Zernike expansion of derivatives and Laplacians of the Zernike circle polynomials

A. J. E. M. Janssen

Department of Mathematics and Computer Science, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands (a.j.e.m.janssen@tue.nl)

Received April 24, 2014; revised May 21, 2014; accepted May 21, 2014; posted May 21, 2014 (Doc. ID 210855); published June 25, 2014

The partial derivatives and Laplacians of the Zernike circle polynomials occur in various places in the literature on computational optics. In a number of cases, the expansion of these derivatives and Laplacians in the circle polynomials are required. For the first-order partial derivatives, analytic results are scattered in the literature. Results start as early as 1942 in Nijboer's thesis and continue until present day, with some emphasis on recursive computation schemes. A brief historic account of these results is given in the present paper. By choosing the unnormalized version of the circle polynomials, with exponential rather than trigonometric azimuthal dependence, and by a proper combination of the two partial derivatives, a concise form of the expressions emerges. This form is appropriate for the formulation and solution of a model wavefront sensing problem of reconstructing a wavefront on the level of its expansion coefficients from (measurements of the expansion coefficients of) the partial derivatives. It turns out that the least-squares estimation problem arising here decouples per azimuthal order m, and per m the generalized inverse solution assumes a concise analytic form so that singular value decompositions are avoided. The preferred version of the circle polynomials, with proper combination of the partial derivatives, also leads to a concise analytic result for the Zernike expansion of the Laplacian of the circle polynomials. From these expansions, the properties of the Laplacian as a mapping from the space of circle polynomials of maximal degree N, as required in the study of the Neumann problem associated with the transport-of-intensity equation, can be read off within a single glance. Furthermore, the inverse of the Laplacian on this space is shown to have a concise analytic form.

OCIS codes: (000.3860) Mathematical methods in physics; (080.1005) Aberration expansions; (050.1970) Diffractive optics; (010.7350) Wave-front sensing; (100.3190) Inverse problems.

http://dx.doi.org/10.1364/JOSAA.31.001604

1. INTRODUCTION

The design and analysis of complex optical imaging systems is commonly carried out with the aid of ray tracing. To obtain information about the imaging quality of an optical system, a number of pencils of rays in the object plane is defined and the rays of each pencil are traced from each object point to the diaphragm of the optical system. The rays that intersect the open area of the diaphragm are followed further through the interior of the optical system, and the point of intersection with the exit pupil sphere is determined. By keeping track of the optical pathlength along each ray, the difference in pathlength is established with respect to a reference ray. As a result of the tracing of a large number of rays belonging to a particular object point, the wavefront in the exit pupil can be computed, for instance, by interpolation. For optical systems with wavefront aberrations that are large with respect to the wavelength, the optical disturbance in the image plane is calculated by tracing rays beyond the exit pupil and calculating the intersection point with the image plane. In this way, the spot diagram is obtained. For the calculation of the ray directions from the wavefront surface data only, the gradient vector of the wavefront is needed. In [1], normalized lateral coordinates (X_1, Y_1) on the exit pupil sphere are used. In the image plane, scaled cartesian coordinates (x_1, y_1) are obtained with division by the diffraction unit λ_0/NA, where λ_0 is the vacuum wavelength and NA is the numerical aperture of the imaging pencils. With these canonical coordinates [1] on the exit pupil sphere and in the image plane, the following compact expression for the transverse ray aberration components in the image plane is obtained,

$$\delta x_1 = \frac{\partial W(X_1, Y_1)}{\partial X_1}, \qquad \delta y_1 = \frac{\partial W(X_1, Y_1)}{\partial Y_1}. \tag{1}$$

In a practical situation, with a more or less circular cross section of a pencil of rays or a propagating wave, the expansion of the wavefront aberration with polynomials that are orthogonal on the unit circle is appropriate (Zernike polynomials). Polynomials defined on the exit pupil sphere that allow an expansion of the transverse aberration components $(\delta x_1, \delta y_1)$ have been proposed by Lukosz [2], but these polynomials are not strictly orthogonal on the exit pupil.

