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Optimal measurements for resolution beyond the Rayleigh limit

J. Rehacek,[1] M. Paúr,[1] B. Stoklasa,[1] Z. Hradil,[1] and L. L. Sánchez-Soto[2,3,*]

[1]Department of Optics, Palacký University, 17. listopadu 12, 771 46 Olomouc, Czech Republic
[2]Departamento de Óptica, Facultad de Física, Universidad Complutense, 28040 Madrid, Spain
[3]Max-Planck-Institut für die Physik des Lichts, Günther-Scharowsky-Straße 1, Bau 24, 91058 Erlangen, Germany
*Corresponding author: lsanchez@fis.ucm.es

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We establish the conditions to attain the ultimate resolution predicted by quantum estimation theory for the case of two incoherent point sources using a linear imaging system. The solution is closely related to the spatial symmetries of the detection scheme. In particular, for real symmetric point spread functions, any complete set of projections with definite parity achieves the goal.

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The spatial resolution of any imaging device is restricted by diffraction [1], which causes a sharp point on the object to blur into a finite-sized spot in the image. This information is encoded in the point spread function (PSF) [2], whose size determines the resolution: two points closer than the PSF width will be difficult to resolve due to the substantial overlap of their images. This is the physical significance of the celebrated Rayleigh criterion [3].

Needless to say, improving this limit has been a source of continuing research. Actually, in the past two decades a number of top-notch techniques have appeared, overcoming Rayleigh limit under particular conditions. They rely on nonconventional strategies, such as near-field imaging or on nonclassical or nonlinear optical properties of the object [4–10]. However, these schemes are often challenging and require careful control of the source, which is not always possible.

Quite recently, Tsang and coworkers [11–13] have looked at this question from the perspective of estimation theory. The idea is to use the Fisher information and the associated Cramér–Rao lower bound (CRLB) to quantify how well the separation between two poorly resolved incoherent point sources can be estimated. When only light intensity at the image plane is measured (the basis of all the standard techniques), the Fisher information falls to zero as the separation between the sources decreases and the CRLB diverges accordingly; this is the Rayleigh curse [11]. However, when the Fisher information of the complete field is calculated, it remains constant and so does the CRLB, evidencing that the Rayleigh limit is subsidiary to the problem.

These stunning predictions prompted a sequence of rapid-fire experimental implementations [14–17] and quantum generalizations [18,19]. Inspired by these developments, in this Letter we derive simple conditions that ensure ultimate resolution by singling out sets of spatial modes such that, when the signal is projected onto them, yield constant Fisher information, thus attaining the CRLB. These measurements not only explain and generalize the known superresolution schemes, but also allow us to devise feasible strategies on demand, so that the separation of the sources can be estimated with the best achievable precision.

The key feature of these modes is the spatial symmetry: for any symmetric PSF, the complete set has a definite (i.e., odd or even) parity.

We follow the basic model in Refs. [11–13] and consider quasi-monochromatic paraxial waves with one specified polarization and one spatial dimension, x, denoting the image–plane coordinate. Here, we focus on the spatial degrees of freedom of the signal and formulate what follows in a quantum language, even though it can be directly applied to a classical scenario. This is justified because wave optics and quantum mechanics share the same mathematical structure. A coherent complex amplitude $U(x)$ can be assigned to a ket $|U\rangle$, such that $U(x) = \langle x|U\rangle$, where $|x\rangle$ represents a point-like source located at x. In this way, we model the wave from a point source as a pure state, which is an excellent approximation for stars in observational astronomy or molecules in localization microscopy.

We take a spatially invariant imaging system. The associated PSF, which is just the normalized intensity response to a point light source, is denoted as $I(x) = |\langle x|\Psi\rangle|^2 = |\Psi(x)|^2$, where $\Psi(x)$ is the amplitude PSF, which we require to be inversion symmetric; i.e., $\Psi(x) = \Psi(-x)$, an assumption met by most aberration-free imaging systems.

