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 projector of a measurement. The saturation of all these bounds results in the saturation of the multi-parameter quantum Cramér-Rao bound. Necessary and sufficient conditions are obtained for the optimal measurements that give rise to the multi-parameter quantum Cramér-Rao bound associated with a general quantum state. We find that nonlocal measurements on replicas of a pure or full ranked state do not help saturate the multi-parameter quantum Cramér-Rao bound if no optimal measurement exists for a single copy of such a 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.

Introduction.—Metrology [1–3], the science of precision measurements, has found wide applications in various fields of physics and engineering, including interferometry [4], atomic clocks [5–7], optical imaging [8–11], and detection of gravitational waves [12]. In classical metrology, the covariance matrix of a maximum likelihood estimator can always asymptotically achieve the classical Cramér-Rao bound proportional to the inverse of the Classical Fisher Information Matrix (CFIM) [13, 14]. In quantum metrology, pioneered by Helstrom [15] and Holevo [16], the CFIM can be further maximized over all possible quantum measurements to yield the Quantum Fisher Information Matrix (QFIM). Throughout this paper, we assume the limit of the large sample size. Therefore the saturation of the quantum Cramér-Rao bound, proportional to the inverse of QFIM, becomes the search for optimal measurements that maximize the CFIM. Braunstein and Caves showed [17] that for single parameter estimation such an optimal measurement always exists and therefore the quantum Cramér-Rao bound can be always achieved in this case. Since then much work has been done in this direction [18–30]. 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 [31].

A different but related topic is the superresolution imaging beyond the subdiffraction limit. This discovery pioneered by Tsang and coworkers [8] has spurred a number of works [32–41]. The realistic superresolution problem in three-dimensional space essentially involves multi-parameter estimation. So a general theory of quantum multi-parameter estimation is desired. Currently much work has been done toward this goal [42–46]. In particular, for a pure state, Matsumoto [46] derived a necessary and sufficient condition for the saturation of the Multi-parameter Quantum Cramér-Rao Bound (MQCRB). More recently Pezzè et al. [42] gave the necessary and sufficient conditions for a measurement consisting of rank one projectors to saturate MQCRB of a pure state, and the recipes of constructing the optimal measurements if the pure state satisfies the Matsumoto condition.

However, for a general mixed state, the necessary and sufficient conditions for a given projective measurement to saturate the MQCRB are still uncharted. In this paper, we solve this problem by generalizing the earlier approach developed by Braunstein and Caves [17] for single parameter estimation to multi-parameter estimation. For the measurement projector corresponding to a zero probability outcome, we find that the saturation of the MQCRB imposes a constraint which is satisfied automatically in the case of single parameter estimation and therefore does not appear there. The necessary and sufficient conditions for saturating the MQCRB we obtain can recover the results for pure states and rank one projectors recently found by Pezzè et al. [42] as a special case. We also find that if optimal measurements do not exist for a single copy of a pure or full-ranked state, they do not exist either for replicas of such a state. Therefore nonlocal measurements on replicas of a pure or full-ranked state do not help saturate the MQCRB. Based on the saturation conditions of the MQCRB, we also construct several local optimal measurements in the problem of estimating the three-dimensional separation of two monochromatic, incoherent point sources. We emphasize that the saturation conditions we find may have possible applications not only in the superresolution of optical imaging, but also in quantum sensing [4].

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 $\rho_{\boldsymbol{\lambda}} = \sum_n p_{n\boldsymbol{\lambda}} |\psi_{n\boldsymbol{\lambda}}\rangle \langle\psi_{n\boldsymbol{\lambda}}|$, where

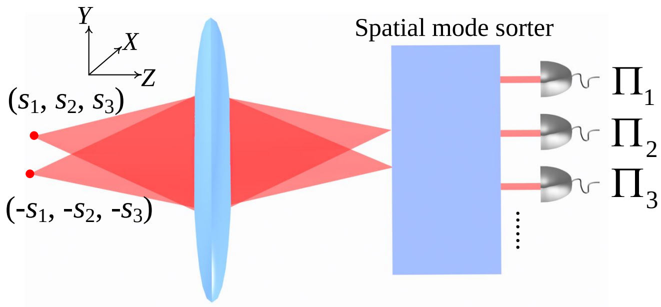

Figure 1. Schematic setup of the estimation of the three-dimensional separation of two point light sources, whose coordinates are denoted as $\pm(s_1, s_2, s_3)$. Π_k denotes a projector of a measurement, which can be implemented by spatial mode sorters [47–49]. The measurement is performed at the image plane. Alternatively, the measurement can also be performed at the pupil plane, i.e., the Fourier transformed plane of the image plane (not shown).

$p_{n\boldsymbol{\lambda}}$'s are *strictly* positive and $|\psi_{n\boldsymbol{\lambda}}\rangle$'s are orthonormal. We denote the kernel (null space) of $\rho_{\boldsymbol{\lambda}}$ as $\ker(\rho_{\boldsymbol{\lambda}}) \equiv \mathrm{span}\{|\psi\rangle : \langle\psi_{n\boldsymbol{\lambda}}|\psi\rangle = 0, \forall n\}$ and the support of $\rho_{\boldsymbol{\lambda}}$ as $\mathrm{supp}(\rho_{\boldsymbol{\lambda}}) \equiv \mathrm{span}\{|\psi_{n\boldsymbol{\lambda}}\rangle\text{'s}\}$. 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 the decomposition $|\psi\rangle = |\psi^0\rangle + |\psi^\perp\rangle$ is unique. (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 $|\partial_i^0\psi_{\boldsymbol{\lambda}}\rangle \equiv |\partial_i\psi_{\boldsymbol{\lambda}}\rangle - |\partial_i^\perp\psi_{\boldsymbol{\lambda}}\rangle$ and $|\partial_i^\perp\psi_{\boldsymbol{\lambda}}\rangle \equiv \sum_n |\psi_{n,\boldsymbol{\lambda}}\rangle\langle\psi_{n,\boldsymbol{\lambda}}|\partial_i\psi_{\boldsymbol{\lambda}}\rangle$. (c) The measurement projector is denoted as $\Pi_k \equiv \sum_\alpha \Pi_{k\alpha}$, where $\Pi_{k\alpha} \equiv |\pi_{k\alpha}\rangle\langle\pi_{k\alpha}|$ is a rank one projector and $\sum_k \Pi_k = \mathbb{I}$. If $\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k) = 0$ then Π_k is called a *null* projector otherwise it is called a *regular* projector. We emphasis that null projectors will make the CFIM elements ill-defined and therefore some regularization is required when calculating their contributions to the CFIM. $|\pi_{k\alpha}\rangle$ is called a *null* or *regular* basis vector if $\Pi_{k\alpha}$ is a null or regular projector. Note that a null basis vector $|\pi_{k\alpha}\rangle$ must lie completely in the subspace $\ker(\rho_{\boldsymbol{\lambda}})$, i.e., $|\pi_{k\alpha}^\perp\rangle = 0$, otherwise, due to the positive definiteness of $\rho_{\boldsymbol{\lambda}}$ on its support, we would obtain $\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_{k\alpha}) = \langle\pi_{k\alpha}^\perp|\rho_{\boldsymbol{\lambda}}|\pi_{k\alpha}^\perp\rangle > 0$.

Recovering the MQCRB.—The CFIM quantifies the sensitivity of a probability distribution to a small change in $\boldsymbol{\lambda}$ [50]. Its matrix element is defined as $F_{ij}(\boldsymbol{\lambda}) = \sum_k \mathcal{F}_{ij}^k(\boldsymbol{\lambda})$, where $\mathcal{F}_{ij}^k(\boldsymbol{\lambda}) \equiv \partial_i\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k)\partial_j\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k)/\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k)$ [13, 14]. Note that null projectors 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 projectors. For regular projectors, we can generalize the technique by Braunstein and Caves [17] to obtain (see Sec. I A in [51] for proofs)

$$\sum_{ij} u_i\mathcal{F}_{ij}^k u_j \le \sum_{ij} u_i u_j \mathrm{Re}[\mathrm{Tr}(\rho_{\boldsymbol{\lambda}} L_i \Pi_k L_j)], \tag{1}$$

where $\boldsymbol{u}$ is an arbitrary, real, and nonzero vector and L_i is the Symmetric Logarithmic Derivative (SLD) with respect to parameter λ_i defined as $[L_i\rho_{\boldsymbol{\lambda}} + \rho_{\boldsymbol{\lambda}}L_i]/2 = \partial_i\rho_{\boldsymbol{\lambda}}$ [15, 16, 52]. Furthermore, we prove in Sec. I B of the Supplemental Materials [51] that Eq. (1) is also true for null projectors. Note that Eq. (1) for null projectors is not discussed in Ref. [17] since it is automatically saturated in the case of single parameter estimation, as we will see subsequently. We define $\mathcal{I}_{ij}^k \equiv \mathrm{Re}[\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}L_i\Pi_k L_j)]$ as the QFIM element corresponding to a measurement projector Π_k, either regular or null. The matrix element of QFIM, which sets the upper bound of the CFIM, can be expressed as [15, 16, 52],

$$I_{ij}(\boldsymbol{\lambda}) \equiv \mathrm{Re}[\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}L_i L_j)]. \tag{2}$$

With these definitions, it is readily checked that summation over k in Eq. (1) yields $\sum_{ij} u_i F_{ij} u_j \le \sum_{ij} u_i I_{ij} u_j$. Therefore we successfully recover the MQCRB proposed by the pioneers of quantum estimation [15, 16].

Saturating the MQCRB.—The physical implications of $\mathcal{F}_{ij}^k$ and $\mathcal{I}_{ij}^k$ are very important in understanding the saturation of the MQCRB: from Eq. (1), we see that for each measurement projector 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 MQCRB requires the saturation of all these matrix bounds. Following this idea, we can derive the saturation conditions of MQCRB by saturating Eq. (1) for regular and null measurement projectors respectively. We summarize our main findings as the theorems below (see Secs. II B and II C of the Supplemental Material [51] for proofs).

Theorem 1: 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

$$\langle\psi_{n\boldsymbol{\lambda}}|L_i^\perp|\pi_{k\alpha}\rangle + 2\langle\partial_i^0\psi_{n\boldsymbol{\lambda}}|\pi_{k\alpha}\rangle = \xi_i^k\langle\psi_{n\boldsymbol{\lambda}}|\pi_{k\alpha}\rangle \;\forall i,\, n,\, \alpha \tag{3}$$

where ξ_i^k is a real number that does not depend on n and α, and $L_i^\perp$ denotes the projection of L_i onto $\mathrm{supp}(\rho_{\boldsymbol{\lambda}})$.

Theorem 2: The matrix bound of the CFIM due to a *null* projector $\Pi_k = \sum_\alpha |\pi_{k\alpha}\rangle\langle\pi_{k\alpha}|$ is saturated, if and only if

$$\langle\partial_i\psi_{n\boldsymbol{\lambda}}|\pi_{k\alpha}\rangle = \eta_{ij}^k\langle\partial_j\psi_{n\boldsymbol{\lambda}}|\pi_{k\alpha}\rangle \;\forall i,\, j,\, n, \alpha \tag{4}$$

where the coefficient η_{ij}^k is a real number that does not depend on n and α.

