol{r}) = e^{\pm i\theta_{\boldsymbol{s}}}\Phi_{\pm\boldsymbol{s}}(\boldsymbol{r}), \tag{B9}$$

$$\Phi_{\boldsymbol{s}}(\boldsymbol{r}) = \mathcal{A}\mathrm{circ}(r/a)\exp[ik(\boldsymbol{s}_\perp\cdot\boldsymbol{r} - s_3 r^2/2)]. \tag{B10}$$

We can write the explicit forms of $\psi_{\pm\boldsymbol{s}}(\boldsymbol{r}) \equiv \langle \boldsymbol{r}|\psi_{\pm\boldsymbol{s}}\rangle$ as

$$\begin{aligned}\psi_{1\boldsymbol{s}}(\boldsymbol{r}) = \frac{\tilde{\psi}_{1\boldsymbol{s}}(\boldsymbol{r})}{\sqrt{4p_{1\boldsymbol{s}}}} &= \frac{2\mathcal{A}\mathrm{circ}(r/a)}{\sqrt{4p_{1\boldsymbol{s}}}}, \\ &\times\cos(\theta_{\boldsymbol{s}} + k\boldsymbol{s}_\perp\cdot\boldsymbol{r} - ks_3r^2/2)\end{aligned} \tag{B11}$$

$$\begin{aligned}\psi_{2\boldsymbol{s}}(\boldsymbol{r}) = \frac{\tilde{\psi}_{2\boldsymbol{s}}(\boldsymbol{r})}{\sqrt{4p_{2\boldsymbol{s}}}} &= \frac{2\mathcal{A}\mathrm{circ}(r/a)}{\sqrt{4p_{2\boldsymbol{s}}}}. \\ &\times\sin(\theta_{\boldsymbol{s}} + k\boldsymbol{s}_\perp\cdot\boldsymbol{r} - ks_3r^2/2)\end{aligned} \tag{B12}$$

Eqs. (B9, B10) immediately tell us

$$\begin{aligned}\langle\partial_i\Psi_{+\boldsymbol{s}}|\Psi_{+\boldsymbol{s}}\rangle &= -\langle\partial_i\Psi_{-\boldsymbol{s}}|\Psi_{-\boldsymbol{s}}\rangle \\ &= -i\partial_i\theta_{\boldsymbol{s}} + i\delta_{i3}ka^2/4,\end{aligned} \tag{B13}$$

$$\begin{aligned}\langle\partial_i\Psi_{-\boldsymbol{s}}|\Psi_{+\boldsymbol{s}}\rangle &= \langle\partial_i\Psi_{+\boldsymbol{s}}|\Psi_{-\boldsymbol{s}}\rangle \\ &= -\partial_i\Delta_{\boldsymbol{s}}/2,\end{aligned} \tag{B14}$$

where δ_{i3} is the Kronecker delta.

From Eqs. (B7, B8) we know that $\psi_{1,2\boldsymbol{s}}(\boldsymbol{r})$ are real. Therefore we conclude $\langle\partial_i\psi_{1\boldsymbol{s}}|\psi_{1\boldsymbol{s}}\rangle$ and $\langle\partial_i\psi_{2\boldsymbol{s}}|\psi_{2\boldsymbol{s}}\rangle$ must be real. On other hand, they must be purely imaginary due to the fact that $\langle\partial_i\psi_{n\boldsymbol{s}}|\psi_{n\boldsymbol{s}}\rangle + \langle\psi_{n\boldsymbol{s}}|\partial_i\psi_{n\boldsymbol{s}}\rangle = 0$ for $n = 1, 2$. So we end up with

$$\langle\partial_i\psi_{1\boldsymbol{s}}|\psi_{1\boldsymbol{s}}\rangle = \langle\partial_i\psi_{2\boldsymbol{s}}|\psi_{2\boldsymbol{s}}\rangle = 0. \tag{B15}$$

Furthermore $\langle\partial_i\psi_{1\boldsymbol{s}}|\psi_{2\boldsymbol{s}}\rangle$ is also real since, upon application of Eqs. (B13, B14),

$$\begin{aligned}\langle\partial_i\psi_{1\boldsymbol{s}}|\psi_{2\boldsymbol{s}}\rangle &= \frac{-\mathrm{i}}{2\sqrt{1-\Delta_{\boldsymbol{s}}^2}}(\langle\partial_i\Psi_{+\boldsymbol{s}}| + \langle\partial_i\Psi_{-\boldsymbol{s}}|) \\ &\quad\times(|\Psi_{+\boldsymbol{s}}\rangle - |\Psi_{-\boldsymbol{s}}\rangle) \\ &= \frac{-\mathrm{i}}{2\sqrt{1-\Delta_{\boldsymbol{s}}^2}}(\langle\partial_i\Psi_{+\boldsymbol{s}}|\Psi_{+\boldsymbol{s}}\rangle - \langle\partial_i\Psi_{-\boldsymbol{s}}|\Psi_{-\boldsymbol{s}}\rangle \\ &\quad\cancel{+ \langle\partial_i\Psi_{-\boldsymbol{s}}|\Psi_{+\boldsymbol{s}}\rangle - \langle\partial_i\Psi_{+\boldsymbol{s}}|\Psi_{-\boldsymbol{s}}\rangle})) \\ &= \frac{-\mathrm{i}\langle\partial_i\Psi_{+\boldsymbol{s}}|\Psi_{+\boldsymbol{s}}\rangle}{\sqrt{1-\Delta_{\boldsymbol{s}}^2}} \\ &= \frac{-\partial_i\theta_{\boldsymbol{s}} + \delta_{i3}ka^2/4}{\sqrt{1-\Delta_{\boldsymbol{s}}^2}}.\end{aligned} \tag{B16}$$