We assume that two mutually incoherent point sources are located at two unknown points $X_{\pm} = \pm \mathfrak{s}/2$ in the object plane. This regular configuration entails no essential loss of generality. Our objective is to estimate the separation $\mathfrak{s} = X_{+} - X_{-}$. In principle, the two sources might have unequal intensities. The density matrix for the image–plane modes is thus

$$\rho_{\mathfrak{s}} = q|\Psi_+\rangle\langle\Psi_+| + (1-q)|\Psi_-\rangle\langle\Psi_-|, \qquad 0 \le q \le 1, \tag{1}$$

where the spatially shifted responses are $\Psi_\pm(x) = \langle x \pm \mathfrak{s}/2|\Psi\rangle$. This $\rho_{\mathfrak{s}}$ gives the normalized mean intensity profile $\rho_{\mathfrak{s}}(x) = q|\Psi(x-\mathfrak{s}/2)|^2 + (1-q)|\Psi(x+\mathfrak{s}/2)|^2$. In general, the spatial modes excited by the two sources are not orthogonal ($\langle\Psi_-|\Psi_+\rangle \neq 0$), which means that they cannot be separated by independent measurements. This is the crux of the problem.

To estimate $\mathfrak{s}$ we must perform appropriate measurements. Complete von Neumann tests [20] will prove sufficient for our purposes. They consist of a set of orthonormal projectors $\{|n\rangle\langle n|\}$ (with $\langle n|n'\rangle = \delta_{nn'}$) resolving the identity $\Sigma_n |n\rangle\langle n| = \mathbb{1}$. Each projector represents a single output channel of the measuring apparatus; the probability of detecting the nth output is given by the Born rule $p_n(\mathfrak{s}) = \langle n|\rho_{\mathfrak{s}}|n\rangle$. The generalization to continuous observables is otherwise straightforward.

The statistics of the quantum measurement carries information about $\mathfrak{s}$. This is aptly encompassed by the Fisher information [21,22], which is a mathematical measure of the sensitivity of an observable quantity to changes in its underlying parameters (the emitter's position). It is defined as

$$\mathcal{F}_{\mathfrak{s}} = \mathbb{E}\left[\left(\frac{\partial \log p_n(\mathfrak{s})}{\partial \mathfrak{s}}\right)^2\right], \tag{2}$$

with $\mathbb{E}[Y]$ being the expectation value of the random variable Y. The CRLB [23,24] ensures that the variance of any unbiased estimator $\hat{\mathfrak{s}}$ of the quantity $\mathfrak{s}$ is bounded by the reciprocal of the Fisher information; viz,

$$\mathrm{Var}(\hat{\mathfrak{s}}) \ge \frac{1}{\mathcal{F}_{\mathfrak{s}}}. \tag{3}$$

Let us take the von Neumann measurement as the continuous projection over $|x\rangle\langle x|$, which corresponds to conventional image–plane intensity detection (or photon counting, in the quantum regime). We stress that this is the information used in any traditional technique, including previous superresolution approaches. The Fisher information (per detection event) for this scheme reads as

$$\mathcal{F}_{\mathfrak{s}} = \int_{-\infty}^{\infty} \frac{1}{\varrho_{\mathfrak{s}}(x)} \left[\frac{\partial \varrho_{\mathfrak{s}}(x)}{\partial \mathfrak{s}}\right]^2 \mathrm{d}x \simeq \mathfrak{s}^2 \int_{-\infty}^{\infty} \frac{[I''(x)]^2}{I(x)} \mathrm{d}x, \tag{4}$$

where, in the second integral we have performed a first-order expansion in $\mathfrak{s}$, which is valid only for points sufficiently close together. Then, $\mathcal{F}_{\mathfrak{s}}$ goes to zero quadratically as $\mathfrak{s} \to 0$. This means that detection of intensity at the image plane is progressively worse at estimating the separation for closer sources, to the point that the variance in this situation is doomed to blow up.

To bypass this obstruction, we need a different measurement that incorporates the information available in the phase discarded by the intensity detection. In what follows, we require our measurement to have a well-defined parity; i.e.,

$$\langle -x|n\rangle = \pm\langle x|n\rangle. \tag{5}$$

This, together with the assumed spatial symmetry of the amplitude PSF, means that

$$a_n = \langle n|\Psi_-\rangle = \int \langle n|x\rangle\langle x - \mathfrak{s}/2|\Psi\rangle \mathrm{d}x$$
$$= \pm \int \langle n|x\rangle\langle x + \mathfrak{s}/2|\Psi\rangle \mathrm{d}x = \pm\langle n|\Psi_+\rangle. \tag{6}$$

Accordingly,

$$p_n \equiv |a_n|^2 = |\langle n|\Psi_\pm\rangle|^2, \tag{7}$$

and the measurement does not feel the two-component structure of the signal. The original two-point resolution problem has been effectively transformed to localization of a single point source.