The explicit formulas of L_i and $L_i^\perp$ are given by Eqs. (S28, S30) in Sec. II A of the Supplement Material [51]. They will be useful when one deals with specific problems, e.g., the problem of superresolution of two incoherent optical point sources we will discuss subsequently. Note that $\eta_{ii}^k = 1$, thus for a null projector in single parameter estimation Eq. (4) is satisfied automatically. Moreover, $\eta_{ij}^k = 1/\eta_{ji}^k$. Thus in order to check whether a null projector satisfies Theorem 2, 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. For a pure state $\rho_{\boldsymbol{\lambda}} = |\psi_{\boldsymbol{\lambda}}\rangle\langle\psi_{\boldsymbol{\lambda}}|$, the dimension of $\text{supp}(\rho_{\boldsymbol{\lambda}})$ is one. Therefore ξ_i^k's naturally do not depend on the index n. To satisfy Theorem 1, we only require the coefficients ξ_i^k be real and independent of α. The SLD for a pure state is $L_i = 2(|\partial_i\psi_{\boldsymbol{\lambda}}\rangle\langle\psi_{\boldsymbol{\lambda}}| + |\psi_{\boldsymbol{\lambda}}\rangle\langle\partial_i\psi_{\boldsymbol{\lambda}}|)$ [17, 52], from which we find $L_i^{\perp} = 0$. With this observation, we obtain the following theorems for pure states by straightforward applications of the preceding two theorems:

Theorem 3: For a pure state $|\psi_{\boldsymbol{\lambda}}\rangle$, 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

$$\langle\partial_i^0\psi_{\boldsymbol{\lambda}}|\pi_{k\alpha}\rangle = \xi_i^k\langle\psi_{\boldsymbol{\lambda}}|\pi_{k\alpha}\rangle\ \forall i,\ \alpha, \tag{5}$$

with ξ_i^k being real and independent of α.

Theorem 4: For a pure state $|\psi_{\boldsymbol{\lambda}}\rangle$, the matrix bound of the CFIM due to a *null* projector $\Pi_k = \sum_\alpha |\pi_{k\alpha}\rangle\langle\pi_{k\alpha}|$, where $|\pi_{k\alpha}\rangle$'s are orthogonal to $|\psi_{\boldsymbol{\lambda}}\rangle$, is saturated if and only if

$$\langle\partial_i\psi_{\boldsymbol{\lambda}}|\pi_{k\alpha}\rangle = \eta_{ij}^k\langle\partial_j\psi_{\boldsymbol{\lambda}}|\pi_{k\alpha}\rangle\ \forall i,\ j,\ \alpha, \tag{6}$$

with η_{ij}^k being real and independent of α.

Theorems 3 and 4 can recover the results for pure states and rank one projectors recently found by Pezzè et al. [42] (see Sec. III of [51]). Theorems 1-4 are our central results. As a first application of these results, we analyze the role of nonlocal measurements in saturating the MQCRB. We ask the following question: if no optimal measurement exists for a single copy of a state $\rho_{\boldsymbol{\lambda}}$, does there exist an optimal measurement for the replicas $\rho_{\boldsymbol{\lambda}}^{\otimes\nu}$ of the state? We show in Sec. IV of [51] for a pure or full ranked mixed state, the answer is no, which indicates nonlocal measurements do not help saturate the MQCRB.

Application to superresolution.—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 since they can be estimated with standard optical measurement in the position basis at the image plane without Rayleigh's curse. Thus without loss of generality, we can assume the centroid is located at the origin and 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 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 $|\Psi_{\pm\boldsymbol{s}}\rangle \equiv e^{i\theta_{\pm\boldsymbol{s}}}|\Phi_{\pm\boldsymbol{s}}\rangle$. The pupil function is $\Phi_{\boldsymbol{s}}(\boldsymbol{r}) \equiv \langle\boldsymbol{r}|\Phi_{\boldsymbol{s}}\rangle = \mathcal{A}\text{circ}(r/a)\exp[ik(\boldsymbol{s}_\perp\cdot\boldsymbol{r} - s_3r^2/2)]$ [33, 53] , where the normalization constant $\mathcal{A} = 1/\sqrt{\pi}a$, $\text{circ}(r/a)$ is one if $0 \leq r \leq a$ and vanishes everywhere else, and $r = \sqrt{x_1^2 + x_2^2}$. The overall phase $\theta_{\boldsymbol{s}}$ is chosen such that $\Delta_{\boldsymbol{s}} \equiv e^{2i\theta_{\boldsymbol{s}}}\int d\boldsymbol{r}\Phi_{\boldsymbol{s}}^2(\boldsymbol{r})$ is real. It is straightforward to show that $\theta_{\boldsymbol{s}} = -\theta_{-\boldsymbol{s}}$ (see Sec. V A of [51]). Therefore 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 $|\psi_{1\boldsymbol{s}}\rangle = (|\Psi_{+\boldsymbol{s}}\rangle + |\Psi_{-\boldsymbol{s}}\rangle)/\sqrt{4p_{1\boldsymbol{s}}}$ and $|\psi_{2\boldsymbol{s}}\rangle = -i(|\Psi_{+\boldsymbol{s}}\rangle - |\Psi_{-\boldsymbol{s}}\rangle)/\sqrt{4p_{2\boldsymbol{s}}}$, where $p_{1,2\boldsymbol{s}} = (1\pm\Delta_{\boldsymbol{s}})/2$ are the corresponding eigenvalues. The QFIM associated with $\rho_{\boldsymbol{s}}$ has been shown in Ref. [32], which is $I_{ij} = 4\text{Re}[\langle\partial_i\Phi_{\boldsymbol{s}}|\partial_j\Phi_{\boldsymbol{s}}\rangle + \langle\Phi_{\boldsymbol{s}}|\partial_i\Phi_{\boldsymbol{s}}\rangle\langle\Phi_{\boldsymbol{s}}|\partial_j\Phi_{\boldsymbol{s}}\rangle]$. 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 our central results, i.e., Theorems 1-4 to this problem to obtain the necessary and sufficient conditions for optimal measurements. We summarize the results as two corollaries below (see Secs. V B, V C, V D of [51] for proofs). Note that our approach to optimal measurements is quite different from the approach of direct calculations by many papers [8, 32, 35, 37], 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 $\boldsymbol{s} = 0$, if and only if

$$\langle\partial_i^0\Phi_{\boldsymbol{s}}|\pi_{k\alpha}\rangle\big|_{\boldsymbol{s}=0} = \xi_i^k\langle\Phi_{\boldsymbol{s}}|\pi_{k\alpha}\rangle\big|_{\boldsymbol{s}=0}\,\forall i,\ \alpha, \tag{7}$$

provided the projector is *regular* and if and only if

$$\langle\partial_i\Phi_{\boldsymbol{s}}|\pi_{k\alpha}\rangle\big|_{\boldsymbol{s}=0} = \eta_{ij}^k\langle\partial_j\Phi_{\boldsymbol{s}}|\pi_{k\alpha}\rangle\big|_{\boldsymbol{s}=0}\,\forall i,\ j\,\alpha, \tag{8}$$

provided the projector is *null*, where ξ_i^k and η_{ij}^k are real and independent of α.

Corollary 2: On the line $\boldsymbol{s}_\perp = 0$ or on the plane $s_3 = 0$, 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

$$\langle\partial_i\psi_{n\boldsymbol{s}}|\pi_{k\alpha}\rangle = \xi_i^k\langle\psi_{n\boldsymbol{s}}|\pi_{k\alpha}\rangle\,,\ i = 1,\,2,\ \forall n,\ \alpha, \tag{9}$$

provided the projector is *regular*, and if and only if

$$\langle\partial_i\psi_{n\boldsymbol{s}}|\pi_{k\alpha}\rangle = \eta_{ij}^k\langle\partial_j\psi_{n\boldsymbol{s}}|\pi_{k\alpha}\rangle\,,\ i,\,j = 1,\,2,\ \forall n,\ \alpha, \tag{10}$$

provided the projector is *null*, where ξ_i^k and η_{ij}^k are real and independent of n and α.

Based on Corollary 1, 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 $\xi_i^{k\alpha}$ defined in Eq. (7) and check whether $\xi_i^{k\alpha}$'s are real for each i. (iii) Assemble regular basis vectors that have the same coefficient $\xi_i^{k\alpha}$ 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 $\langle\partial_i\Phi_{\boldsymbol{s}}|\pi_{k\alpha}\rangle = 0$ for all 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 (excluding diagonal) matrix elements $\eta_{ij}^{k\alpha}$ defined in Eq. (8) and check whether they are all real. If both $\langle\partial_i\Phi_{\boldsymbol{s}}|\pi_{k\alpha}\rangle$ and $\langle\partial_j\Phi_{\boldsymbol{s}}|\pi_{k\alpha}\rangle$ vanishes for some i and j, $\eta_{ij}^{k\alpha}$ 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 2, except that (a) one needs to check that $\xi_{ij}^{k\alpha}$ and $\eta_{ij}^{k\alpha}$ do not depend on the index n of the two eigenstates $|\psi_{n\boldsymbol{s}}\rangle$ of $\rho_{\boldsymbol{s}}$. (b) A null basis vector $|\pi_{k\alpha}\rangle$ in this case is said to be *flexible* if $\langle\partial_i\psi_{n\boldsymbol{s}}|\pi_{k\alpha}\rangle = 0$ for all n and i. It is clear from Theorems 1 and 2 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 $|Z_n^m\rangle$ [54], where $|Z_0^0\rangle = |\Phi_{\boldsymbol{s}}\rangle\big|_{\boldsymbol{s}=\boldsymbol{0}}$. Following the recipe above (details can be found in Sec. V B of [51]): (i) $|Z_0^0\rangle$ is the only regular basis vector and the remaining basis vectors are null. (ii) We find $\xi_i^{(00)} = \langle\partial_i^0\Phi_{\boldsymbol{s}}|Z_0^0\rangle\big|_{\boldsymbol{s}=0}/\langle\Phi_{\boldsymbol{s}}|Z_0^0\rangle\big|_{\boldsymbol{s}=0} = 0$ 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 $(n, m) \neq (1, \pm1), (2, 0)$, we find $\langle\partial_i\Phi_{\boldsymbol{s}}|Z_n^m\rangle = 0$ for all i. Thus they are flexible and can be lumped to the previous regular projector. So the new regular projector is $|\Pi_1\rangle = |Z_0^0\rangle\langle Z_0^0| + \sum_{n'm'}|Z_{n'}^{m'}\rangle\langle Z_{n'}^{m'}|$, where the prime means $(n', m') \neq (1, \pm1), (2, 0)$. (v) We find $\eta_{12}^{(1,-1)} = \langle\partial_1\Phi_{\boldsymbol{s}}|Z_1^{-1}\rangle/\langle\partial_2\Phi_{\boldsymbol{s}}|Z_1^{-1}\rangle = 0$, $\eta_{32}^{(1,-1)} = \langle\partial_3\Phi_{\boldsymbol{s}}|Z_1^{-1}\rangle/\langle\partial_2\Phi_{\boldsymbol{s}}|Z_1^{-1}\rangle = 0$ and $\eta_{13}^{(1,-1)}$ can be set arbitrarily since $\langle\partial_1\Phi_{\boldsymbol{s}}|Z_1^{-1}\rangle = \langle\partial_3\Phi_{\boldsymbol{s}}|Z_1^{-1}\rangle = 0$. Similarly, we find $\eta_{21}^{(1,1)} = \eta_{31}^{(1,1)} = \eta_{23}^{(2,0)} = \eta_{13}^{(2,0)} = 0$, $\eta_{23}^{(1,1)}$ and $\eta_{12}^{(2,0)}$ can be set arbitrarily. (vi) Since the η matrices corresponding to basis vectors $|Z_1^{\pm1}\rangle$ and $|Z_2^0\rangle$ are all distinct, we obtain three null projectors $|\Pi_2\rangle = |Z_1^1\rangle\langle Z_1^1|$, $|\Pi_3\rangle = |Z_1^{-1}\rangle\langle Z_1^{-1}|$, and $|\Pi_4\rangle = |Z_2^0\rangle\langle Z_2^0|$.