The fact that $\partial_i\langle\psi_{2\boldsymbol{s}}|\psi_{1\boldsymbol{s}}\rangle = 0$ gives $\langle\partial_i\psi_{2\boldsymbol{s}}|\psi_{1\boldsymbol{s}}\rangle = -\langle\psi_{2\boldsymbol{s}}|\partial_i\psi_{1\boldsymbol{s}}\rangle$. On the other hand Eq. (B16) tells us $\langle\psi_{2\boldsymbol{s}}|\partial_i\psi_{1\boldsymbol{s}}\rangle = \langle\partial_i\psi_{1\boldsymbol{s}}|\psi_{2\boldsymbol{s}}\rangle$. Thus we know

$$\langle\partial_i\psi_{2\boldsymbol{s}}|\psi_{1\boldsymbol{s}}\rangle = -\langle\partial_i\psi_{1\boldsymbol{s}}|\psi_{2\boldsymbol{s}}\rangle. \tag{B17}$$

2. The case $\boldsymbol{s} = 0$

We first apply Theorem 3 in the main text to obtain the following Lemmas, which will be useful subsequently.

Lemma 3. *For the mixed state $\rho_{\boldsymbol{s}}$, the matrix bound of the CFIM due to a regular projector $\Pi_k = \sum_\alpha|\pi_{k\alpha}\rangle\langle\pi_{k\alpha}|$ is saturated if and only if*

$$\begin{aligned}&\frac{\partial_i p_{1\boldsymbol{s}}}{p_{1\boldsymbol{s}}}\langle\psi_{1\boldsymbol{s}}|\pi_{k\alpha}\rangle - 4p_{2\boldsymbol{s}}\langle\partial_i\psi_{1\boldsymbol{s}}|\psi_{2\boldsymbol{s}}\rangle\langle\psi_{2\boldsymbol{s}}|\pi_{k\alpha}\rangle \\ &\quad+2\langle\partial_i\psi_{1\boldsymbol{s}}|\pi_{k\alpha}\rangle = \xi_i^k\langle\psi_{1\boldsymbol{s}}|\pi_{k\alpha}\rangle,\end{aligned} \tag{B18}$$

$$\begin{aligned}&\frac{\partial_i p_{2\boldsymbol{s}}}{p_{2\boldsymbol{s}}}\langle\psi_{2\boldsymbol{s}}|\pi_{k\alpha}\rangle - 4p_{1\boldsymbol{s}}\langle\partial_i\psi_{2\boldsymbol{s}}|\psi_{1\boldsymbol{s}}\rangle\langle\psi_{1\boldsymbol{s}}|\pi_{k\alpha}\rangle \\ &\quad+2\langle\partial_i\psi_{2\boldsymbol{s}}|\pi_{k\alpha}\rangle = \xi_i^k\langle\psi_{2\boldsymbol{s}}|\pi_{k\alpha}\rangle,\end{aligned} \tag{B19}$$

holds $\forall i$, α, where $p_{1,2\boldsymbol{s}} = (1\pm\Delta_{\boldsymbol{s}})/2$ and ξ_i^k is real and independent of n and α.

Proof. According to Eqs. (A8, B15), we find

$$\begin{aligned}L_{i\boldsymbol{s}}^\perp &= \frac{\partial_i\Delta_{\boldsymbol{s}}}{1+\Delta_{\boldsymbol{s}}}|\psi_{1\boldsymbol{s}}\rangle\langle\psi_{1\boldsymbol{s}}| - \frac{\partial_i\Delta_{\boldsymbol{s}}}{1-\Delta_{\boldsymbol{s}}}|\psi_{2\boldsymbol{s}}\rangle\langle\psi_{2\boldsymbol{s}}| \\ &\quad+2\Delta_{\boldsymbol{s}}\langle\partial_i\psi_{1\boldsymbol{s}}|\psi_{2\boldsymbol{s}}\rangle|\psi_{1\boldsymbol{s}}\rangle\langle\psi_{2\boldsymbol{s}}| \\ &\quad-2\Delta_{\boldsymbol{s}}\langle\partial_i\psi_{2\boldsymbol{s}}|\psi_{1\boldsymbol{s}}\rangle|\psi_{2\boldsymbol{s}}\rangle\langle\psi_{1\boldsymbol{s}}|.\end{aligned} \tag{B20}$$

