Optimal Metagrating for Position Metrology under Poisson Shot Noise

Zheng Xi, Sander Konijnenberg, and H.P. Urbach
Optics Research Group, Delft University of Technology
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We introduce an optimal metagrating design for position metrology under Poisson shot noise. By using electric and magnetic resonances inside the metagrating, the position of the metagrating within an interference field can be extracted with high precision in the presence of shot noise, leading to nearly three orders of magnitude improvement compared to the centroid-fitting-based position metrology with the same number of detected photons. Furthermore, we find that the improvement in precision is closely related to the formation of a phase vortex in the diffraction orders around the optimal design in the parameter space. The connection between the metagrating design, the formation of a phase vortex and the fundamental precision limit using classical light gives new insights to all of these fields.

Metadevices consisting of artificially designed subwavelength resonant structures can have unique and useful functionality beyond classical devices\cite{6,7}. In particular, the control over optical beam properties such as phase, amplitude, and polarization using dielectric metadevices with electric and magnetic resonances have shown tremendous progress surpassing limits of conventional methods\cite{6,7}.

One particular important research area of optics is to develop sensitive metrology to measure a very small displacement around a certain point\cite{8–21}. This problem is basic for pushing the limit in fields such as interferometry\cite{14–17}, metrology\cite{12} and super-resolution microscopy\cite{3,4,11}. This amounts to a parameter estimation problem in the presence of measurement noise, which can either be due to imperfections of the setup, or more fundamentally, be the intrinsic fluctuations due to photon shot noise. The finite precision of inferring the position in the presence of noise is described by statistics, giving a lower bound on the measurement uncertainty called the Cramér-Rao lower bound (CRLB)\cite{22}. Given $N$ independently detected photons, this bound implies a minimum uncertainty given by $\sigma/\sqrt{N}$, where $\sigma^2$ is the variance of the measurement result per photon\cite{23}. Depending on the measurement scheme, $\sigma^2$ has different values and sets a restriction on the maximum precision that can be achieved, especially for weak signals where the total number of detected photons is low. For example, in fluorescence microscopy, the position of the fluorescent molecule is obtained by centroid fitting and $\sigma^2$ is then governed by the point spread function (PSF) whose minimum size is limited by the diffraction limit\cite{24,25}. While a lot of research has been done to optimize the PSF to obtain a lower CRLB\cite{26,27,28}, these techniques often require complex and precise shaping of the field. Recently, a very promising approach was proposed to improve the localization precision to $\sim 1\text{nm}$ by the use of an intensity minimum\cite{30}. However, this approach requires sequential scans which increases the measurement time\cite{31}.

In this Letter, we introduce a specially designed resonant metagrating to minimize the restriction imposed by $\sigma^2$ without the need for additional scans. By optimizing the unit cell resonances, we encode the position information of the metagrating inside an illumination field into the intensities of the reflected diffraction orders. Photon shot noise is considered in the model to investigate the fundamental precision limit that can be achieved using classical light. By writing the field scattered by the unit cell of the metagrating as a superposition of fields of linear and rotating electric and magnetic dipoles, it can be shown that at the resonance of these dipoles, the reflected order of interest has a phase vortex as function of certain design parameters. The center of the phase vortex corresponds to the optimized design with improved position precision. The connection between the formation of a phase vortex due to the multipole resonances of the metagrating and the fundamental precision limit for position metrology set by the CRLB opens new possibilities for metadevices to surpass current limits in metrology.

We use a silicon nanowire with refractive index $n = 3.5$ of radius $R$ as the constituting element for the metagrating, because of its potential for controlling the far-field scattering properties\cite{32–37}. The metagrating is placed inside an interference field produced by two plane waves with an initial phase shift of $\pi$ as shown in Fig.1(a). The wavelength used is $650\text{nm}$ throughout this Letter. The illumination of the metagrating is chosen such that the $x$-component of the incident wave vectors satisfies $k_x = \pi/P$, where $P$ is the pitch of the metagrating. Under this condition, the two reflected orders $P_+$ and $P_-$ are parallel to the incident angles. The metagrating is designed to make $P_+$ and $P_-$ vanish when displaced by $+x_0$ and $-x_0$ respectively. Because the displacement $x_0$ is equivalent to adding a phase shift of $2k_x x_0$ to one of the two beams, this requirement can be expressed as:

$$r_0 - r_1 e^{-2ik_x x_0} = 0,$$

where $r_0$ and $r_1$ are the reflection coefficients of the 0th and 1st orders and the minus sign is due to the initial phase shift of $\pi$. Assuming each incident beam has a power $\mathcal{P}$, for other displacements $x$, the power of the
two diffraction orders are:
\[
P_+ = 4r_0^2 P \sin^2 k_x (x - x_0), \\
P_- = 4r_0^2 P \sin^2 k_x (x + x_0).
\] (2)