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 $\psi_{1,2\boldsymbol{s}}(\boldsymbol{r})\big|_{\boldsymbol{s}_\perp=0}$

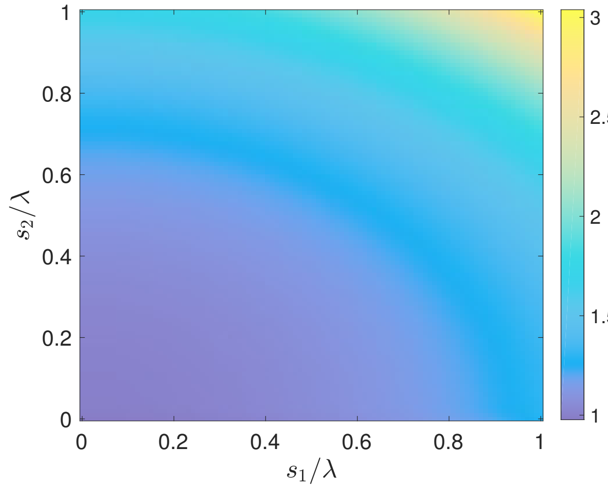

Figure 2. Numerical simulation of the classical Cramér-Rao bound associated with the optimal measurement: $\Pi_1 = \sum_{n=0}^\infty |Z_{2n+1}^1\rangle\langle Z_{2n+1}^1|$, $\Pi_2 = \sum_{n=0}^\infty |Z_{2n+1}^{-1}\rangle\langle Z_{2n+1}^{-1}|$ and $\Pi_3 = 1 - \Pi_1 - \Pi_2$. Note that the QFIM of estimating 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.

are even and $e\partial_i\psi_{1,2\boldsymbol{s}}(\boldsymbol{r})\big|_{\boldsymbol{s}_\perp=0}$ are odd. We still consider Zernike basis vectors $|Z_n^m\rangle$. Following the previously proposed recipe (details can be found in Sec. V C of [51]): (i) Even basis vectors are either regular or flexible. Odd basis vectors are null and they are also flexible except for $m = \pm1$. (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 $|\psi_{1,2\boldsymbol{s}}\rangle$. (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. (iii) We add all the rank one projectors formed by flexible basis vectors to the previous regular projector to obtain a regular projector $\Pi_1 = 1 - \sum_{n=0}^\infty |Z_{2n+1}^{\pm1}\rangle\langle Z_{2n+1}^{\pm1}|$. (iv) For the remaining null basis vectors, where $m = \pm1$, we find $\eta_{21}^{(2n+1,1)} = 0$ and $\eta_{12}^{(2n+1,-1)} = 0$ for $|\psi_{1,2\boldsymbol{s}}\rangle$. (v) 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 $\Pi_1 = \sum_{n=0}^\infty |Z_{2n+1}^1\rangle\langle Z_{2n+1}^1|$, $\Pi_2 = \sum_{n=0}^\infty |Z_{2n+1}^{-1}\rangle\langle Z_{2n+1}^{-1}|$. 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 $\langle\psi|\Pi_1|\psi\rangle = 1/\pi\int_0^\infty rdr\left|\int_0^{2\pi}d\phi\psi(r,\phi)\cos\phi\right|^2$ and $\langle\psi|\Pi_2|\psi\rangle = 1/\pi\int_0^\infty rdr\left|\int_0^{2\pi}d\phi\psi(r,\phi)\sin\phi\right|^2$, 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 Cramér-Rao bound of estimating s_1 associated with this measurement. As we clearly see from Fig. 2, the quantum Cramér-Rao bound of estimating s_1 is saturated near the origin where $\boldsymbol{s}_\perp = 0$. Note that the quantum Cramér-Rao bound of estimating s_2 is the same as that of estimating s_1 and hence is omitted here.

On the plane $s_3 = 0$, we still restrict to the case of $i = 1, 2$, i.e., estimating the transverse separation. It is readily shown that $\psi_{1\boldsymbol{s}}(\boldsymbol{r})\big|_{s_3=0}$, $\partial_i\psi_{1\boldsymbol{s}}(\boldsymbol{r})\big|_{s_3=0}$ are even and $\psi_{2\boldsymbol{s}}(\boldsymbol{r})\big|_{s_3=0}$, $\partial_i\psi_{2\boldsymbol{s}}(\boldsymbol{r})\big|_{s_3=0}$ are odd. Again following the previous recipe (see Sec. V D of [51] for details) we find a measurement consisting of rank one, real and parity definite basis vectors is optimal on the plane $s_3 = 0$. This result is a generalization of previous one on one-dimensional transverse estimation [35].

Conclusion.—We derived a matrix bound of the CFIM due to each measurement projector. The saturation of the MQCRB requires the saturation of all these matrix bounds, whose sum adds up to the QFIM. We also gave necessary and sufficient conditions for a measurement to give the MQCRB. Based on these saturation conditions, we predict 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. Our work has potential applications in quantum sensing, quantum enhanced imaging, in particular may shed light on investigating the attainability of MQCRB and moment estimation in quantum imaging of objects of finite size.

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SUPPLEMENTAL MATERIAL

I. PROOF OF EQ. (1) IN THE MAIN TEXT

A. For regular projectors

For regular projectors, we prove Eq. (1) in the main text by generalizing the technique by Braunstein and Caves [17]. The Classical Fisher Information Matrix (QFIM) element corresponding to a regular projector Π_k is defined as

$$\mathcal{F}_{ij}^k(\boldsymbol{\lambda}) = \partial_i \mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k)\partial_j \mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k)/\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k). \tag{S1}$$

Using the definition of Symmetric Logarithmic Derivative (SLD)

$$[L_i\rho_{\boldsymbol{\lambda}} + \rho_{\boldsymbol{\lambda}}L_i]/2 = \partial_i\rho_{\boldsymbol{\lambda}}, \tag{S2}$$

and the cyclic property of trace, i.e.,

$$\mathrm{Tr}(L_i\rho_{\boldsymbol{\lambda}}\Pi_k) = \mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k L_i) = [\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}L_i\Pi_k)]^*, \tag{S3}$$

we obtain [17, 52]

$$\partial_i \mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k) = \mathrm{Tr}(\partial_i\rho_{\boldsymbol{\lambda}}\Pi_k) = \frac{1}{2}[\mathrm{Tr}(L_i\rho_{\boldsymbol{\lambda}}\Pi_k) + \mathrm{Tr}(\rho_{\boldsymbol{\lambda}}L_i\Pi_k)] = \mathrm{Re}[\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k L_i)]. \tag{S4}$$

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

$$\begin{aligned}
\sum_{ij} u_i\mathcal{F}_{ij}^k u_j &= \frac{[\mathrm{Re}\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k \sum_i u_i L_i)]^2}{\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k)} \\
&\le \frac{\left|\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k \sum_i u_i L_i)\right|^2}{\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k)} \\
&\le \sum_{ij} u_i u_j \mathrm{Tr}(\rho_{\boldsymbol{\lambda}}L_i\Pi_k L_j) \\
&= \frac{1}{2}\sum_{ij} u_i u_j \left(\mathrm{Tr}[\rho_{\boldsymbol{\lambda}}(L_i\Pi_k L_j + L_j\Pi_k L_i)]\right) \\
&= \sum_{ij} u_i u_j \mathrm{Re}[\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}L_i\Pi_k L_j)],
\end{aligned} \tag{S5}$$

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 $B \equiv \sum_i \sqrt{\Pi_k} u_i L_i \sqrt{\rho_{\boldsymbol{\lambda}}}$. Due to the fact $u_i u_j$ is symmetric in indices i, j, we have symmetrized $\mathrm{Tr}(\rho_{\boldsymbol{\lambda}} L_i \Pi_k L_j)$ in the second last equality and used $\mathrm{Tr}(\rho_{\boldsymbol{\lambda}} L_j \Pi_k L_i) = [\mathrm{Tr}(\rho_{\boldsymbol{\lambda}} L_i \Pi_k L_j)]^*$ to obtain the last equality. □

B. For null projectors

Introducing short hand notation

$$g_{ij}^k(\boldsymbol{\lambda}') \equiv \mathrm{Tr}(\partial_i \rho_{\boldsymbol{\lambda}'} \Pi_k)\mathrm{Tr}(\partial_j \rho_{\boldsymbol{\lambda}'} \Pi_k), \tag{S6}$$

$$h^k(\boldsymbol{\lambda}') \equiv \mathrm{Tr}(\rho_{\boldsymbol{\lambda}'} \Pi_k), \tag{S7}$$

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

$$\mathcal{F}_{ij}^k(\boldsymbol{\lambda}) \equiv \lim_{\boldsymbol{\lambda}' \to \boldsymbol{\lambda}} \frac{g_{ij}^k(\boldsymbol{\lambda}')}{h^k(\boldsymbol{\lambda}')}. \tag{S8}$$

Since the right hand side of Eq. (S8) is of the type 0/0, we need to Taylor expand both the numerator and denominator, which will involve the derivatives of $\rho_{\boldsymbol{\lambda}}$. So let us calculate the derivatives of $\rho_{\boldsymbol{\lambda}}$ first. We consider a general state $\rho_{\boldsymbol{\lambda}} = \sum_n p_{n\boldsymbol{\lambda}} \left|\psi_{n\boldsymbol{\lambda}}\right\rangle \left\langle\psi_{n\boldsymbol{\lambda}}\right|$, where $p_{n\boldsymbol{\lambda}}$'s are strictly positive. It is straightforward to calculate

$$\partial_i \rho_{\boldsymbol{\lambda}} = \sum_n \partial_i p_{n\boldsymbol{\lambda}} \left|\psi_{n\boldsymbol{\lambda}}\right\rangle \left\langle\psi_{n\boldsymbol{\lambda}}\right| + \sum_n p_{n\boldsymbol{\lambda}} \left|\partial_i \psi_{n\boldsymbol{\lambda}}\right\rangle \left\langle\psi_{n\boldsymbol{\lambda}}\right| + \sum_n p_{n\boldsymbol{\lambda}} \left|\psi_{n\boldsymbol{\lambda}}\right\rangle \left\langle\partial_i \psi_{n\boldsymbol{\lambda}}\right|. \tag{S9}$$