Other computational problems can be imagined in which wave gradients are needed. For instance, in electromagnetic problems, to calculate the energy and momentum flow, the wave normal has to be calculated over the area of the wavefront [3]. In the case of adaptive optics wavefront correction, the local slope components of a wavefront are measured by means of a Shack–Hartmann sensor [4]. In such a measurement problem, the gradient components of a wavefront, sampled at a sufficiently large number of points, have to be integrated to obtain the wavefront. The correction of turbulence in the atmosphere during stellar observation is an example of such a combined measurement and computational task.

Fast and efficient algorithms are needed because of the high temporal bandwidth of the turbulence effects [5].

Higher-order derivatives of the wavefront function are used to improve the reliability of the measurement data. For instance, second-order derivatives occur in [6], where the Euler principal curvatures and the azimuths of the two corresponding principal planes are used in an enhanced wavefront reconstruction method for adaptive optics. Higher-order derivatives of the wavefront function W are also needed when approximate solutions of Maxwell's equations are pursued in free space [7]. For field solutions that are valid far away from diffracting obstacles, at least in terms of the wavelength of the light, an approximate solution $U(x,y,z;t) = Q(x,y,z)\exp\{i(kz-\omega t)\}$ is used, with $Q(x,y,z) = A(x,y,z)\exp\{ikW(x,y,z)\}$. It should be a slowly varying solution of the (paraxial) wave equation,

$$\nabla_t^2 Q + 2ik\frac{\partial Q}{\partial z} = 0, \tag{2}$$

where the subscript t means that only the derivatives with respect to the transverse coordinates (x,y) need to be considered. The wavenumber k equals nk_0 where n is the refractive index under consideration and k_0 is the wavenumber of the radiation in vacuum.

The intensity function $I = |A|^2$ can be shown to satisfy the intensity transport equation [7,8],

$$-k\frac{\partial I}{\partial z} = \nabla_t \cdot [I\nabla_t(kW)] = I\nabla_t^2(kW) + \nabla_t I \cdot \nabla_t(kW), \tag{3}$$

in which second-order derivatives of the wavefront function W need to be made available.

In this paper, we present analytic results for the gradients and Laplacians of the Zernike circle polynomials Z_n^m, in the unnormalized version with exponential azimuthal dependence, into which any wavefront function W can be thought to be expanded. These results are useful in formulating and solving the reconstruction problem of wavefront functions from their first-order partial derivatives, and for tracking the solution of the transport-of-intensity equation on the level of Zernike expansion coefficients. Choosing normalized Cartesian coordinates ν, μ on the unit disk $\nu^2 + \mu^2 \le 1$, it turns out to be convenient to combine the partial derivatives $(\partial W/\partial\nu)$, $(\partial W/\partial\mu)$ according to $(\partial W/\partial\nu) + i(\partial W/\partial\mu)$ and $(\partial W/\partial\nu) - i(\partial W/\partial\mu)$ in accordance with two formulas for derivatives of the circle polynomials in polar coordinates as presented by Lukosz [2], Anhang II. Assuming the availability of (measurements of the) Zernike coefficients of the two combinations $(\partial W/\partial\nu) \pm i(\partial W/\partial\mu)$, the least-squares problem of estimating the Zernike coefficients of the wavefront function itself has a very tractable form. The problem decouples per m, and, for any m, the pseudo-inverse solution $(A^H A)^{-1}A^H\mathbf{c}$ can be computed explicitly. The least-squares estimate of the expansion coefficient for azimuthal order m and degree n is an explicit linear combination of the empirical coefficients of $(\partial W/\partial\nu) + i(\partial W/\partial\mu)$ of order $m+1$ and degrees $n-1$, $n+1$, and of $(\partial W/\partial\nu) - i(\partial W/\partial\mu)$ of order $m-1$ and degrees $n-1$, $n+1$. Second, the Laplacian $\Delta = \nabla^2$ can be written as $((\partial/\partial\nu) + i(\partial/\partial\mu)((\partial/\partial\nu) - i(\partial/\partial\mu)$, and this yields a very concise and explicit formula for the Laplacian of the Zernike circle polynomials, and, hence, for any wavefront function W developed into the circle polynomials. Moreover, $\Delta^{-1}Z_n^m$ can be shown to be an explicit linear combination of three circle polynomials of azimuthal order m.