In Fig. 1(b) we show the normalized power difference of the two reflected orders defined by \( D(x) = (P_+ - P_-)/(P_+ + P_-) \). The value of displacement \( x \) can be inferred by measuring \( D(x) \) without scanning, provided that \( x \) is in the interval \([-x_0, x_0]\). For a region \( d \) shown in Fig. 1(b), \( D(x) \) can be linearized with the slope given by 
\[
\frac{dp_0(x; x_0)}{dx} = 2k_x \sqrt{N},
\] (3)

The uncertainty \( \sigma(x; x_0) \) in retrieving position \( x \) is highly dependent on the uncertainty of inferring \( p_0(x; x_0) \) from the binomial distribution. The latter is characterized by the reciprocal of the Fisher information 
\[
J(p_0(x; x_0)) \approx \frac{N}{p_0(x_0)(1 - p_0(x; x_0))} \text{ for a binomial distribution.}
\] By applying the chain rule, the CRLB is given by:
\[
\sigma_{\text{CRLB}}(x; x_0) = \sqrt{\frac{dp_0(x; x_0)}{dx} / \sqrt{J(p_0(x; x_0))}}.
\] (4)

If one is interested in knowing the position for \( x = 0 \), e.g. for alignment, Eq.(4) becomes:
\[
\sigma_{\text{CRLB}}(0; x_0) \approx \frac{k_x x_0}{2k_x \sqrt{N}},
\] (5)

This shows the key advantage of the metagrating design. For centroid-fitting-based microscopy, the CRLB is given by 
\[
\sigma_{\text{CRLB}}(0; x_0) = \frac{\lambda}{2\pi \sqrt{N}}
\] and is thus limited by the wavelength for \( N \) detected photons. In contrast, for the metagrating based measurement with \( N \) detected photons, the uncertainty around the origin scales linearly with \( x_0 \) (a parameter which can be designed to be much smaller than the wavelength). In Fig. 1(c), we compare the two schemes in detail. The value of \( x_0 \) is tuned from 0.08nm to 50nm. By reducing \( x_0 \), the measurement scheme based error \( \sigma \) can be reduced significantly, resulting in more than three orders of magnitude improvement.

The question now is how to design a metagrating that fulfills Eq.(1). The rich resonances contained in the unit cell consisting of the silicon nanowire offer extra freedom to realize the desired properties. Because the reflected field is fully determined by the scattered field from the unit cell, we first expand the scattered field \( G_{\text{cell}}(\phi) \) of a single nanowire within the metagrating array using multipole expansion:
\[
G_{\text{cell}}(\phi) = \sum_{m=-\infty}^{\infty} A_m e^{im\phi},
\] (7)

with \( A_m \) corresponding to the multiple-scattered coefficients for different multipoles. Note here the difference between the multipole expansion of the scattered field from an isolated nanowire: 
\[
G_{\text{iso}}(\phi) = \sum_{m=-\infty}^{\infty} a_m e^{im\phi},
\] where \( a_m \) correspond to the strength of single-scattered multipoles, and the scattered field \( G_{\text{cell}}(\phi) \) from a single nanowire as part of the metagrating. For \( G_{\text{iso}}(\phi) \), the excitation field is only a plane wave whereas for \( G_{\text{cell}}(\phi) \), the excitation field is the superposition of the plane wave and
two reflected orders. For sufficiently small radii, one can
\[ \phi \]
where
\[ \text{Eq.(1)} \]
leads to:
\[ (c), (d) \]
Absolute value and phase of the complex reflection
for each multipole for TM polarization. (b) Far-field scattering
|a nanowire within the metagrating:
for
\[ \text{Fig.2(a)} \]
scatter the fields from other nanowires in the metagrating.
In other words, multiple scattering is fully taken into
account in calculating \( A_m \). Substituting \( G_{\text{far}}(\phi) \)
into Eq.(1) leads to:
\[ G_{\text{far}}(\phi_0) - G_{\text{far}}(\phi_1) e^{-2ik_x x_0} = 0, \]  
where \( \phi_0 = \phi_{\text{in}} \) and \( \phi_1 = \pi - \phi_{\text{in}} \)
are the angles of the two reflected orders. For sufficiently small radii, one can keep
only the first three terms \( A_{-1,0,1} \) in the expansion
and Eq.(8) becomes:
\[ A_0 \sin(\Delta) - i A_1 \cos(\phi_{\text{in}} + \Delta) - i A_{-1} \cos(\phi_{\text{in}} - \Delta) = 0, \]  
with \( \Delta = k_x x_0 \).