Therefore for a null measurement projector $\Pi_k \equiv \sum_\alpha \Pi_{k\alpha} = \sum_\alpha \left|\pi_{k\alpha}\right\rangle \left\langle\pi_{k\alpha}\right|$ defined in the main text, where$\langle\psi_{n\boldsymbol{\lambda}}|\pi_{k\alpha}\rangle = 0$, one obtains

$$\mathrm{Tr}(\partial_i \rho_{\boldsymbol{\lambda}} \Pi_{k\alpha}) = \left\langle\pi_{k\alpha}\middle|\partial_i \rho_{\boldsymbol{\lambda}}\middle|\pi_{k\alpha}\right\rangle = 0, \tag{S10}$$

$$\mathrm{Tr}(\partial_i \rho_{\boldsymbol{\lambda}} \Pi_k) = \sum_\alpha \mathrm{Tr}(\partial_i \rho_{\boldsymbol{\lambda}} \Pi_{k\alpha}) = 0, \tag{S11}$$

$$\mathrm{Tr}(\partial_i \partial_j \rho_{\boldsymbol{\lambda}} \Pi_{k\alpha}) = \left\langle\pi_{k\alpha}\middle|\partial_i \partial_j \rho_{\boldsymbol{\lambda}}\middle|\pi_{k\alpha}\right\rangle = \sum_n p_{n\boldsymbol{\lambda}} \left\langle\pi_{k\alpha}\middle|\partial_i \psi_{n\boldsymbol{\lambda}}\right\rangle \left\langle\partial_j \psi_{n\boldsymbol{\lambda}}\middle|\pi_{k\alpha}\right\rangle + \text{c.c.}, \tag{S12}$$

where "c.c." denotes the complex conjugate of the preceding term. Due to Eq. (S11), the first order derivatives of $g_{ij}^k(\boldsymbol{\lambda}')$ and $h^k(\boldsymbol{\lambda}')$ vanish at $\boldsymbol{\lambda}$, i.e.,

$$\partial_p g_{ij}^k(\boldsymbol{\lambda}) = \mathrm{Tr}(\partial_p \partial_i \rho_{\boldsymbol{\lambda}} \Pi_k)\cancel{\mathrm{Tr}(\partial_j \rho_{\boldsymbol{\lambda}} \Pi_k)} + \cancel{\mathrm{Tr}(\partial_i \rho_{\boldsymbol{\lambda}} \Pi_k)}\mathrm{Tr}(\partial_p \partial_j \rho_{\boldsymbol{\lambda}} \Pi_k) = 0, \tag{S13}$$

$$\partial_p h^k(\boldsymbol{\lambda}) = \mathrm{Tr}(\partial_p \rho_{\boldsymbol{\lambda}} \Pi_k) = 0, \tag{S14}$$

where the cancellations of the terms are due to the facts that Π_k is a null projector and therefore $\rho_{\boldsymbol{\lambda}} \Pi_k = 0$. 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.,

$$\partial_p \partial_q g_{ij}^k(\boldsymbol{\lambda}) = \mathrm{Tr}(\partial_p \partial_i \rho_{\boldsymbol{\lambda}} \Pi_k)\mathrm{Tr}(\partial_q \partial_j \rho_{\boldsymbol{\lambda}} \Pi_k) + \mathrm{Tr}(\partial_q \partial_i \rho_{\boldsymbol{\lambda}} \Pi_k)\mathrm{Tr}(\partial_p \partial_j \rho_{\boldsymbol{\lambda}} \Pi_k), \tag{S15}$$

$$\partial_p \partial_q h^k(\boldsymbol{\lambda}) = \mathrm{Tr}(\partial_p \partial_q \rho_{\boldsymbol{\lambda}} \Pi_k). \tag{S16}$$

If we define

$$T_{ij}^k \equiv \frac{1}{2}\mathrm{Tr}(\partial_i \partial_j \rho_{\boldsymbol{\lambda}} \Pi_k), \tag{S17}$$

$$z_{ni}^{k\alpha} \equiv \sqrt{p_{n\boldsymbol{\lambda}}} \left\langle \partial_i \psi_{n\boldsymbol{\lambda}} \middle| \pi_{k\alpha} \right\rangle, \tag{S18}$$

it is readily shown that

$$T_{ij}^k = \mathrm{Re}[\sum_{n\alpha} (z_{ni}^{k\alpha})^* z_{nj}^{k\alpha}]. \tag{S19}$$

Substitution of Eq. (S17) into Eqs. (S15, S16) gives

$$\partial_p \partial_q g_{ij}^k(\boldsymbol{\lambda}) = 4(T_{pi}^k T_{qj}^k + T_{qi}^k T_{pj}^k), \tag{S20}$$

$$\partial_p \partial_q h^k(\boldsymbol{\lambda}') = 2T_{pq}^k. \tag{S21}$$

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. (S8), with notice of Eqs. (S20, S21), we arrive at

$$\mathcal{F}_{ij}^k(\boldsymbol{\lambda}) = \frac{2\sum_{pq}(T_{pi}^k T_{qj}^k + T_{qi}^k T_{pj}^k)\delta\lambda_p \delta\lambda_q}{\sum_{pq} T_{pq}^k \delta\lambda_p \delta\lambda_q}. \tag{S22}$$

Next we calculate the QFIM corresponding to the null projector $\Pi_k = \sum_\alpha |\pi_{k\alpha}\rangle \langle \pi_{k\alpha}|$. According to Eq. (S2) we find

$$\begin{aligned}
\mathcal{I}_{ij}^k &\equiv \mathrm{ReTr}(\rho_{\boldsymbol{\lambda}} L_i \Pi_k L_j) \\
&= \frac{1}{2}[\mathrm{Tr}(\rho_{\boldsymbol{\lambda}} L_i \Pi_k L_j) + \mathrm{c.c.}] \\
&= \frac{1}{2}[\mathrm{Tr}(L_j \rho_{\boldsymbol{\lambda}} L_i \Pi_k) + \mathrm{Tr}(L_i \rho_{\boldsymbol{\lambda}} L_j \Pi_k)] \\
&= \mathrm{Tr}(L_j \partial_i \rho_{\boldsymbol{\lambda}} \Pi_k) + \mathrm{Tr}(\partial_i \rho_{\boldsymbol{\lambda}} L_j \Pi_k) - \cancel{\mathrm{Tr}(L_j L_i \rho_{\boldsymbol{\lambda}} \Pi_k)} - \cancel{\mathrm{Tr}(L_i L_j \rho_{\boldsymbol{\lambda}} \Pi_k)} \\
&= \mathrm{Tr}(\partial_i (L_j \rho_{\boldsymbol{\lambda}}) \Pi_k) + \mathrm{Tr}(\partial_i (\rho_{\boldsymbol{\lambda}} L_j) \Pi_k) - \cancel{2\mathrm{Tr}(\partial_i L_j \rho_{\boldsymbol{\lambda}} \Pi_k)} - \cancel{2\mathrm{Tr}(\rho_{\boldsymbol{\lambda}} \partial_i L_j \Pi_k)} \\
&= \mathrm{Tr}(\partial_i (L_j \rho_{\boldsymbol{\lambda}} + \rho_{\boldsymbol{\lambda}} L_j) \Pi_k) \\
&= 2\mathrm{Tr}(\partial_i \partial_j \rho_{\boldsymbol{\lambda}} \Pi_k),
\end{aligned} \tag{S23}$$

where the cancellations of the terms are due to the facts that Π_k is a null projector and therefore $\rho_{\boldsymbol{\lambda}} \Pi_k = 0$. In view of Eq. (S17), we arrive at

$$\mathcal{I}_{ij}^k = 4T_{ij}^k. \tag{S24}$$

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

$$\begin{aligned}
(\sum_{ij} \delta\lambda_i T_{ij}^k u_j)^2 &= \left[\mathrm{Re}(\sum_{n\alpha} [\sum_i z_{ni}^{k\alpha} \delta\lambda_i]^* [\sum_j z_{nj}^{k\alpha} u_j]) \right]^2 \\
&\leq \Big| \sum_{n\alpha} [\sum_i z_{ni}^{k\alpha} \delta\lambda_i]^* [\sum_j z_{nj}^{k\alpha} u_j] \Big|^2 \\
&\leq \left(\sum_{n\alpha} [\sum_i (z_{ni}^{k\alpha})^* \delta\lambda_i] [\sum_p z_{np}^{k\alpha} \delta\lambda_p] \right) \times \left(\sum_{n\alpha} [\sum_j (z_{nj}^{k\alpha})^* u_j] [\sum_q z_{nq}^{k\alpha} u_q] \right) \\
&= \left(\sum_{ip} \mathrm{Re}[\sum_{n\alpha} (z_{ni}^{k\alpha})^* z_{np}^{k\alpha}] \delta\lambda_i \delta\lambda_p \right) \times \left(\sum_{jq} u_j u_q \mathrm{Re}[\sum_{n\alpha} (z_{nj}^{k\alpha})^* z_{nq}^{k\alpha}] \right) \\
&= (\sum_{ip} T_{ip}^k \delta\lambda_i \delta\lambda_p) \sum_{jq} u_j u_q T_{jq}^k,
\end{aligned} \tag{S25}$$

where we have used the Cauchy-Swartz inequality $\left|\sum_{n\alpha} a^*_{n\alpha} b_{n\alpha}\right|^2 \leq (\sum_{n\alpha} a^*_{n\alpha} a_{n\alpha})(\sum_{n\alpha} b^*_{n\alpha} b_{n\alpha})$ in the second inequality with $a_{n\alpha} \equiv \sum_i z^{k\alpha}_{ni}\delta\lambda_i$ and $b_{n\alpha} \equiv \sum_j z^{k\alpha}_{nj} u_j$ and performed symmetrization to obtain the second last equality. Note that the denominator of Eq. (S22) can be rewritten as, upon substitution of Eq. (S19),

$$\sum_{pq} T^k_{pq}\delta\lambda_p\delta\lambda_q = \mathrm{Re}[\sum_{n\alpha}(\sum_p z^{k\alpha}_{np}\delta\lambda_p)^*(\sum_q z^{k\alpha}_{nq}\delta\lambda_q)] = \sum_{n\alpha}\Big|\sum_p z^{k\alpha}_{np}\delta\lambda_p\Big|^2. \tag{S26}$$