Thus

$$L^{\perp}_{i\boldsymbol{s}}\left|\pi_{k\alpha}\right\rangle = \left|\psi_{1\boldsymbol{s}}\right\rangle\left[\frac{\partial_i\Delta_{\boldsymbol{s}}}{1+\Delta_{\boldsymbol{s}}}\left\langle\psi_{1\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle + 2\Delta_{\boldsymbol{s}}\left\langle\partial_i\psi_{1\boldsymbol{s}}\middle|\psi_{2\boldsymbol{s}}\right\rangle\left\langle\psi_{2\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle\right] + \left|\psi_{2\boldsymbol{s}}\right\rangle\left[-\frac{\partial_i\Delta_{\boldsymbol{s}}}{1-\Delta_{\boldsymbol{s}}}\left\langle\psi_{2\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle - 2\Delta_{\boldsymbol{s}}\left\langle\partial_i\psi_{2\boldsymbol{s}}\middle|\psi_{1\boldsymbol{s}}\right\rangle\left\langle\psi_{1\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle\right], \tag{B21}$$

which can be rewritten as upon noting Eq. (B15),

$$L^{\perp}_{i\boldsymbol{s}}\left|\pi_{k\alpha}\right\rangle = \left|\psi_{1\boldsymbol{s}}\right\rangle\left[\frac{\partial_i\Delta_{\boldsymbol{s}}}{1+\Delta_{\boldsymbol{s}}}\left\langle\psi_{1\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle + 2\Delta_{\boldsymbol{s}}\left\langle\partial_i^{\perp}\psi_{1\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle\right] + \left|\psi_{2\boldsymbol{s}}\right\rangle\left[-\frac{\partial_i\Delta_{\boldsymbol{s}}}{1-\Delta_{\boldsymbol{s}}}\left\langle\psi_{2\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle - 2\Delta_{\boldsymbol{s}}\left\langle\partial_i^{\perp}\psi_{2\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle\right]. \tag{B22}$$

In order to saturate the Helstrom CR bound, according to Theorem 4 in the main text, every regular projector $\Pi_k = \sum_\alpha \left|\pi_{k\alpha}\right\rangle\left\langle\pi_{k\alpha}\right|$ must satisfy

$$\frac{\partial_i\Delta_{\boldsymbol{s}}}{1+\Delta_{\boldsymbol{s}}}\left\langle\psi_{1\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle + 2\Delta_{\boldsymbol{s}}\left\langle\partial_i^{\perp}\psi_{1\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle + 2\left\langle\partial_i^{0}\psi_{1\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle = \xi_i^k\left\langle\psi_{1\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle, \tag{B23}$$

$$-\frac{\partial_i\Delta_{\boldsymbol{s}}}{1-\Delta_{\boldsymbol{s}}}\left\langle\psi_{2\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle - 2\Delta_{\boldsymbol{s}}\left\langle\partial_i^{\perp}\psi_{2\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle + 2\left\langle\partial_i^{0}\psi_{2\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle = \xi_i^k\left\langle\psi_{2\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle, \tag{B24}$$

where ξ_i^k is real. With the facts that $\left\langle\partial_i^{\perp}\psi_{1,\,2\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle + \left\langle\partial_i^{0}\psi_{1,\,2\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle = \left\langle\partial_i\psi_{1,\,2\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle$ and $p_{1,\,2\boldsymbol{s}} = (1\pm\Delta_{\boldsymbol{s}})/2$, one can easily concludes the proof. □

a. *Proof of Corollary 1 in the main text*

Proof. We find at $\boldsymbol{s}=0$

$$\Delta_{\boldsymbol{s}} = 1 \tag{B25}$$

and $p_{1\boldsymbol{s}}\big|_{\boldsymbol{s}=0} = 1$ and $p_{2\boldsymbol{s}}\big|_{\boldsymbol{s}=0} = 0$. Therefore $p_{1\boldsymbol{s}}$ and $p_{2\boldsymbol{s}}$ attain their local maximum and minimum respectively at $\boldsymbol{s}=0$, i.e., $\partial_i p_{1\boldsymbol{s}} = \partial_i p_{2\boldsymbol{s}} = 0$, which indicates

$$\partial_i\Delta_{\boldsymbol{s}} = 0,\ i = 1,\ 2,\ 3. \tag{B26}$$

We recognize that $\boldsymbol{s}=0$ is the critical point of the change of the rank of $\rho_{\boldsymbol{s}}$. In this case, both the normalized vector $\left|\psi_{2\boldsymbol{s}}\right\rangle$ and the first term on the left hand side of Eq. (B19) is not well-defined. Therefore Eqs. (B18, B19) should be understood in the sense of the limit $\boldsymbol{s}\to 0$. It can be also shown that for $i = 1,\ 2,\ 3$,

$$\partial_i\tilde{\psi}_{1\boldsymbol{s}}(\boldsymbol{r})\big|_{\boldsymbol{s}=0} = \partial_i\psi_{1\boldsymbol{s}}(\boldsymbol{r})\big|_{\boldsymbol{s}=0} = 0, \tag{B27}$$

$$\left|\tilde{\psi}_{2\boldsymbol{s}}\right\rangle\big|_{\boldsymbol{s}=0} = 0 \tag{B28}$$

With these facts, the second term of the left hand side of Eq. (B18) reads

$$4p_{2\boldsymbol{s}}\left\langle\partial_i\psi_{1\boldsymbol{s}}\middle|\psi_{2\boldsymbol{s}}\right\rangle\left\langle\psi_{2\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle = \left\langle\partial_i\psi_{1\boldsymbol{s}}\middle|\tilde{\psi}_{2\boldsymbol{s}}\right\rangle\left\langle\tilde{\psi}_{2\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle = 0, \tag{B29}$$

which immediately tells us that for a regular projector Π_k that saturates its matrix bound $\xi_i^k = 0\,\forall i = 1,\ 2\ 3$. In order to saturate the matrix bound, it remains to show Eq. (B19) is consistent with the result $\xi_i^k = 0$. It is readily checked that