The paper is organized as follows. In Section 2, we present the basic formulas concerning the first-order partial derivatives of Zernike circle polynomials and first-order derivatives of the radial polynomials. We use here the Born-and-Wolf convention [3] with upper index m as the azimuthal order and lower index n as the degree, and with exponential azimuthal dependence $\exp(im\vartheta)$. We also give in Section 2 an account of the development of the results on first-order partial derivatives. In Section 3, we consider the problem of estimating the Zernike coefficients of a wavefront function W from (estimates of) the Zernike coefficients of the partial derivatives of the first-order of W. In Section 4, we compute the Laplacians and the inverse Laplacians of the circle polynomials, and we make a connection with the work of Gureyev *et al.* [8] on the Neumann problem associated with the transport-of-intensity equation. In Appendix A, we present the proofs of the results that give the action of the operators $(\partial/\partial\nu) \pm i(\partial/\partial\mu)$ in terms of the Zernike coefficients of a wavefront function W, the associated adjoint operators, and the generalized inverse required in the estimation problem of Section 3. In Appendix B, we present the results on the inversion of certain special matrices that give rise to the explicit results in Sections 3 and 4 on the inverse operators.

2. FIRST-ORDER DERIVATIVES OF THE CIRCLE POLYNOMIALS

For integer n and m with $n-|m|$ even and non-negative, we let (permitting ourselves some notational liberty),

$$Z_n^m(\nu,\mu) = Z_n^m(\rho,\vartheta) = R_n^{|m|}(\rho)e^{im\vartheta}, \tag{4}$$

where we have set for real ν, μ with $\nu^2 + \mu^2 \le 1$

$$\nu + i\mu = \rho\exp(i\vartheta); \qquad \nu = \rho\cos\vartheta, \qquad \mu = \rho\sin\vartheta, \tag{5}$$

and where the radial polynomials $R_n^{|m|}$ are given as

$$R_n^{|m|}(\rho) = P^{(0,|m|)}_{\frac{n-|m|}{2}}(2\rho^2 - 1) \tag{6}$$

with $P_k^{(\alpha,\beta)}(x)$ the Jacobi polynomial of degree k corresponding to the weight function $(1-x)^\alpha(1+x)^\beta$ on $[-1,1]$. We set, furthermore, $Z_n^m \equiv 0$ for all integers n and m, with $n-|m|$ odd or negative.

A. Basic Identities for First-Order Derivatives

Let n and m be integers with $n-|m|$ even and non-negative. It follows from basic considerations about product functions as in Eq. (4) in Cartesian and polar coordinates that

$$\begin{aligned}&\left(\frac{\partial}{\partial\nu} \pm i\frac{\partial}{\partial\mu}\right)Z_n^m(\nu,\mu)\\ &= \left(\frac{\partial}{\partial\nu} \pm i\frac{\partial}{\partial\mu}\right)[R_n^{|m|}((\nu^2+\mu^2)^{1/2})\exp[im\arctan(\mu/\nu)]]\\ &= \left((R_n^{|m|})'(\rho) \mp \frac{m}{\rho}R_n^{|m|}(\rho)\right)\exp[i(m\pm1)\vartheta],\end{aligned} \tag{7}$$

where the prime on the last line of Eq. (7) denotes differentiation with respect to ρ. Next (see Subsection 2.B for comments), there is the identity

$$\left(\frac{d}{d\rho}\pm\frac{m}{\rho}\right)(R_n^{|m|}-R_{n-2}^{|m|})=2nR_{n-1}^{|m\mp1|},\tag{8}$$

where we recall the conventions of the beginning of this section. Using Eq. (8) with $n-2l$ where $l=0,1,\ldots,(1/2)(n-1-|m\mp1|)$, instead of n, summing over l, and using the observation that

$$\left(\frac{d}{d\rho}\pm\frac{m}{\rho}\right)R_{n-2-(n-1-|m\mp1|)}^{|m|}=\left(\frac{d}{d\rho}\pm\frac{m}{\rho}\right)R_{|m\mp1|-1}^{|m|}=0,\tag{9}$$

in all cases, we get

$$\left(\frac{d}{d\rho}\pm\frac{m}{\rho}\right)R_n^{|m|}=2\sum_{l=0}^{\frac{1}{2}(n-1-|m\mp1|)}(n-2l)R_{n-1-2l}^{|m\mp1|}.\tag{10}$$