Therefore for any $\delta\boldsymbol{\lambda}$ the denominator of Eq. (S22) is non-negative. With these observations, next we find

$$\begin{aligned}\sum_{ij} u_i \mathcal{F}^k_{ij} u_j &= \frac{4\sum_{ij} u_i u_j \sum_{pq} T^k_{pi} T^k_{qj}\delta\lambda_p\delta\lambda_q}{\sum_{pq} T^k_{pq}\delta\lambda_p\delta\lambda_q} \\ &= \frac{4(\sum_{pi}\delta\lambda_p T^k_{pi} u_i)^2}{\sum_{pq} T^k_{pq}\delta\lambda_p\delta\lambda_q} \\ &\leq \frac{4(\sum_{pq} T^k_{pq}\delta\lambda_p\delta\lambda_q)\sum_{ij} u_i u_j T^k_{ij}}{\sum_{pq} T^k_{pq}\delta\lambda_p\delta\lambda_q} \\ &= \sum_{ij} u_i u_j \mathcal{I}^k_{ij},\end{aligned} \tag{S27}$$

where we have used Eq. (S25) in the inequality to get the upper bound.□

II. PROOFS OF THEOREM 1 AND 2 IN THE MAIN TEXT

A. Matrix representation of the SLD

For a general pure state $\rho_{\boldsymbol{\lambda}} = \sum_n p_{n\boldsymbol{\lambda}} |\psi_{n\boldsymbol{\lambda}}\rangle\langle\psi_{n\boldsymbol{\lambda}}|$, where $p_{n\boldsymbol{\lambda}}$ is strictly greater than zero. We denote the basis vectors of the null space of $\rho_{\boldsymbol{\lambda}}$ as $|e_{m\boldsymbol{\lambda}}\rangle$. Then in the basis formed by $\{|\psi_{n\boldsymbol{\lambda}}\rangle, |e_{m\boldsymbol{\lambda}}\rangle\}_{nm}$, a matrix representation of the SLD,

$$\begin{aligned}L_i = &\sum_n \frac{\partial_i p_{n,\boldsymbol{\lambda}}}{p_{n,\boldsymbol{\lambda}}} |\psi_{n\boldsymbol{\lambda}}\rangle\langle\psi_{n\boldsymbol{\lambda}}| + 2\sum_{m,n}\frac{p_{m\boldsymbol{\lambda}} - p_{n\boldsymbol{\lambda}}}{p_{m\boldsymbol{\lambda}} + p_{n\boldsymbol{\lambda}}}\langle\partial_i\psi_{m\boldsymbol{\lambda}}|\psi_{n\boldsymbol{\lambda}}\rangle|\psi_{m\boldsymbol{\lambda}}\rangle\langle\psi_{n\boldsymbol{\lambda}}| \\ &+ \left[2\sum_m\sum_n^N\langle\partial_i\psi_{n\boldsymbol{\lambda}}|e_{m\boldsymbol{\lambda}}\rangle|\psi_{n\boldsymbol{\lambda}}\rangle\langle e_{m\boldsymbol{\lambda}}| + \text{c.c.}\right],\end{aligned} \tag{S28}$$

can be found by solving the matrix equation $L_i\rho_{\boldsymbol{\lambda}} + \rho_{\boldsymbol{\lambda}} L_i = \partial_i\rho_{\boldsymbol{\lambda}}$ [52]. With Eq. (S28), it is straightforward to calculate, for a state $|\psi\rangle = |\psi^0\rangle + |\psi^\perp\rangle$,

$$L_i|\psi\rangle = L_i^\perp|\psi\rangle + 2\sum_m\sum_n\langle\partial_i\psi_{n\boldsymbol{\lambda}}|e_{m\boldsymbol{\lambda}}\rangle\langle e_{m\boldsymbol{\lambda}}|\psi^0\rangle|\psi_{n\boldsymbol{\lambda}}\rangle + 2\sum_m^M\sum_n^N\langle e_{m\boldsymbol{\lambda}}|\partial_i\psi_{n\boldsymbol{\lambda}}\rangle\langle\psi_{n,\boldsymbol{\lambda}}|\psi^\perp\rangle|e_{m,\boldsymbol{\lambda}}\rangle, \tag{S29}$$

where

$$L_i^\perp \equiv \sum_n\frac{\partial_i p_{n\boldsymbol{\lambda}}}{p_{n\boldsymbol{\lambda}}}|\psi_{n\boldsymbol{\lambda}}\rangle\langle\psi_{n\boldsymbol{\lambda}}| + 2\sum_{m,n}\frac{p_{m\boldsymbol{\lambda}} - p_{n\boldsymbol{\lambda}}}{p_{m\boldsymbol{\lambda}} + p_{n\boldsymbol{\lambda}}}\langle\partial_i\psi_{m\boldsymbol{\lambda}}|\psi_{n\boldsymbol{\lambda}}\rangle|\psi_{m\boldsymbol{\lambda}}\rangle\langle\psi_{n\boldsymbol{\lambda}}|, \tag{S30}$$

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

$$\langle\partial_i\psi_{n\boldsymbol{\lambda}}|e_{m\boldsymbol{\lambda}}\rangle = \langle\partial_i^0\psi_{n\boldsymbol{\lambda}}|e_{m\boldsymbol{\lambda}}\rangle, \tag{S31}$$

$$\sum_m\langle\partial_i^0\psi_{n\boldsymbol{\lambda}}|e_{m\boldsymbol{\lambda}}\rangle\langle e_{m\boldsymbol{\lambda}}|\psi^0\rangle = \langle\partial_i^0\psi_{n\boldsymbol{\lambda}}|\psi^0\rangle, \tag{S32}$$

we obtain

$$\begin{aligned}(L_i|\psi\rangle)^\perp &= L_i^\perp|\psi\rangle + 2\sum_n\langle\partial_i^0\psi_{n\boldsymbol{\lambda}}|\psi^0\rangle|\psi_{n\boldsymbol{\lambda}}\rangle \\ &= L_i^\perp|\psi\rangle + 2\sum_n\langle\partial_i^0\psi_{n\boldsymbol{\lambda}}|\psi\rangle|\psi_{n\boldsymbol{\lambda}}\rangle.\end{aligned} \tag{S33}$$

B. Proof of Theorem 1

Proof: The saturation of the first inequality of Eq. (S5) requires that $\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k\sum_i u_iL_i)$ must be real for any arbitrary real and nonzero vector $\boldsymbol{u}$. Therefore $\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k L_i)$ must be real for each i. The saturation of the second inequality of Eq. (S5) requires that $\sqrt{\Pi_k}\sqrt{\rho_{\boldsymbol{\lambda}}}$ must be proportional to $\sqrt{\Pi_k}\sum_i u_iL_i\sqrt{\rho_{\boldsymbol{\lambda}}}$ for any arbitrary, non-zero and real $\boldsymbol{u}$. Thus $\sqrt{\Pi_k}\sqrt{\rho_{\boldsymbol{\lambda}}}$ must be proportional to $\sqrt{\Pi_k}L_i\sqrt{\rho_{\boldsymbol{\lambda}}}$ for each i, i.e.,

$$\xi_i^k\sqrt{\Pi_k}\sqrt{\rho_{\boldsymbol{\lambda}}} = \sqrt{\Pi_k}L_i\sqrt{\rho_{\boldsymbol{\lambda}}},\ \forall i. \tag{S34}$$

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. (S34), i.e.,

$$\xi_i^k = \mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k L_i)/\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k),\ \forall i. \tag{S35}$$

Since the projector is regular, $\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k)$ is a real and positive. Eq. (S34) can be rewritten as

$$\sqrt{\Pi_k}(L_i - \xi_i^k)\sqrt{\rho_{\boldsymbol{\lambda}}} = 0,\ \forall i. \tag{S36}$$

Since for a projector $\sqrt{\Pi_k} = \Pi_k = \sum_\alpha |\pi_{k\alpha}\rangle\langle\pi_{k\alpha}|$, Eq. (S36) becomes

$$\sum_\alpha \left[|\pi_{k\alpha}\rangle\langle\pi_{k\alpha}|(L_i - \xi_i^k)\sqrt{\rho_{\boldsymbol{\lambda}}}\right] = 0,\ \forall i. \tag{S37}$$

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

$$\langle\pi_{k\alpha}|(L_i - \xi_i^k)\sqrt{\rho_{\boldsymbol{\lambda}}} = 0,\ \forall i,\ \alpha. \tag{S38}$$

Note that according to Eq. (S35) the condition of $\mathrm{Tr}(\rho_{\boldsymbol{\lambda}}\Pi_k L_i)$ being real is equivalent to that ξ_i^k is real. Furthermore, the kernel of $\sqrt{\rho_{\boldsymbol{\lambda}}}$ is the same as that of $\rho_{\boldsymbol{\lambda}}$. Thus we conclude $[L_i - \xi_i^k]|\pi_{k\alpha}\rangle \in \ker(\rho_{\boldsymbol{\lambda}})$, $\forall i$. It follows that the projections onto $\mathrm{supp}(\rho_{\boldsymbol{\lambda}})$ of $L_i|\pi_{k\alpha}\rangle$ and $\xi_i^k|\pi_{k\alpha}\rangle$ must be equal such that their subtraction only lies on $\ker(\rho_{\boldsymbol{\lambda}})$, i.e.,

$$(L_i|\pi_{k\alpha}\rangle)^\perp = \xi_i^k|\pi_{k\alpha}^\perp\rangle,\ \forall i,\ \alpha. \tag{S39}$$

Applying Eq. (S33) and $|\pi_{k\alpha}^\perp\rangle = \sum_n |\psi_{n\boldsymbol{\lambda}}\rangle\langle\psi_{n\boldsymbol{\lambda}}|\pi_{k\alpha}\rangle$ concludes the proof. □

C. Proof of Theorem 2

Proof: Since the saturation of Eq. (S27) is equivalent as the saturation of the two inequalities in Eq. (S25), we will work with Eq. (S25) subsequently. The saturation of the first inequality in Eq. (S25) requires $T_{ij}^k = \sum_{n\alpha}(z_{nj}^{k\alpha})^* z_{ni}^{k\alpha}$ is real for any i, j. That is, according to Eq. (S18),

$$\mathrm{Im}[\sum_{n\alpha}(z_{nj}^{k\alpha})^* z_{ni}^{k\alpha}] = 0,\ \forall i,\ j. \tag{S40}$$

The saturation of the second inequality in Eq. (S25) requires $\sum_i z_{ni}^{k\alpha}\delta\lambda_i$ be proportional to $\sum_j z_{nj}^{k\alpha}u_j$ with the proportionality constant independent of n, α, i.e.,

$$\sum_i z_{ni}^{k\alpha}\delta\lambda_i / \sum_j z_{nj}^{k\alpha}u_j = \sum_i z_{mi}^{k\beta}\delta\lambda_i / \sum_j z_{mj}^{k\beta}u_j,\ \forall n,\ m,\ \alpha,\ \beta. \tag{S41}$$

Eq. (S41) can be recast into

$$\sum_{ij}(z_{ni}^{k\alpha}z_{mj}^{k\beta} - z_{nj}^{k\alpha}z_{mi}^{k\beta})\delta\lambda_i u_j = 0,\ \forall n,\ m,\ \alpha,\ \beta. \tag{S42}$$