In addition, we impose the condition that the probability amplitudes a_n have to fulfill

$$\mathrm{Im}\left(a_n \frac{\partial a_n^*}{\partial \mathfrak{s}}\right) = 0, \qquad \forall\ n, \mathfrak{s}. \tag{8}$$

We emphasize that, for infinitesimal separations $\mathfrak{s}$ this becomes the optimality condition found in Ref. [25] for resolving two neighboring pure states. The more stringent constraint Eq. (8) extends the optimality of the measurement to all separations. Indeed, by Eq. (8), the Fisher information becomes

$$\mathcal{F}_{\mathfrak{s}} = 4\sum_n \left|\frac{\partial a_n}{\partial \mathfrak{s}}\right|^2. \tag{9}$$

Next, we note that $|\Psi_\pm\rangle = \exp(\pm i\mathfrak{s}P/2)|\Psi\rangle$. Here, P is the momentum operator that generates displacements in the x variable, so it acts as a derivative $P = -i\partial_x$, much in the same way as in quantum optics. In the momentum representation

$$a_n = \int \langle n|p\rangle\langle p|\Psi\rangle e^{-i\mathfrak{s}p/2} \mathrm{d}p, \tag{10}$$

which, upon inserting this in Eq. (9), performing the derivative, and using the completeness, gives the final compact expression

$$\mathcal{F}_{\mathfrak{s}} = \int p^2 |\Psi(p)|^2 \mathrm{d}p = \langle P^2\rangle, \tag{11}$$

where $\Psi(p)$ is the Fourier transform of the PSF amplitude $\Psi(x)$. This is known to be the quantum limit for the problem in hand [25,26]. The Fisher information appears then as the second moment of P with respect to the PSF and is therefore independent of the separation of the points. Consequently, the variance in the CRLB remains constant and one lifts the Rayleigh curse, as heralded. Hence, we have identified optimal conditions, Eqs. (5) and (8), enabling two-point resolution to attain the quantum CRLB and the ultimate resolution limit.

Next, we address the problem of finding the optimal measurements for a given PSF. By writing $a_n = |a_n|\exp(i\alpha_n)$, the condition in Eq. (8) requires the phases α_n to be independent of $\mathfrak{s}$. As these phases can be absorbed in the basis $|n\rangle$, this is tantamount to requiring real probability amplitudes a_n. For real $\Psi(x)$, this can be satisfied by restricting the choice of the measurement basis to modes with real amplitudes $\langle x|n\rangle$, as it is clear from Eq. (6).

We have thus come to an interesting observation: for an optical system with a real symmetric amplitude PSF, the ultimate resolution is achieved by projecting the signal onto any complete set of real spatial modes $\langle x|n\rangle$ with a well-defined parity. As there are many such choices, the ultimate resolution should not be considered as a rarity, but rather as a feature shared by many permissible detection schemes. Furthermore, these detections are universal; i.e., they attain the quantum limit for all real and symmetric PSFs, and hence irrespective of the knowledge of the true PSF.

When the amplitude PSF becomes complex, but still spatially symmetric, we may proceed as follows. As the spatial parity is preserved by the Fourier transform, the required real-valuedness of a_n is ensured by

$$\langle n|p\rangle\langle p|\Psi\rangle = \pm(\langle n|p\rangle\langle p|\Psi\rangle)^*. \tag{12}$$

Hence, optimal measurements can be constructed starting from a complete set of real modes with definite parity in momentum representation and rephasing them to absorb the momentum symmetric phase of the $\langle p|\Psi\rangle$ term. This adjustment preserves the required spatial symmetry of the modes.