$$\left\langle\partial_i\psi_{2\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle = \frac{\left\langle\partial_i\tilde{\psi}_{2\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle}{\sqrt{4p_{2\boldsymbol{s}}}} - \frac{\partial_i p_{2\boldsymbol{s}}}{2p_{2\boldsymbol{s}}}\frac{\left\langle\tilde{\psi}_{2\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle}{\sqrt{4p_{2\boldsymbol{s}}}} \tag{B30}$$

$$\lim_{\boldsymbol{s}\to 0} p_{1\boldsymbol{s}}\left\langle\partial_i\psi_{2\boldsymbol{s}}\middle|\psi_{1\boldsymbol{s}}\right\rangle\left\langle\psi_{1\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle = -\lim_{\boldsymbol{s}\to 0}\frac{\left\langle\tilde{\psi}_{2\boldsymbol{s}}\middle|\partial_i\psi_{1\boldsymbol{s}}\right\rangle}{\sqrt{4p_{2\boldsymbol{s}}}}\left\langle\psi_{1\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle \tag{B31}$$

the left hand and right hand sides of Eq. (B19) can be written as

$$\text{LHS} = \lim_{\boldsymbol{s}\to 0}\frac{2\left\langle\tilde{\psi}_{2\boldsymbol{s}}\middle|\partial_i\psi_{1\boldsymbol{s}}\right\rangle}{\sqrt{p_{2\boldsymbol{s}}}}\left\langle\psi_{1\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle + \frac{\left\langle\partial_i\tilde{\psi}_{2\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle}{\sqrt{p_{2\boldsymbol{s}}}} \tag{B32}$$

$$\text{RHS} = \xi_i^k\lim_{\boldsymbol{s}\to 0}\left\langle\psi_{2\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle = \xi_i^k\lim_{\boldsymbol{s}\to 0}\frac{\left\langle\tilde{\psi}_{2\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle}{\sqrt{4p_{2\boldsymbol{s}}}} \tag{B33}$$

Upon eliminating the factor $1/\sqrt{p_{2\boldsymbol{s}}}$ in both equations and noting that $\lim_{\boldsymbol{s}\to 0}\left\langle\tilde{\psi}_{2\boldsymbol{s}}\middle|\partial_i\psi_{1\boldsymbol{s}}\right\rangle = \lim_{\boldsymbol{s}\to 0}\left\langle\tilde{\psi}_{2\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle = 0$, we find that LHS = RHS is the consistent with the result $\xi_i^k = 0$ if and only if

$$\lim_{\boldsymbol{s}\to 0}\left\langle\partial_i\tilde{\psi}_{2\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle = \left\langle\partial_i\tilde{\psi}_{2\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle\big|_{\boldsymbol{s}=0} = 0,\ \forall i,\ \alpha. \tag{B34}$$

It is straightforward to calculate for $i = 1,\ 2,\ 3$, we have

$$\partial_i\tilde{\psi}_{2\boldsymbol{s}}(\boldsymbol{r})\big|_{\boldsymbol{s}=0} = -\mathrm{i}[\partial_i\Psi_{+\boldsymbol{s}}(\boldsymbol{r}) - \partial_i\Psi_{-\boldsymbol{s}}(\boldsymbol{r})]\big|_{\boldsymbol{s}=0} = [2\partial_i\theta_{\boldsymbol{s}}\Phi_{\boldsymbol{s}}(\boldsymbol{r}) - 2\mathrm{i}\partial_i\Phi_{\boldsymbol{s}}(\boldsymbol{r})]\big|_{\boldsymbol{s}=0} \tag{B35}$$

On the other hand, at $\boldsymbol{s}=0$, according to Eqs. (B2, B3), the explicit forms of $v_{\boldsymbol{s}}$ and $w_{\boldsymbol{s}}$ can be expressed as

$$v_{\boldsymbol{s}}\big|_{\boldsymbol{s}=0} = \pi\mathcal{A}^2a^2, \tag{B36}$$

$$w_{\boldsymbol{s}}\big|_{\boldsymbol{s}=0} = 0, \tag{B37}$$

According to Eq. (B4), we obtain

$$\theta_{\boldsymbol{s}}\big|_{\boldsymbol{s}=0} = 0. \tag{B38}$$

Differentiating both sides of Eq. (B1), we obtain

$$\partial_i \Delta_{\boldsymbol{s}} = 2\mathrm{i}\partial_i\theta_{\boldsymbol{s}} \int d\boldsymbol{r}\Phi_{\boldsymbol{s}}^2(\boldsymbol{r}) + 2e^{2\mathrm{i}\theta_{\boldsymbol{s}}} \int d\boldsymbol{r}\Phi_{\boldsymbol{s}}(\boldsymbol{r})\partial_i\Phi_{\boldsymbol{s}}(\boldsymbol{r}) \tag{B39}$$

So at $\boldsymbol{s}=0$, $\int d\boldsymbol{r}\Phi_{\boldsymbol{s}}^2(\boldsymbol{r})\big|_{\boldsymbol{s}=0} = 1$ and $\Phi_{\boldsymbol{s}}(\boldsymbol{r})\big|_{\boldsymbol{s}=0} =$ is real and therefor

$$\begin{aligned}\partial_i\theta_{\boldsymbol{s}}\big|_{\boldsymbol{s}=0} &= \mathrm{i}\int d\boldsymbol{r}\Phi_{\boldsymbol{s}}(\boldsymbol{r})\partial_i\Phi_{\boldsymbol{s}}(\boldsymbol{r})\big|_{\boldsymbol{s}=0} \\ &= \mathrm{i}\left\langle\Phi_{\boldsymbol{s}}\middle|\partial_i\Phi_{\boldsymbol{s}}\right\rangle\big|_{\boldsymbol{s}=0}\end{aligned} \tag{B40}$$