It must hold for any arbitrary nonzero $\boldsymbol{u}$ and nonzero $\delta\boldsymbol{\lambda}$, so we are left with $z_{ni}^{k\alpha}z_{mj}^{k\beta} - z_{nj}^{k\alpha}z_{mi}^{k\beta} = 0$, $\forall i,\ j,\ n,\ m,\ \alpha,\ \beta$. Thus the ratio

$$\eta_{ij}^k \equiv z_{ni}^{k\alpha}/z_{nj}^{k\alpha} \tag{S43}$$

should not depend on n, α. Substitution of Eq. (S18) into Eqs. (S43, S40) gives

$$\langle \partial_i \psi_{n,\boldsymbol{\lambda}} | \pi_{k\alpha} \rangle = \eta_{ij}^k \langle \partial_j \psi_{n,\boldsymbol{\lambda}} | \pi_{k\alpha} \rangle \, \forall i,\, j,\, n, \alpha, \tag{S44}$$

$$\mathrm{Im}[\eta_{ij}^k \sum_{n\alpha} (z_{ni}^{k\alpha})^* z_{ni}^{k\alpha}] = \mathrm{Im}[\eta_{ij}^k] \sum_{n\alpha} \left| z_{ni}^{k\alpha} \right|^2 = 0, \tag{S45}$$

from which we immediately identify that $\mathrm{Im}\eta_{ij}^k = 0$. □

III. RECOVER THE RESULTS BY PEZZÈ ET AL. [42]

Pezzè et al. [42] obtained the necessary and sufficient conditions for a measurement consisting of rank one projectors to saturate the MQCRB for pure states. Here we show that our Theorems 3 and 4 in the main text is consistent with their results. For rank one projectors, we suppress the subscript α in the basis vector $|\pi_{k\alpha}\rangle$. Multiplying both sides of Eq. (5) in the main text by $\langle \pi_k | \psi_{\boldsymbol{\lambda}} \rangle$, the only requirement that ξ_i^k be real gives

$$\mathrm{Im}[\langle \partial_i^0 \psi_{\boldsymbol{\lambda}} | \pi_k \rangle \langle \pi_k | \psi_{\boldsymbol{\lambda}} \rangle] = 0. \tag{S46}$$

This equation is equivalent as the Eq. (8) in Pezzè et al. [42] and is a generalization of Eq. (29) in Braunstein and Caves [17]. Similarly, multiplying both sides of Eq. (6) in the main text by $\langle \pi_k | \partial_j \psi_{\boldsymbol{\lambda}} \rangle$, the only requirement that η_{ij}^k be real gives

$$\mathrm{Im}[\langle \partial_i \psi_{\boldsymbol{\lambda}} | \pi_k \rangle \langle \pi_k | \partial_j \psi_{\boldsymbol{\lambda}} \rangle] = 0, \tag{S47}$$

which recovers Eq. (7) of Pezzè et al. [42].

IV. THE ROLE OF NONLOCAL MEASUREMENTS IN THE SATURATION OF THE MQCRB

We first consider measurements on ν replicas of a single pure state, denoted as $|\phi_{\boldsymbol{\lambda}}\rangle = |\psi_{\boldsymbol{\lambda}}\rangle^{\otimes \nu}$, where ν is the number of replicas of the pure state. A straightforward calculation gives

$$\langle \partial_i \phi_{\boldsymbol{\lambda}} | \partial_j \phi_{\boldsymbol{\lambda}} \rangle = \sum_{n=1}^{\nu} \langle \partial_i \psi_{\boldsymbol{\lambda}}^{(n)} | \partial_j \psi_{\boldsymbol{\lambda}}^{(n)} \rangle + \sum_{n,\, m,\, n \neq m} \langle \partial_i \psi_{\boldsymbol{\lambda}}^{(n)} | \psi_{\boldsymbol{\lambda}}^{(n)} \rangle \langle \psi_{\boldsymbol{\lambda}}^{(m)} | \partial_i \psi_{\boldsymbol{\lambda}}^{(m)} \rangle \,, \forall i,\, j, \tag{S48}$$

where $|\psi_{\boldsymbol{\lambda}}^{(n)}\rangle$ is the state of n-th copy. According to Matsumoto condition [46], an optimal measurement exists if and only if

$$\mathrm{Im} \langle \partial_i \phi_{\boldsymbol{\lambda}} | \partial_j \phi_{\boldsymbol{\lambda}} \rangle = \nu \mathrm{Im} \langle \partial_i \psi_{\boldsymbol{\lambda}} | \partial_j \psi_{\boldsymbol{\lambda}} \rangle = 0,\, \forall i,\, j, \tag{S49}$$

where we have used the fact that $\langle \partial_i \psi_{\boldsymbol{\lambda}}^{(n)} | \psi_{\boldsymbol{\lambda}}^{(n)} \rangle$ is purely imaginary. Therefore if a single copy of a pure state violates the Matsumoto condition, meaning the MQCRB is not achievable by any measurement, then any measurement including nonlocal ones on the replicas of the pure state will not achieve the MQCRB either.

The opposite limit is that $\rho_{\boldsymbol{\lambda}}$ is full ranked such that the support of $\rho_{\boldsymbol{\lambda}}$ is the total Hilbert space of the states. In this case, every basis vector is regular since

$$\langle \psi | \rho_{\boldsymbol{\lambda}} | \psi \rangle > 0,\, \forall \, |\psi\rangle \neq 0, \tag{S50}$$

and so does every measurement projector. Furthermore, in this case we have $L_i^{\perp} = L_i$, $\langle \partial_i^0 \psi_{n\boldsymbol{\lambda}} | = 0$ and $|\pi_{k\alpha}^{\perp}\rangle = |\pi_{k\alpha}\rangle$. Theorem 1 in the main text gives

$$\langle \psi_{n\boldsymbol{\lambda}} | L_i | \pi_{k\alpha} \rangle = \xi_i^k \langle \psi_{n\boldsymbol{\lambda}} | \pi_{k\alpha} \rangle \,, \forall i,\, n,\, \alpha. \tag{S51}$$

Since $\{|\psi_{n\boldsymbol{\lambda}}\rangle\}$ is complete in this case, we obtain

$$L_i \, |\pi_{k\alpha}\rangle = \xi_i^k \, |\pi_{k\alpha}\rangle \,, \forall i,\, \alpha. \tag{S52}$$

Now the requirement ξ_i^k being real is satisfied automatically since L_i is Hermitian. If the MQCRB is achievable by a set of measurement basis, then the L_i's will have common eigenvector $|\pi_{k\alpha}\rangle$. Note that the basis $\{|\pi_{k\alpha}\rangle\}$ is complete and orthonormal. Thus an optimal measurement exists if and only if

$$[L_i,\, L_j] = 0,\, \forall i,\, j. \tag{S53}$$

Let us now consider nonlocal measurements on the replicas of the full-ranked mixed state, denoted as as $\varrho_{\boldsymbol{\lambda}} = \rho_{\boldsymbol{\lambda}}^{\otimes\nu}$. If $\rho_{\boldsymbol{\lambda}}$ is full-ranked then $\varrho_{\boldsymbol{\lambda}}$ is also full-ranked. The SLD's associated with $\varrho_{\boldsymbol{\lambda}}$ are denoted by $\mathscr{L}_i$'s. By mathematical induction, it is readily shown that [15, 18]

$$\mathscr{L}_i = \sum_{n=1}^{\nu} L_i^{(n)},\, \forall i, \tag{S54}$$

where $L_i^{(n)} \equiv \mathbb{I}\otimes\cdots\otimes L_i \otimes\cdots\otimes\mathbb{I}$ is the SLD acting on the n-th copy of the probe states corresponding to parameter λ_i. Upon replacing $L_i \to \mathscr{L}_i$ in Eq. (S53) we know that the MQCRB is saturable if and only if

$$[\mathscr{L}_i,\, \mathscr{L}_j] = \sum_{n=1}^{\nu}[L_i^{(n)},\, L_j^{(n)}] = 0. \tag{S55}$$

But this condition is equivalent to $[L_i,\, L_j] = 0$. Thus we know if $\rho_{\boldsymbol{\lambda}}$ is full ranked and L_i's do not commute, which implies that no optimal measurements exist for the single copy, then nonlocal measurements on replicas of the full ranked mixed state do not help saturate the MQCRB.

V. OPTIMAL MEASUREMENTS IN ESTIMATING THE SEPARATIONS OF TWO POINT INCOHERENT SOURCES OF LIGHT

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

We mention in the main text that $\theta_{\boldsymbol{s}}$ is chosen such that $\Delta_{\boldsymbol{s}} \equiv e^{2i\theta_{\boldsymbol{s}}}\int d\boldsymbol{r}\Phi_{\boldsymbol{s}}^2(\boldsymbol{r})$ is real. Defining

$$v_{\boldsymbol{s}} \equiv \mathrm{Re}[\int d\boldsymbol{r}\Phi_{\boldsymbol{s}}^2(\boldsymbol{r})] = \mathcal{A}^2\int d\boldsymbol{r}\mathrm{circ}(r/a)\cos(2k\boldsymbol{s}_\perp\cdot\boldsymbol{r})\cos(ks_3r^2), \tag{S56}$$

$$w_{\boldsymbol{s}} \equiv \mathrm{Im}[\int d\boldsymbol{r}\Phi_{\boldsymbol{s}}^2(\boldsymbol{r})] = -\mathcal{A}^2\int d\boldsymbol{r}\mathrm{circ}(r/a)\cos(2k\boldsymbol{s}_\perp\cdot\boldsymbol{r})\sin(ks_3r^2), \tag{S57}$$

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

$$\tan 2\theta_{\boldsymbol{s}} = -\frac{w_{\boldsymbol{s}}}{v_{\boldsymbol{s}}}, \tag{S58}$$

$$\Delta_{\boldsymbol{s}} = \sqrt{v_{\boldsymbol{s}}^2 + w_{\boldsymbol{s}}^2}. \tag{S59}$$

As is clear from Eqs. (S56, S57), $v_{\boldsymbol{s}}$ is even in $\boldsymbol{s}$ while $w_{\boldsymbol{s}}$ is odd in $\boldsymbol{s}$. Thus according to Eq. (S58), we know $\theta_{\boldsymbol{s}}$ is odd in $\boldsymbol{s}$, i.e.,

$$\theta_{\boldsymbol{s}} = -\theta_{-\boldsymbol{s}}. \tag{S60}$$

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

$$\psi_{1\boldsymbol{s}}(\boldsymbol{r}) = \frac{1}{\sqrt{2(1+\Delta_{\boldsymbol{s}})}}[\Psi_{+\boldsymbol{s}}(\boldsymbol{r}) + \Psi_{-\boldsymbol{s}}(\boldsymbol{r})], \tag{S61}$$

$$\psi_{2\boldsymbol{s}}(\boldsymbol{r}) = \frac{-i}{\sqrt{2(1-\Delta_{\boldsymbol{s}})}}[\Psi_{+\boldsymbol{s}}(\boldsymbol{r}) - \Psi_{-\boldsymbol{s}}(\boldsymbol{r})], \tag{S62}$$

where

$$\Psi_{\pm\boldsymbol{s}}(\boldsymbol{r}) = e^{\pm i\theta_{\boldsymbol{s}}}\Phi_{\pm\boldsymbol{s}}(\boldsymbol{r}), \tag{S63}$$

$$\Phi_{\boldsymbol{s}}(\boldsymbol{r}) = \mathcal{A}\mathrm{circ}(r/a)\exp[ik(\boldsymbol{s}_{\perp}\cdot\boldsymbol{r} - s_3 r^2/2)]. \tag{S64}$$

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

$$\psi_{1\boldsymbol{s}}(\boldsymbol{r}) = \frac{\mathcal{A}\mathrm{circ}(r/a)\cos(\theta_{\boldsymbol{s}} + k\boldsymbol{s}_{\perp}\cdot\boldsymbol{r} - ks_3 r^2/2)}{\sqrt{2(1+\Delta_{\boldsymbol{s}})}}, \tag{S65}$$

$$\psi_{2\boldsymbol{s}}(\boldsymbol{r}) = \frac{\mathcal{A}\mathrm{circ}(r/a)\sin(\theta_{\boldsymbol{s}} + k\boldsymbol{s}_{\perp}\cdot\boldsymbol{r} - ks_3 r^2/2)}{\sqrt{2(1-\Delta_{\boldsymbol{s}})}}. \tag{S66}$$

Eqs. (S63, S64) immediately tell us

$$\langle\partial_i\Psi_{+\boldsymbol{s}}|\Psi_{+\boldsymbol{s}}\rangle = -\langle\partial_i\Psi_{-\boldsymbol{s}}|\Psi_{-\boldsymbol{s}}\rangle = -i\partial_i\theta_{\boldsymbol{s}} + i\delta_{i3}ka^2/4, \tag{S67}$$

$$\langle\partial_i\Psi_{-\boldsymbol{s}}|\Psi_{+\boldsymbol{s}}\rangle = \langle\partial_i\Psi_{+\boldsymbol{s}}|\Psi_{-\boldsymbol{s}}\rangle = -\partial_i\Delta_{\boldsymbol{s}}/2, \tag{S68}$$

where δ_{i3} is the Kronecker delta.