The above derivation works for both TE and TM polarization. For TM polarization, the term \( A_0 \)
corresponds to the multiple-scattered linearly polarized magnetic dipole in the array. Because of the broken symmetry, the \( A_{-1} \) and \( A_1 \) terms are different when \( \phi_{\text{in}} \neq 90^\circ \). Since their scattered fields carry different topological charges \(-1\) and 
\(+1\) as shown in the insets of Fig.2(a), they can be associated with the multiple-scattered left-rotating and right-
rotating electric dipoles. For TE polarization, \( A_0 \)
corresponds to the multiple-scattered linearly polarized electric
dipole while \( A_{\pm1} \) are the rotating magnetic dipoles.

On the left-hand-side of Eq.(9) is the complex amplitude
of reflection order \( F_\pm \) at position \( x = x_0 \). To make
this order vanish at \( x_0 \), there should be a proper balance
of the different multipole components. Of particular interest
is the factor \( i \) in front of \( A_{\pm1} \) which implies that
a phase difference of \( \pi/2 \) is required. When one of
the multipoles experiences a resonance, the phase around
this resonance changes rapidly, by which this requirement can be fulfilled.

To verify this, we show in Fig.2(a) the behavior of different
multipoles as a function of the radius \( R \) of the
nanowire for \( \phi_{\text{in}} = 60^\circ \), with insets being the phase map
of each multipole component. The incident angle is
chosen to be \( \phi_{\text{in}} = 60^\circ \) as in Fig.1(b). A clear resonance
in \( |A_0| \) is seen at \( R = 70 \text{nm} \), which corresponds to
the multiple-scattered magnetic dipole resonance. We plot the far-field scattering pattern \( |G_{\text{far}}(\phi)|^2 \) at this radius in Fig.2(b). For comparison, the scattering pattern \( |G_{\text{far}}(\phi)|^2 \) of the isolated nanowire is also plotted. Eq.(1)
implies that \( |r_0| = |r_1| \), i.e. the amplitude of the scattered
field in the directions \( \phi = 60^\circ, 120^\circ \) should be the
same in Fig.2(b). This is not possible for the isolated
case, because the far-field scattering pattern \( |G_{\text{far}}(\phi)|^2 \) is
symmetric with respect to the incident direction \( \phi = 60^\circ \).
However, because of the coupling inside the metagrating,
the symmetry between \( A_{\pm1} \) is broken and the interference
of these multipole moments produces a far-field pattern
with \( |G_{\text{far}}(60^\circ)|^2 = |G_{\text{far}}(120^\circ)|^2 \).

In Fig.2(c) and Fig.2(d) the absolute value and phase
of the complex amplitude of the reflection order \( P_\pi \)
are shown for as a function of position \( x \) and radius \( R \). At
\( x = 22 \text{nm} \) and \( R = 70 \text{nm} \) the amplitude is zero meaning
that for these values Eq. (1) is satisfied, which is in agreement with the zero of \( D(x) \) in Fig.1(b). It is particularly interesting to look at the phase distribution
around this zero-amplitude point. Due to the presence of the multiple-scattered magnetic dipole resonance in \( |A_0| \),
the phase changes very rapidly, forming a phase vortex
topological charge \(+1\) in Fig.2(d). It is at this phase
vortex point that the metagrating satisfies the design requirement. Because such a phase vortex is topologically
stable\[41–44\], it follows that by continuous variation of
parameters such as the incident angle \( \phi_{\text{in}} \), Eq. (1) is
again satisfied for some \( R \) and \( x_0 \).

Therefore, we can utilize this topological robustness to minimize \( x_0 \) and thus minimize \( \sigma^{\text{CR-LB}}(0; x_0) \) for the
alignment. Besides, different incident polarizations have
different multipole coefficients which also influence how small \( x_0 \) can be obtained.