According to Eqs. (B35, B40), we know

$$\begin{aligned}\left|\partial_i\tilde{\psi}_{2\boldsymbol{s}}\right\rangle\big|_{\boldsymbol{s}=0} &= 2\mathrm{i}(\left|\Phi_{\boldsymbol{s}}\right\rangle\left\langle\Phi_{\boldsymbol{s}}\middle|\partial_i\Phi_{\boldsymbol{s}}\right\rangle - \left|\partial_i\Phi_{\boldsymbol{s}}\right\rangle)\big|_{\boldsymbol{s}=0} \\ &= -2\mathrm{i}\left|\partial_i^0\Phi_{\boldsymbol{s}}\right\rangle\end{aligned} \tag{B41}$$

where $|\partial_i^0\Phi_{\boldsymbol{s}}\rangle$ is the projection of $|\partial_i\Phi_{\boldsymbol{s}}\rangle$ onto the kernel of $|\Phi_{\boldsymbol{s}}\rangle\langle\Phi_{\boldsymbol{s}}|$. Therefore the satisfaction of Eq. (B34) is equivalent as

$$\left\langle\partial_i^0\Phi_{\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle\big|_{\boldsymbol{s}=0} = 0,\ \forall i,\ \alpha \tag{B42}$$

The saturation of the matrix bound associated with a null projector requires that

$$\left\langle\partial_i\tilde{\psi}_{1\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle\big|_{\boldsymbol{s}=0} = \eta_{ij}^k\left\langle\partial_j\tilde{\psi}_{1\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle\big|_{\boldsymbol{s}=0},\ \forall i,\ j,\ \alpha, \tag{B43}$$

$$\left\langle\partial_i\tilde{\psi}_{2\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle\big|_{\boldsymbol{s}=0} = \eta_{ij}^k\left\langle\partial_j\tilde{\psi}_{2\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle\big|_{\boldsymbol{s}=0},\ \forall i,\ j,\ \alpha. \tag{B44}$$

Due to Eq. (B27), Eq. (B43) is trivially satisfied. Note that for null projectors $\langle\Phi_{\boldsymbol{s}}|\pi_{k\alpha}\rangle\big|_{\boldsymbol{s}=0} = 0$ and therefore according to Eq. (B41), we find

$$\left\langle\partial_i\tilde{\psi}_{2\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle\big|_{\boldsymbol{s}=0} = 2\mathrm{i}\left\langle\partial_i\Phi_{\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle\big|_{\boldsymbol{s}=0}. \tag{B45}$$

Now the satisfaction of Eq. (B34) is equivalent as is

$$\left\langle\partial_i\Phi_{\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle\big|_{\boldsymbol{s}=0} = \eta_{ij}^k\left\langle\partial_j\Phi_{\boldsymbol{s}}\middle|\pi_{k\alpha}\right\rangle\big|_{\boldsymbol{s}=0},\ \forall i,\ j,\ \alpha. \tag{B46}$$

□

b. *Details of constructing the optimal measurement in the main text*

It is easily calculated that

$$\left|\Phi_{\boldsymbol{s}}\right\rangle\big|_{\boldsymbol{s}=0} = \left|Z_0^0\right\rangle, \tag{B47}$$

$$\left|\partial_1\Phi_{\boldsymbol{s}}\right\rangle\big|_{\boldsymbol{s}=0} = ik\left|Z_1^1\right\rangle/2, \tag{B48}$$

$$\left|\partial_2\Phi_{\boldsymbol{s}}\right\rangle\big|_{\boldsymbol{s}=0} = ik\left|Z_1^{-1}\right\rangle/2, \tag{B49}$$

$$\left|\partial_3\Phi_{\boldsymbol{s}}\right\rangle\big|_{\boldsymbol{s}=0} = -ik(\left|Z_2^0\right\rangle/3 + \left|Z_0^0\right\rangle)/2. \tag{B50}$$

With Eqs. (B47-B50), one can easily understand the details in the construction recipes in the main text. For example, the following facts can be obtained:

$$\left\langle\partial_i^0\Phi_{\boldsymbol{s}}\middle|Z_0^0\right\rangle\big|_{\boldsymbol{s}=0} = \left\langle\partial_i\Phi_{\boldsymbol{s}}\middle|Z_0^0\right\rangle\big|_{\boldsymbol{s}=0} = 0,\ i=1,\ 2, \tag{B51}$$

$$\begin{aligned}\left\langle\partial_3^0\Phi_{\boldsymbol{s}}\middle|Z_0^0\right\rangle\big|_{\boldsymbol{s}=0} &= \left\langle\partial_3\Phi_{\boldsymbol{s}}\middle|Z_0^0\right\rangle\big|_{\boldsymbol{s}=0} \\ &\quad - \left\langle\partial_3\Phi_{\boldsymbol{s}}\middle|\Phi_{\boldsymbol{s}}\right\rangle\big|_{\boldsymbol{s}=0}\left\langle\Phi_{\boldsymbol{s}}\middle|Z_0^0\right\rangle\big|_{\boldsymbol{s}=0} \\ &= 0.\end{aligned} \tag{B52}$$