From Eqs. (S61, S62) 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

$$\langle\partial_i\psi_{1\boldsymbol{s}}|\psi_{1\boldsymbol{s}}\rangle = \langle\partial_i\psi_{2\boldsymbol{s}}|\psi_{2\boldsymbol{s}}\rangle = 0. \tag{S69}$$

Furthermore $\langle\partial_i\psi_{1\boldsymbol{s}}|\psi_{2\boldsymbol{s}}\rangle$ is also real since, upon application of Eqs. (S67, S68),

$$\begin{aligned}
\langle\partial_i\psi_{1\boldsymbol{s}}|\psi_{2\boldsymbol{s}}\rangle &= \frac{-i}{2\sqrt{1-\Delta_{\boldsymbol{s}}^2}}\left(\left(\langle\partial_i\Psi_{+\boldsymbol{s}}| + \langle\partial_i\Psi_{-\boldsymbol{s}}|\right)\left(|\Psi_{+\boldsymbol{s}}\rangle - |\Psi_{-\boldsymbol{s}}\rangle\right)\right) \\
&= \frac{-i}{2\sqrt{1-\Delta_{\boldsymbol{s}}^2}}\left(\langle\partial_i\Psi_{+\boldsymbol{s}}|\Psi_{+\boldsymbol{s}}\rangle + \cancel{\langle\partial_i\Psi_{-\boldsymbol{s}}|\Psi_{+\boldsymbol{s}}\rangle - \langle\partial_i\Psi_{+\boldsymbol{s}}|\Psi_{-\boldsymbol{s}}\rangle} - \langle\partial_i\Psi_{-\boldsymbol{s}}|\Psi_{-\boldsymbol{s}}\rangle\right) \\
&= \frac{-i\langle\partial_i\Psi_{+\boldsymbol{s}}|\Psi_{+\boldsymbol{s}}\rangle}{\sqrt{1-\Delta_{\boldsymbol{s}}^2}} = \frac{-\partial_i\theta_{\boldsymbol{s}} + \delta_{i3}ka^2/4}{\sqrt{1-\Delta_{\boldsymbol{s}}^2}}.
\end{aligned} \tag{S70}$$

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. (S70) 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

$$\langle\partial_i\psi_{2\boldsymbol{s}}|\psi_{1\boldsymbol{s}}\rangle = -\langle\partial_i\psi_{1\boldsymbol{s}}|\psi_{2\boldsymbol{s}}\rangle. \tag{S71}$$

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

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

Proof: Note that for $\boldsymbol{s} = 0$, $\langle\boldsymbol{r}|\Psi_{+\boldsymbol{s}}\rangle\big|_{\boldsymbol{s}=0} = \langle\boldsymbol{r}|\Psi_{-\boldsymbol{s}}\rangle\big|_{\boldsymbol{s}=0}$ and therefore the state becomes pure, which can be written as $\rho_{\boldsymbol{s}}\big|_{\boldsymbol{s}=0} = |\Phi_{\boldsymbol{s}}\rangle\langle\Phi_{\boldsymbol{s}}|_{\boldsymbol{s}=0}$. For a regular projector, one needs to apply Theorem 3 in the main text. For a null projector one needs to apply Theorem 4 in the main text. □

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

It is easily calculated that

$$|\Phi_{\boldsymbol{s}}\rangle\big|_{\boldsymbol{s}=0} = |Z_0^0\rangle, \tag{S72}$$

$$|\partial_1\Phi_{\boldsymbol{s}}\rangle\big|_{\boldsymbol{s}=0} = ik|Z_1^1\rangle/2, \tag{S73}$$

$$|\partial_2\Phi_{\boldsymbol{s}}\rangle\big|_{\boldsymbol{s}=0}=ik\,|Z_1^{-1}\rangle/2, \tag{S74}$$

$$|\partial_3\Phi_{\boldsymbol{s}}\rangle\big|_{\boldsymbol{s}=0}=-ik(|Z_2^0\rangle/3+|Z_0^0\rangle)/2. \tag{S75}$$

With Eqs. (S72-S75), one can easily understand the details in the construction recipes. For example, $\xi_i^{00}=0$ for all i follow from the following facts:

$$\langle\partial_i^0\Phi_{\boldsymbol{s}}|Z_0^0\rangle\big|_{\boldsymbol{s}=0}=\langle\partial_i\Phi_{\boldsymbol{s}}|Z_0^0\rangle\big|_{\boldsymbol{s}=0}=0,\, i=1,\,2, \tag{S76}$$

$$\langle\partial_3^0\Phi_{\boldsymbol{s}}|Z_0^0\rangle\big|_{\boldsymbol{s}=0}=\langle\partial_3\Phi_{\boldsymbol{s}}|Z_0^0\rangle\big|_{\boldsymbol{s}=0}-\langle\partial_3\Phi_{\boldsymbol{s}}|\Phi_{\boldsymbol{s}}\rangle\big|_{\boldsymbol{s}=0}\langle\Phi_{\boldsymbol{s}}|Z_0^0\rangle\big|_{\boldsymbol{s}=0}=0. \tag{S77}$$

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

1. *The necessary and sufficient conditions for optimal measurements when the state is mixed*

Lemma 1: For a mixed state $\rho_{\boldsymbol{s}}$, where the true value $\boldsymbol{s}\neq 0$ and therefore $\Delta_{\boldsymbol{s}}\neq 1$, 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

$$\frac{\partial_i\Delta_{\boldsymbol{s}}}{2p_{1\boldsymbol{s}}}\langle\psi_{1\boldsymbol{s}}|\pi_{k\alpha}\rangle-4p_{2\boldsymbol{s}}\langle\partial_i\psi_{1\boldsymbol{s}}|\psi_{2\boldsymbol{s}}\rangle\langle\psi_{2\boldsymbol{s}}|\pi_{k\alpha}\rangle+2\langle\partial_i\psi_{1\boldsymbol{s}}|\pi_{k\alpha}\rangle=\xi_i^k\langle\psi_{1\boldsymbol{s}}|\pi_{k\alpha}\rangle, \tag{S78}$$

$$-\frac{\partial_i\Delta_{\boldsymbol{s}}}{2p_{2\boldsymbol{s}}}\langle\psi_{2\boldsymbol{s}}|\pi_{k\alpha}\rangle-4p_{1\boldsymbol{s}}\langle\partial_i\psi_{2\boldsymbol{s}}|\psi_{1\boldsymbol{s}}\rangle\langle\psi_{1\boldsymbol{s}}|\pi_{k\alpha}\rangle+2\langle\partial_i\psi_{2\boldsymbol{s}}|\pi_{k\alpha}\rangle=\xi_i^k\langle\psi_{2\boldsymbol{s}}|\pi_{k\alpha}\rangle, \tag{S79}$$

holds $\forall i,\,\alpha$, 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. (S30, S69), we find

$$L_i^\perp=\frac{\partial_i\Delta_{\boldsymbol{s}}}{1+\Delta_{\boldsymbol{s}}}|\psi_{1\boldsymbol{s}}\rangle\langle\psi_{1\boldsymbol{s}}|-\frac{\partial_i\Delta_{\boldsymbol{s}}}{1-\Delta_{\boldsymbol{s}}}|\psi_{2\boldsymbol{s}}\rangle\langle\psi_{2\boldsymbol{s}}|+2\Delta_{\boldsymbol{s}}\langle\partial_i\psi_{1\boldsymbol{s}}|\psi_{2\boldsymbol{s}}\rangle|\psi_{1\boldsymbol{s}}\rangle\langle\psi_{2\boldsymbol{s}}|-2\Delta_{\boldsymbol{s}}\langle\partial_i\psi_{2\boldsymbol{s}}|\psi_{1\boldsymbol{s}}\rangle|\psi_{2\boldsymbol{s}}\rangle\langle\psi_{1\boldsymbol{s}}|. \tag{S80}$$

Thus

$$\begin{aligned}L_i^\perp|\pi_k\rangle=&|\psi_{1\boldsymbol{s}}\rangle\left[\frac{\partial_i\Delta_{\boldsymbol{s}}}{1+\Delta_{\boldsymbol{s}}}\langle\psi_{1\boldsymbol{s}}|\pi_{k\alpha}\rangle+2\Delta_{\boldsymbol{s}}\langle\partial_i\psi_{1\boldsymbol{s}}|\psi_{2\boldsymbol{s}}\rangle\langle\psi_{2\boldsymbol{s}}|\pi_{k\alpha}\rangle\right]\\&+|\psi_{2\boldsymbol{s}}\rangle\left[-\frac{\partial_i\Delta_{\boldsymbol{s}}}{1-\Delta_{\boldsymbol{s}}}\langle\psi_{2\boldsymbol{s}}|\pi_{k\alpha}\rangle-2\Delta_{\boldsymbol{s}}\langle\partial_i\psi_{2\boldsymbol{s}}|\psi_{1\boldsymbol{s}}\rangle\langle\psi_{1\boldsymbol{s}}|\pi_{k\alpha}\rangle\right],\end{aligned} \tag{S81}$$

which can be rewritten as upon noting Eq. (S69),

$$L_i^\perp|\pi_k\rangle=|\psi_{1\boldsymbol{s}}\rangle\left[\frac{\partial_i\Delta_{\boldsymbol{s}}}{1+\Delta_{\boldsymbol{s}}}\langle\psi_{1\boldsymbol{s}}|\pi_{k\alpha}\rangle+2\Delta_{\boldsymbol{s}}\langle\partial_i^\perp\psi_{1\boldsymbol{s}}|\pi_{k\alpha}\rangle\right]+|\psi_{2\boldsymbol{s}}\rangle\left[-\frac{\partial_i\Delta_{\boldsymbol{s}}}{1-\Delta_{\boldsymbol{s}}}\langle\psi_{2\boldsymbol{s}}|\pi_{k\alpha}\rangle-2\Delta_{\boldsymbol{s}}\langle\partial_i^\perp\psi_{2\boldsymbol{s}}|\pi_{k\alpha}\rangle\right]. \tag{S82}$$