Because of the ambiguity inherent in the conditions in Eqs. (5) and (8), there is ample room for further refinement. In particular, finding efficient measurements that for a given PSF quickly saturate the CRLB with a small number of projections may be crucial for implementing ultimate imaging in practice. It is known that in the limit of small $\mathfrak{s}$, all the information can be extracted with a single projection proportional to the first derivative of $\Psi(x)$ [17]. This suggests that one could try to project the signal on a set of orthonormalized derivatives of $\Psi(x)$. Indeed, we propose to construct the efficient measurement basis $|n\rangle$ in momentum space as

$$\Phi_n(p) \equiv \langle p|n\rangle = Q_n(p)\Psi(p), \tag{13}$$

where $Q_n(p)$ is a system of orthogonal polynomials, with respect to the measure $|\Psi(p)|^2 dp$. Since this measure is symmetric, they satisfy the symmetry property $Q_n(-p) = (-1)^n Q_n(p)$ [27].

One can check that this generates a *bona fide* measurement basis. Truly, for the states in Eq. (13), the condition in Eq. (5) trivially holds, the probability amplitudes $a_n = \langle n|\Psi_\pm\rangle$ are real, and Eq. (8) is fulfilled. Of course, one would expect that the number of significant projections is small, and even the first derivative is sufficient in the superresolution regime.

The efficient PSF-adapted modes attaining the CRLB in Eq. (11) for all separations are obtained by an inverse Fourier transform

$$\Phi_n(x) \equiv \langle x|n\rangle = \frac{1}{\sqrt{2\pi}}\int Q_n(p)\Psi(p)e^{\mathrm{i}px}\mathrm{d}p. \tag{14}$$

The general rules in Eqs. (13) and (14) of finding the PSF-adapted scheme make the second main result of this Letter.

As a first, important example, we consider a Gaussian PSF amplitude $\Psi(x) = (2\pi)^{-1/4}\exp(-x^2/4)$, with unit variance ($\sigma = 1$). Although a circular diaphragm produces Airy rings, these are routinely approximated by a Gaussian PSF, so this is more than a curiosity. The Fourier transform of $\Psi(x)$ is again a Gaussian, and a direct calculation gives $\mathcal{F}_{\mathfrak{s}} = 1/4$. The optimal PSF-adapted set consists of Hermite–Gauss polynomials, which are orthonormal with respect to the PSF.

As a second example, we take a slit aperture with $\Psi(x) = \frac{1}{\sqrt{\pi}}\operatorname{sinc}(x)$ and Fourier transform $\Psi(p) = \frac{1}{\sqrt{2}}\operatorname{rect}(p/2)$. Here, $\operatorname{sinc}(x) = \sin(x)/x$ and $\operatorname{rect}(p)$ is 0 outside the interval $[-1/2, 1/2]$ and 1 inside it. The set $\Phi_n(p)$ is now the Legendre polynomials $L_n(p)$, which are complete in the unit interval. In this way,

$$a_n = \langle n|\Psi_\pm\rangle = \frac{\sqrt{2n+1}}{2}\int_{-1}^{1} L_n(p)e^{-i\mathfrak{s}p/2}\mathrm{d}p. \tag{15}$$

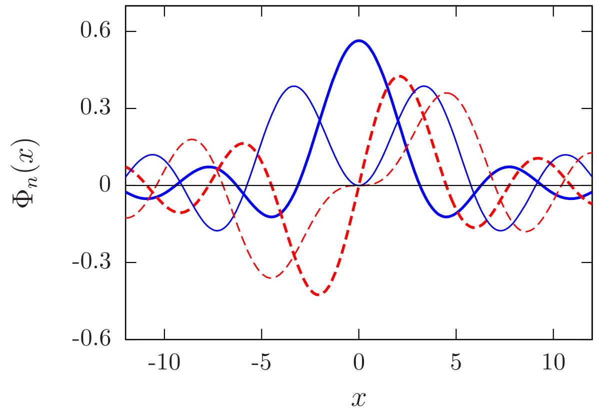

Fig. 1. First PSF-adapted modes from Eq. (16) for a sinc response. In blue solid lines we plot the symmetric modes [$n = 0$ (thick) and $n = 2$ (thin)] and in red broken lines we have the antisymmetric ones [$n = 1$ (thick) and $n = 3$ (thin)].

By Eq. (11), the Fisher information is $\mathcal{F}_{\mathfrak{s}} = 1/3$ and, by Eq. (14), the efficient measurement modes are given as

$$\Phi_n(x) = \sqrt{n + 1/2}\,\frac{J_{n+\frac{1}{2}}(x)}{\sqrt{x}}, \tag{16}$$

where $J_k(x)$ is the Bessel function of the first kind. For $n = 1$, the measurement reduces to the first derivative of the sinc function, as expected. In Fig. 1 we plot the first PSF-adapted modes from Eq. (16).