The results of exploring the above possibilities are summarized
in Fig.3(a). On the horizontal axes, the radius \( R \) and incident angle \( \phi_{\text{in}} \) are varied and the absolute value
of the normalized power difference \( D(x_0) \) is plotted as different
colors at different \( x_0 \). Each red point in Fig.3(a)
corresponds to a good metagrating design with \( |D(x_0)| \approx 1 \).
By continuous variation of \( \phi_{\text{in}} \), the good design which
results to the formation of the phase vortex is always satisfied for some other \( R \) and \( x_0 \).
FIG. 3. (a) The achievable $x_0$ for different combination of $R$ and $\phi_{in}$ for both TE and TM polarizations using metagrating designs. (b) Absolute value of the normalized power difference $D(x)$ for TE and TM polarizations at the optimum design with minimum $x_0$. The insets show the formation of a phase vortex around the optimum design. (c) Multipole amplitude strength for TE and TM polarizations at minimal $x_0$. (d) Achievable $\sigma^\text{CRLB}(0)$ for TE and TM polarizations under N photons with using good metagrating designs shown as the red points in Fig. 3(a).

There are three distinct curves giving good metagrating designs, which correspond to the trajectories of phase vortexes. The origins of the three curves can be identified by comparing them with the position of multipole resonances as indicated in the plot. It can be seen that good designs can also be obtained from resonances with $m = -1, 1$ for TE polarization. In this case, it is the resonances from the two rotating dipoles that provide the required $\pi/2$ phase shift. A small change of $R$ gives a large change in $x_0$ for the $m = -1, 1$ branch as follows from the dotted line in Fig. 3(a) (which is not continuous due to insufficient sampling in $R$). We therefore focus on the two $m = 0$ branches.

Although an explicit expression for the dependence of $x_0$ on $R$ and $\phi_{in}$ is complicated, to make $x_0$ small, a smaller $R$ and a relatively large $\phi_{in}$ are needed. We restrict $\phi_{in}$ to be smaller than $70^\circ$, to present the occurrence of a second reflection order. By imposing this constraint, the minimum $x_0$ is determined for each polarization. The normalized power difference $D(x)$ is plotted in Fig. 3(b) for both polarizations for the design of the minimum $x_0$. With TE polarization, a much smaller $x_0$ (0.08nm) can be achieved than with TM (15nm). It is further confirmed that for both cases, a phase vortex occurs around the desired design shown in insets of Fig. 3(b).

To understand the difference in performance between both polarizations, we take the absolute value of Eq.(9) and assume $|A_{-1}| \approx |A_{1}|$ and $k_2 x_0 << 1$ at the $A_0$ resonance for small $x_0$. After some derivations, one finds:

$$x_0 \approx \frac{\lambda}{2\pi} |A_1|/|A_0|.$$  \hspace{1cm} (10)

In Fig.3(c), we plot the amplitudes of $|A_{-1}|, |A_0|$ and $|A_{1}|$ at the angle for which the smallest $x_0$ can be achieved for both polarizations. For TE polarization, the two dipole resonances are further apart and the ratio $|A_{1}|/|A_0| \approx 0.001$ is smaller at the $A_0$ resonance than for TM case where $|A_{1}|/|A_0| \approx 0.15$. The difference in this ratio leads to approximately two orders of magnitude difference in $x_0$, which in turn explains the difference in the achievable precision limit plotted in Fig. 3(d).

In many applications, we are not only interested in knowing the position information around one point, but also within a certain range. Let this range be $[-x_r, x_r]$, when $k_2 x_r << 1$, the total uncertainty is:

$$\int_{-x_r}^{x_r} \sigma^\text{CRLB}(x; x_0)dx = \frac{1}{\sqrt{N}}(x_0x_r + x_r^3/3x_0),$$  \hspace{1cm} (11)

with $\sigma^\text{CRLB}(x; x_0) = \frac{1}{\sqrt{N}}(x_0/2 + x^2/2x_0)$. We therefore look for an optimum $x_0$ that minimizes Eq.(11) under the constraint $x_0 \geq x_r$, this guarantees that the retrieved position is unique as illustrated in Fig. 1(b). In Fig. 4, we plot the total standard uncertainty as a function of $x_0/x_r$ with $x_r = 20\text{nm}$. The total uncertainty reaches a minimum at $x_0/x_r = 1/\sqrt{3}$. However this point does not satisfy the uniqueness constraint $x_0 \geq x_r$. Since the total uncertainty is monotonically increasing for $x_0 \geq x_r$, the optimum $x_0$ is $x_r$.

In summary, we have proposed a metagrating for high precision position metrology under Poisson noise. By exploring the resonance inside the metagrating, we have shown that the fundamental position uncertainty limited by CRLB in the presence of photon shot noise can be
greatly reduced. The optimum design parameters are closely related to the formation of a phase vortex, which shows the topological robustness of the principle. We believe there is a great potential for using optimized meta-grating to surpass the limit of current position metrology.

* z.xi@tudelft.nl

† On leave from Optics Research Group at TU-Delft, now at ASML Research

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