In order to saturate the MQCRB, according to Theorem 1 in the main text, every regular projector $\Pi_k=\sum_\alpha|\pi_{k\alpha}\rangle\langle\pi_{k\alpha}|$ must satisfy

$$\frac{\partial_i\Delta_{\boldsymbol{s}}}{1+\Delta_{\boldsymbol{s}}}\langle\psi_{1\boldsymbol{s}}|\pi_{k\alpha}\rangle+2\Delta_{\boldsymbol{s}}\langle\partial_i^\perp\psi_{1\boldsymbol{s}}|\pi_{k\alpha}\rangle+2\langle\partial_i^0\psi_{1\boldsymbol{s}}|\pi_{k\alpha}\rangle=\xi_i^k\langle\psi_{1\boldsymbol{s}}|\pi_{k\alpha}\rangle, \tag{S83}$$

$$-\frac{\partial_i\Delta_{\boldsymbol{s}}}{1-\Delta_{\boldsymbol{s}}}\langle\psi_{2\boldsymbol{s}}|\pi_{k\alpha}\rangle-2\Delta_{\boldsymbol{s}}\langle\partial_i^\perp\psi_{2\boldsymbol{s}}|\pi_{k\alpha}\rangle+2\langle\partial_i^0\psi_{2\boldsymbol{s}}|\pi_{k\alpha}\rangle=\xi_i^k\langle\psi_{2\boldsymbol{s}}|\pi_{k\alpha}\rangle, \tag{S84}$$

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

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

Proof: For a null projector, one can apply Theorem 2 in the main text straightforwardly. Let us focus on the case of regular projectors. The explicit forms of $v_{\boldsymbol{s}}$ and $w_{\boldsymbol{s}}$ can be expressed as

$$v_{\boldsymbol{s}}\big|_{\boldsymbol{s}_\perp=0} = \frac{\pi\mathcal{A}^2}{ks_3}\sin(ks_3a^2), \tag{S85}$$

$$w_{\boldsymbol{s}}\big|_{\boldsymbol{s}_\perp=0} = -\frac{\pi\mathcal{A}^2}{ks_3}[1-\cos(ks_3a^2)], \tag{S86}$$

$$\partial_i v_{\boldsymbol{s}}\big|_{\boldsymbol{s}_\perp=0} = \partial_i w_{\boldsymbol{s}}\big|_{\boldsymbol{s}_\perp=0} = 0,\ i=1,\ 2. \tag{S87}$$

According to Eqs. (S58, S59), we obtain

$$\theta_{\boldsymbol{s}}\big|_{\boldsymbol{s}_\perp=0} = \frac{ks_3a^2}{4}, \tag{S88}$$

$$\Delta_{\boldsymbol{s}}\big|_{\boldsymbol{s}_\perp=0} = \left[\frac{2}{ks_3a^2}\sin\left(\frac{ks_3a^2}{2}\right)\right]^2, \tag{S89}$$

$$\left.\frac{2\partial_i\theta_{\boldsymbol{s}}}{1+4\theta_{\boldsymbol{s}}^2}\right|_{\boldsymbol{s}_\perp=0} = -\left.\frac{\partial_i w_{\boldsymbol{s}} v_{\boldsymbol{s}} - w_{\boldsymbol{s}}\partial_i v_{\boldsymbol{s}}}{v_{\boldsymbol{s}}^2}\right|_{\boldsymbol{s}_\perp=0}, \tag{S90}$$

$$\partial_i\Delta_{\boldsymbol{s}}\big|_{\boldsymbol{s}_\perp=0} = \left.\frac{v_{\boldsymbol{s}}\partial_i v_{\boldsymbol{s}} + w_{\boldsymbol{s}}\partial_i w_{\boldsymbol{s}}}{\delta_{\boldsymbol{s}}}\right|_{\boldsymbol{s}_\perp=0}. \tag{S91}$$

Therefore, we arrive at

$$\partial_i\theta_{\boldsymbol{s}}\big|_{\boldsymbol{s}_\perp=0} = \partial_i\Delta_{\boldsymbol{s}}\big|_{\boldsymbol{s}_\perp=0} = 0,\ i=1,\ 2. \tag{S92}$$

Substituting Eq. (S92) into Eqs. (S78, S79), one obtains the condition for regular projectors in Corollary 2 in the main text. In addition, at $s_3 = 0$ the condition is also consistent with that in Corollary 1 in the main text. □

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

It can be calculated that according to Eqs. (S65, S66, S88, S92),

$$\psi_{1\boldsymbol{s}}(\boldsymbol{r})\big|_{\boldsymbol{s}_\perp=0} = \frac{\mathcal{A}\mathrm{circ}(r/a)\cos[ks_3(a^2-2r^2)/4]}{\sqrt{p_{1\boldsymbol{s}}}}, \tag{S93}$$

$$\psi_{2\boldsymbol{s}}(\boldsymbol{r})\big|_{\boldsymbol{s}_\perp=0} = \frac{\mathcal{A}\mathrm{circ}(r/a)\sin[ks_3(a^2-2r^2)/4]}{\sqrt{p_{2\boldsymbol{s}}}}, \tag{S94}$$

$$\partial_i\psi_{1,\,2\boldsymbol{s}}(\boldsymbol{r})\big|_{\boldsymbol{s}_\perp=0} = \mp kx_i\psi_{2,\,1\boldsymbol{s}}(\boldsymbol{r}),\ i=1,\ 2. \tag{S95}$$

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

$$\langle\psi_{1\boldsymbol{s}}|Z_{2n+1}^{2m+1}\rangle = \langle\psi_{2\boldsymbol{s}}|Z_{2n+1}^{2m+1}\rangle = 0, \tag{S96}$$

$$\langle \partial_i \psi_{1\boldsymbol{s}} \big| Z_{2n}^{2m} \rangle = \langle \partial_i \psi_{2\boldsymbol{s}} \big| Z_{2n}^{2m} \rangle = 0, \tag{S97}$$

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

$$\partial_1 \psi_{n\boldsymbol{s}}(\boldsymbol{r})\big|_{\boldsymbol{s}_\perp=0} \propto f(r)\cos\phi,\ n=1,\ 2, \tag{S98}$$

$$\partial_2 \psi_{n\boldsymbol{s}}(\boldsymbol{r})\big|_{\boldsymbol{s}_\perp=0} \propto f(r)\sin\phi,\ n=1,\ 2, \tag{S99}$$

we obtain

$$\langle \partial_1 \psi_{n\boldsymbol{s}} \big| Z_{2n+1}^{-1} \rangle = 0,\ n=1,\ 2, \tag{S100}$$

$$\langle \partial_2 \psi_{n\boldsymbol{s}} \big| Z_{2n+1}^{1} \rangle = 0,\ n=1,\ 2. \tag{S101}$$

D. The case $s_3 = 0$

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

For a null projector, one can apply Theorem 2 in the main text straightforwardly. Let us focus on the case of regular projectors. It is easily calculated that

$$v_{\boldsymbol{s}}\big|_{s_3=0} = \mathcal{A}^2 \int d\boldsymbol{r} \mathrm{circ}(r/a)\cos(2k\boldsymbol{s}_\perp\cdot\boldsymbol{r}), \tag{S102}$$

$$w_{\boldsymbol{s}}\big|_{s_3=0} = 0, \tag{S103}$$

$$\partial_i v_{\boldsymbol{s}}\big|_{s_3=0} = \partial_i w_{\boldsymbol{s}}\big|_{s_3=0} = 0,\ i=1,\ 2. \tag{S104}$$

According to Eqs. (S58, S59), we obtain

$$\theta_{\boldsymbol{s}}\big|_{s_3=0} = 0, \tag{S105}$$

$$\partial_i \theta_{\boldsymbol{s}}\big|_{s_3=0} = \partial_i \Delta_{\boldsymbol{s}}\big|_{s_3=0} = 0,\ i=1,\ 2. \tag{S106}$$

Substituting Eq. (S106) into Eqs. (S78, S79), one obtains the condition for regular projectors in Corollary 2 in the main text. In addition, at $\boldsymbol{s}_\perp = 0$ the condition is also consistent with that in Corollary 1 in the main text. □

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

It can be calculated according to Eqs. (S65, S66, S105, S106) that,

$$\psi_{1\boldsymbol{s}}(\boldsymbol{r})\big|_{s_3=0} = \frac{\mathcal{A}\mathrm{circ}(r/a)\cos(k\boldsymbol{s}_\perp\cdot\boldsymbol{r})}{\sqrt{p_{1\boldsymbol{s}}}}, \tag{S107}$$

$$\psi_{2\boldsymbol{s}}(\boldsymbol{r})\big|_{s_3=0} = \frac{\mathcal{A}\mathrm{circ}(r/a)\sin(k\boldsymbol{s}_\perp\cdot\boldsymbol{r})}{\sqrt{p_{2\boldsymbol{s}}}}, \tag{S108}$$

$$\partial_i \psi_{1,\,2\boldsymbol{s}}(\boldsymbol{r})\big|_{s_3=0} = \mp k x_i \psi_{2,\,1\boldsymbol{s}}(\boldsymbol{r}),\ i=1,\ 2. \tag{S109}$$

We see that for $i = 1, 2$, both $\psi_{1\boldsymbol{s}}(\boldsymbol{r})\big|_{s_3=0}$ and $\partial_i\psi_{1\boldsymbol{s}}(\boldsymbol{r})\big|_{s_3=0}$ are even while both $\psi_{2\boldsymbol{s}}(\boldsymbol{r})\big|_{s_3=0}$ and $\partial_i\psi_{2\boldsymbol{s}}(\boldsymbol{r})\big|_{s_3=0}$ are odd. Note that they are all real as well as the basis functions $\pi_{\pm\alpha}(\boldsymbol{r}) = \langle \boldsymbol{r}|\pi_{\pm\alpha}\rangle$. If an even basis vector $|\pi_{+\alpha}\rangle$ is regular, then we find $\langle \partial_i\psi_{2\boldsymbol{s}}|\pi_{+\alpha}\rangle = \langle \psi_{2\boldsymbol{s}}|\pi_{+\alpha}\rangle = 0$ and

$$\xi_i^{+\alpha} = \frac{\langle \partial_i\psi_{1\boldsymbol{s}}|\pi_{+\alpha}\rangle}{\langle \psi_{1\boldsymbol{s}}|\pi_{+\alpha}\rangle} \tag{S110}$$

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 $\langle \partial_1\psi_{2\boldsymbol{s}}|\pi_{+\alpha}\rangle = \langle \partial_2\psi_{2\boldsymbol{s}}|\pi_{+\alpha}\rangle = 0$ and

$$\eta_{21}^{+\alpha} = \frac{\langle \partial_2\psi_{1\boldsymbol{s}}|\pi_{+\alpha}\rangle}{\langle \partial_1\psi_{1\boldsymbol{s}}|\pi_{+\alpha}\rangle} \tag{S111}$$

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 vectors, either regular or null and 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 $s_3 = 0$.