3. The case $\boldsymbol{s}_\perp = 0$

a. *Proof of Corollary 2 in the main text for the case of* $\boldsymbol{s}_\perp = 0$

Proof. We assume $\boldsymbol{s}_\perp = 0$ and $s_3 \neq 0$, where the rank of the state is strictly two. In this case, according to Eqs. (B2, B3), the explicit forms of $v_{\boldsymbol{s}}$ and $w_{\boldsymbol{s}}$ can be expressed as

$$v_{\boldsymbol{s}}\big|_{\boldsymbol{s}_\perp=0} = \frac{\pi\mathcal{A}^2}{ks_3}\sin(ks_3a^2), \tag{B53}$$

$$w_{\boldsymbol{s}}\big|_{\boldsymbol{s}_\perp=0} = -\frac{\pi\mathcal{A}^2}{ks_3}[1-\cos(ks_3a^2)], \tag{B54}$$

$$\partial_i v_{\boldsymbol{s}}\big|_{\boldsymbol{s}_\perp=0} = \partial_i w_{\boldsymbol{s}}\big|_{\boldsymbol{s}_\perp=0} = 0,\ i=1,\ 2. \tag{B55}$$

According to Eqs. (B4, B5), we obtain

$$\theta_{\boldsymbol{s}}\big|_{\boldsymbol{s}_\perp=0} = \frac{ks_3a^2}{4}, \tag{B56}$$

$$\Delta_{\boldsymbol{s}}\big|_{\boldsymbol{s}_\perp=0} = \left[\frac{2}{ks_3a^2}\sin\left(\frac{ks_3a^2}{2}\right)\right]^2, \tag{B57}$$

$$\left.\frac{2\partial_i\theta_{\boldsymbol{s}}}{1+4\theta_{\boldsymbol{s}}^2}\right|_{\boldsymbol{s}_\perp=0} = -\left.\frac{\partial_i w_{\boldsymbol{s}} v_{\boldsymbol{s}} - w_{\boldsymbol{s}}\partial_i v_{\boldsymbol{s}}}{v_{\boldsymbol{s}}^2}\right|_{\boldsymbol{s}_\perp=0}, \tag{B58}$$

$$\partial_i\Delta_{\boldsymbol{s}}\big|_{\boldsymbol{s}_\perp=0} = \left.\frac{v_{\boldsymbol{s}}\partial_i v_{\boldsymbol{s}} + w_{\boldsymbol{s}}\partial_i w_{\boldsymbol{s}}}{\Delta_{\boldsymbol{s}}}\right|_{\boldsymbol{s}_\perp=0}. \tag{B59}$$

Therefore, we arrive at

$$\partial_i\theta_{\boldsymbol{s}}\big|_{\boldsymbol{s}_\perp=0} = \partial_i\Delta_{\boldsymbol{s}}\big|_{\boldsymbol{s}_\perp=0} = 0,\ i=1,\ 2. \tag{B60}$$

According to Eqs. (B7, B8), we know

$$|\partial_i\psi_{n\boldsymbol{s}}\rangle = \frac{|\partial_i\tilde{\psi}_{n\boldsymbol{s}}\rangle}{\sqrt{4p_{n\boldsymbol{s}}}},\ n,\ i = 1,\ 2. \tag{B61}$$

Substituting Eqs. (B16, B17, B60) into Eqs. (B18, B19), one obtains the saturation condition for regular projectors. One can direct apply Theorem 4 in the main text to obtain the saturation condition for a null projector.

Furthermore, if near the critical point $\boldsymbol{s} = 0$ the QFIM is saturated, then by taking the limit $\boldsymbol{s} \to 0$, it is also saturated at $\boldsymbol{s} = 0$. □

b. *Details of constructing the optimal measurement in the main text*

It can be calculated that according to Eqs. (B11, B12, B56, B60),

$$\tilde{\psi}_{1\boldsymbol{s}}(\boldsymbol{r})\big|_{\boldsymbol{s}_\perp=0} = 2\mathcal{A}\mathrm{circ}(r/a)\cos[ks_3(a^2 - 2r^2)/4], \tag{B62}$$

$$\tilde{\psi}_{2\boldsymbol{s}}(\boldsymbol{r})\big|_{\boldsymbol{s}_\perp=0} = 2\mathcal{A}\mathrm{circ}(r/a)\sin[ks_3(a^2 - 2r^2)/4], \tag{B63}$$

$$\partial_i\tilde{\psi}_{1\boldsymbol{s}}(\boldsymbol{r})\big|_{\boldsymbol{s}_\perp=0} = -kx_i\tilde{\psi}_{2\boldsymbol{s}}(\boldsymbol{r})\big|_{\boldsymbol{s}_\perp=0}\, i = 1,\ 2, \tag{B64}$$

$$\partial_i\tilde{\psi}_{2\boldsymbol{s}}(\boldsymbol{r})\big|_{\boldsymbol{s}_\perp=0} = kx_i\tilde{\psi}_{1\boldsymbol{s}}(\boldsymbol{r})\big|_{\boldsymbol{s}_\perp=0},\ i = 1,\ 2. \tag{B65}$$