Each projection contributes with a piece of information,

$$\mathcal{F}_{\mathfrak{s},n} = \frac{\pi\left[nJ_{n-\frac{1}{2}}(\mathfrak{s}/2) - (n+1)J_{n+\frac{3}{2}}(\mathfrak{s}/2)\right]^2}{(2n+1)\mathfrak{s}}, \tag{17}$$

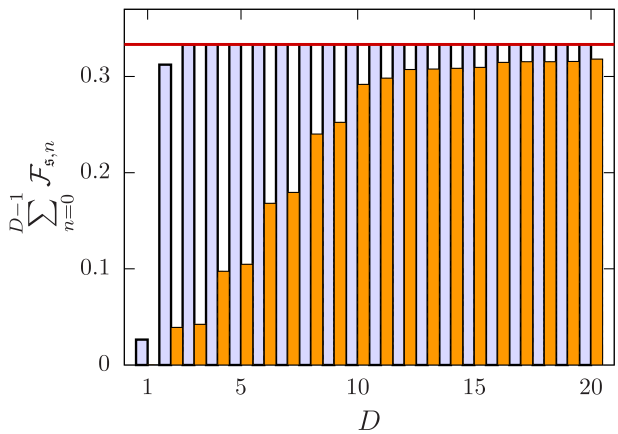

Fig. 2. Fisher information attained by the first D projections on the Hermite–Gauss basis with arbitrarily chosen $\sigma = \pi$ (orange bars) and the PSF-adapted measurement Eq. (16), when applied to a system with a sinc impulse response. The separation and the corresponding Rayleigh limit are $\mathfrak{s} = 1$ and $\mathfrak{s} = \pi$, respectively. More than a hundred of Hermite–Gauss projections must be measured to access 98.5% of the quantum Fisher information (indicated by a horizontal red line), whereas just three projections of the PSF-adapted measurement are sufficient.

and, interestingly, these complicated terms sum up to a total of $\mathcal{F}_{\mathfrak{s}} = 1/3$.

The advantage of this approach can be illustrated by comparing the performance of two optimal detections: the PSF-adapted measurement from Eq. (16) and the generic Hermite–Gauss projections, for the same sinc aperture. Figure 2 shows the information obtained by summing the Fisher information over the first D projections. Both measurements attain the quantum CRLB; however, the number of effective projections to be measured is considerably less for the former.

Finally, we mention in passing that since orthogonality of the measurement modes is not required for deriving the quantum limit from Eq. (11), the same resolution can be obtained in principle with over-complete detections (rank-one probability operator measures), such as the modes comprised of the real and imaginary parts of plane waves that correspond to measuring the real and imaginary parts of the Fourier spectrum of the signal.

The experimental realization of PSF-adapted measurements can be in principle achieved with a spatial mode demultiplexer; i.e., an optical system converting a given set of optimal modes $\Phi_n(x)$ into a set of spatially disentangled modes $\Phi'_n(x) \equiv \langle x|n'\rangle = \langle x|\mathcal{R}|n\rangle$ (with $\Phi'_n(x)\Phi'_{n'}(x) \approx 0$ for $n \neq n'$), followed by a direct intensity measurement. For example, to project the signal on a set of Hermite–Gauss modes, the signal can be subject to conversion from Hermite–Gauss to Laguerre–Gauss modes and, subsequently, to transverse-momentum modes [28,29]. Those are focused on a CCD camera to produce spatially separated spots whose total intensities become proportional to $p_n(\mathfrak{s})$. For other sets of modes, the mode converter transformation U can always be approximated with a sequence of phase modulations and free propagations [30] and realized with a digital-holography setup similar to that used in Ref. [17].

In conclusion, we have shown that an optimal sub-Rayleigh two-point resolution limit can be achieved with an optical system having a symmetric amplitude PSF, provided the system output is projected onto a suitable complete set of modes with definite parity. Particularly useful modes can be generated from the derivatives of the system PSF, which in the limit of small separation can access all available information with a single projection.

The above formalism can be generalized to other transformations provided the frequency spectrum is replaced with a suitable representation, in which the assumed transformation becomes a simple phase shift.

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