We see that both $\tilde{\psi}_{1\boldsymbol{s}}(\boldsymbol{r})\big|_{\boldsymbol{s}_\perp=0}$ and $\tilde{\psi}_{2\boldsymbol{s}}(\boldsymbol{r})\big|_{\boldsymbol{s}_\perp=0}$ are even while both $\partial_i\tilde{\psi}_{1\boldsymbol{s}}(\boldsymbol{r})\big|_{\boldsymbol{s}_\perp=0}$ and $\partial_i\tilde{\psi}_{2\boldsymbol{s}}(\boldsymbol{r})\big|_{\boldsymbol{s}_\perp=0}$ for $i = 1, 2$ are odd. Therefore,

$$\langle\tilde{\psi}_{1\boldsymbol{s}}|Z_{2n+1}^{2m+1}\rangle\,\big|_{\boldsymbol{s}_\perp=0} = \langle\tilde{\psi}_{2\boldsymbol{s}}|Z_{2n+1}^{2m+1}\rangle\,\big|_{\boldsymbol{s}_\perp=0} = 0, \tag{B66}$$

$$\langle\partial_i\tilde{\psi}_{1\boldsymbol{s}}|Z_{2n}^{2m}\rangle\,\big|_{\boldsymbol{s}_\perp=0} = \langle\partial_i\tilde{\psi}_{2\boldsymbol{s}}|Z_{2n}^{2m}\rangle\,\big|_{\boldsymbol{s}_\perp=0} = 0, \tag{B67}$$

where $Z_{2n+1}^{2m+1}(\boldsymbol{r})$ is of odd parity and $Z_{2n}^{2m}(\boldsymbol{r})$ is of even parity. Furthermore, since

$$\partial_1\tilde{\psi}_{k\boldsymbol{s}}(\boldsymbol{r})\big|_{\boldsymbol{s}_\perp=0} \propto f(r)\cos\phi,\ k = 1,\ 2, \tag{B68}$$

$$\partial_2\tilde{\psi}_{k\boldsymbol{s}}(\boldsymbol{r})\big|_{\boldsymbol{s}_\perp=0} \propto f(r)\sin\phi,\ k = 1,\ 2, \tag{B69}$$

we obtain for $m \neq \pm 1$

$$\langle\partial_1\tilde{\psi}_{k\boldsymbol{s}}|Z_{2n+1}^{m}\rangle\,\big|_{\boldsymbol{s}_\perp=0} = 0,\ k = 1,\ 2, \tag{B70}$$

while

$$\langle\partial_1\tilde{\psi}_{k\boldsymbol{s}}|Z_{2n+1}^{\pm 1}\rangle\,\big|_{\boldsymbol{s}_\perp=0} \neq 0,\ k = 1,\ 2. \tag{B71}$$

4. The case $s_3 = 0$

a. *The saturation conditions for the case of $s_3 = 0$*

Let us focus on the case where $s_3 = 0$ and $\boldsymbol{s}_\perp \neq 0$. According to Eqs. (B2, B3), it is easily calculated that

$$v_{\boldsymbol{s}}\big|_{s_3=0} = \mathcal{A}^2\int d\boldsymbol{r}\mathrm{circ}(r/a)\cos(2k\boldsymbol{s}_\perp\cdot\boldsymbol{r}), \tag{B72}$$

$$w_{\boldsymbol{s}}\big|_{s_3=0} = 0, \tag{B73}$$

and for $i = 1,\ 2$

$$\partial_i v_{\boldsymbol{s}}\big|_{s_3=0} = -2k\mathcal{A}^2\int d\boldsymbol{r}x_i\mathrm{circ}(r/a)\sin(2k\boldsymbol{s}_\perp\cdot\boldsymbol{r}), \tag{B74}$$

$$\partial_i w_{\boldsymbol{s}}\big|_{s_3=0} = 0. \tag{B75}$$

According to Eqs. (B4, B5), we obtain

$$\theta_{\boldsymbol{s}}\big|_{s_3=0} = 0, \tag{B76}$$

and for $i = 1,\ 2$

$$\partial_i\theta_{\boldsymbol{s}}\big|_{s_3=0} = 0. \tag{B77}$$

Substituting Eq. (B16, B17, B77) into Eqs. (B18, B19), one obtains the following saturation condition for a regular projector $\Pi_k = \sum_\alpha |\pi_{k\alpha}\rangle\langle\pi_{k\alpha}|$ where $\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k) > 0$ and the estimation of the transverse separation s_1 and s_2,

$$\frac{\partial_i p_{1\boldsymbol{s}}}{p_{1\boldsymbol{s}}}\langle\psi_{1\boldsymbol{s}}|\pi_{k\alpha}\rangle + 2\langle\partial_i\psi_{1\boldsymbol{s}}|\pi_{k\alpha}\rangle = \xi_i^k\langle\psi_{1\boldsymbol{s}}|\pi_{k\alpha}\rangle\,, \tag{B78}$$

$$\frac{\partial_i p_{2\boldsymbol{s}}}{p_{2\boldsymbol{s}}}\langle\psi_{2\boldsymbol{s}}|\pi_{k\alpha}\rangle + 2\langle\partial_i\psi_{2\boldsymbol{s}}|\pi_{k\alpha}\rangle = \xi_i^k\langle\psi_{2\boldsymbol{s}}|\pi_{k\alpha}\rangle\,. \tag{B79}$$

One can direct apply Theorem 4 in the main text to obtain the following saturation condition for a null projector $\Pi_k = \sum_\alpha |\pi_{k\alpha}\rangle\langle\pi_{k\alpha}|$ where $\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k) = 0$,

$$\langle\partial_i\tilde{\psi}_{n\boldsymbol{s}}|\pi_{k\alpha}\rangle = \eta_{ij}\langle\partial_j\tilde{\psi}_{n\boldsymbol{s}}|\pi_{k\alpha}\rangle\,,\ i,\ j = 1,\ 2, \forall n, \alpha. \tag{B80}$$

Note that if near the critical point $\boldsymbol{s} = 0$ the QFIM is saturated by some optimal measurement, then by taking the limit $\boldsymbol{s} \to 0$, it is also saturated at $\boldsymbol{s} = 0$.□

b. *Details of constructing the optimal measurement in the main text*

It can be calculated that according to Eqs. (B11, B12, B76, B77) that,

$$\tilde{\psi}_{1\boldsymbol{s}}(\boldsymbol{r})\big|_{s_3=0} = 2\mathcal{A}\mathrm{circ}(r/a)\cos(k\boldsymbol{s}_\perp\cdot\boldsymbol{r}), \tag{B81}$$

$$\tilde{\psi}_{2\boldsymbol{s}}(\boldsymbol{r})\big|_{s_3=0} = 2\mathcal{A}\mathrm{circ}(r/a)\sin(k\boldsymbol{s}_\perp\cdot\boldsymbol{r}), \tag{B82}$$

$$\partial_i\tilde{\psi}_{1\boldsymbol{s}}(\boldsymbol{r})\big|_{s_3=0} = -kx_i\tilde{\psi}_{2\boldsymbol{s}}(\boldsymbol{r})\big|_{s_3=0},\ i=1,\,2, \tag{B83}$$

$$\partial_i\tilde{\psi}_{2\boldsymbol{s}}(\boldsymbol{r})\big|_{s_3=0} = kx_i\tilde{\psi}_{1\boldsymbol{s}}(\boldsymbol{r})\big|_{s_3=0},\ i=1,\,2. \tag{B84}$$

We see that for $i = 1, 2$, both $\tilde{\psi}_{1\boldsymbol{s}}(\boldsymbol{r})\big|_{s_3=0}$ and $\partial_i\tilde{\psi}_{1\boldsymbol{s}}(\boldsymbol{r})\big|_{s_3=0}$ are even while both $\tilde{\psi}_{2\boldsymbol{s}}(\boldsymbol{r})\big|_{s_3=0}$ and $\partial_i\tilde{\psi}_{2\boldsymbol{s}}(\boldsymbol{r})\big|_{s_3=0}$ are odd. We choose real basis with definite parity where the real even and basis functions are denoted as $\pi_{\pm\alpha}(\boldsymbol{r}) = \langle\boldsymbol{r}|\pi_{\pm\alpha}\rangle$ respectively. For an even and regular basis vector $|\pi_{+\alpha}\rangle$, we can obtain $\langle\psi_{2\boldsymbol{s}}|\pi_{k\alpha}\rangle = 0$ and $\langle\partial_i\psi_{2\boldsymbol{s}}|\pi_{k\alpha}\rangle = 0$ by the parities of these functions. Thus both sides of Eq. (B79) vanish and set no constraint on the constant ξ_i^k. From Eq. (B78) we find

$$\xi_i^{+\alpha} = \left(\frac{\langle\partial_i\psi_{1\boldsymbol{s}}|\pi_{+\alpha}\rangle}{\langle\psi_{1\boldsymbol{s}}|\pi_{+\alpha}\rangle} + \frac{\partial_i p_{1\boldsymbol{s}}}{p_{1\boldsymbol{s}}}\right)\Bigg|_{s_3=0} \tag{B85}$$

is also real. For different regular even basis vectors, the coefficients $\xi_i^{+\alpha}$ are not necessarily equal. Thus according to the recipe in the main text, we obtain one regular projector $\Pi_{+\alpha} = |\pi_{+\alpha}\rangle\langle\pi_{+\alpha}|$ corresponding to each of these vectors for the optimal measurement. If an even basis vector $|\pi_{+\alpha}\rangle$ is null, then we see that $\langle\partial_1\tilde{\psi}_{2\boldsymbol{s}}|\pi_{+\alpha}\rangle = \langle\partial_2\tilde{\psi}_{2\boldsymbol{s}}|\pi_{+\alpha}\rangle = 0$ and

$$\eta_{21}^{+\alpha} = \frac{\langle\partial_2\tilde{\psi}_{1\boldsymbol{s}}|\pi_{+\alpha}\rangle}{\langle\partial_1\tilde{\psi}_{1\boldsymbol{s}}|\pi_{+\alpha}\rangle}\Bigg|_{s_3=0} \tag{B86}$$

is real. Again for different null even basis vectors, the coefficients $\eta_{21}^{+\alpha}$ are not necessarily equal. We obtain one null projector $\Pi_{+\alpha} = |\pi_{+\alpha}\rangle\langle\pi_{+\alpha}|$ for each of these vectors for the optimal measurement. Similar analysis can be done for odd basis functions, either regular or null. Therefore one can construct the optimal projectors $\Pi_{-\alpha} = |\pi_{-\alpha}\rangle\langle\pi_{-\alpha}|$. So we conclude that rank one projectors formed by real and parity definite basis vectors are optimal on the plane $s_3 = 0$.

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