It is sometimes convenient to realize that, in all cases, we can replace the upper summation limit in the series at the right-hand side of Eq. (10) by $(1/2)(n-|m|)$ since all terms additionally included or excluded vanish by our conventions. We will also write the right-hand side of Eq. (10) as

$$2\sum_{n'=|m\mp1|(2)(n-1)}(n'+1)R_{n'}^{|m\mp1|},\tag{11}$$

where for integer j, i with $j-i$ is even and non-negative:

$$k=i(2)j\quad\text{means}\quad k=i,i+2,\ldots,j.\tag{12}$$

We get from Eqs. (7) and (10), using in the latter upper summation limit $(1/2)(n-|m|)$ as explained:

$$\left(\frac{\partial}{\partial\nu}\pm i\frac{\partial}{\partial\mu}\right)Z_n^m(\nu,\mu)=2\sum_{l=0}^{\frac{1}{2}(n-|m|)}(n-2l)Z_{n-1-2l}^{m\pm1}.\tag{13}$$

Adding and subtracting the two identities in Eq. (13), we get

$$\frac{\partial Z_n^m}{\partial\nu}=\sum_{l=0}^{\frac{1}{2}(n-|m|)}(n-2l)Z_{n-1-2l}^{m-1}+\sum_{l=0}^{\frac{1}{2}(n-|m|)}(n-2l)Z_{n-1-2l}^{m+1},\tag{14}$$

and

$$\frac{\partial Z_n^m}{\partial\mu}=i\sum_{l=0}^{\frac{1}{2}(n-|m|)}(n-2l)Z_{n-1-2l}^{m-1}-i\sum_{l=0}^{\frac{1}{2}(n-|m|)}(n-2l)Z_{n-1-2l}^{m+1}.\tag{15}$$

Alternatively, from Eqs. (7) and (8), we get the recursive relation

$$\left(\frac{\partial}{\partial\nu}\pm i\frac{\partial}{\partial\mu}\right)Z_n^m=\left(\frac{\partial}{\partial\nu}\pm i\frac{\partial}{\partial\mu}\right)Z_{n-2}^m+2nZ_{n-1}^{m\pm1},\tag{16}$$

from which the recursions

$$\frac{\partial Z_n^m}{\partial\nu}=\frac{\partial Z_{n-2}^m}{\partial\nu}+n(Z_{n-1}^{m-1}+Z_{n-1}^{m+1})\tag{17}$$

and

$$\frac{\partial Z_n^m}{\partial\mu}=\frac{\partial Z_{n-2}^m}{\partial\mu}+in(Z_{n-1}^{m-1}-Z_{n-1}^{m+1})\tag{18}$$

for the separate first-order partial derivatives follow.

B. History of the Basic Identities

The basic identities in Subsection 2.A have been (re)discovered in one or another form at various places in the optics literature from 1942 onward. We give here a brief historic survey of what we have found in this respect. While the basic identities, as presented in Subsection 2.A, are given for the general integer m, almost all writers on the subject make the restriction $m=0,1,\ldots$. Showing validity of these identities for the general m from validity for $m=0,1,\ldots$ is straightforward but requires some care. For instance, for showing that Eq. (8) holds generally from validity of it for $m=0,1,\ldots$ ($-$ sign on the left-hand side) and for $m=1,2,\ldots$ ($+$ sign on the left-hand side), one has to consider the cases $m=0$ and $m<0$ separately. For $m=0$, one then uses the valid identity with $m=0$ and the $-$ sign on the left-hand side. For $m<0$ one uses the valid identities with $-m$ instead of m and uses that $-m-1=|m+1|$, $-m+1=|m-1|$.

The series identity in Eq. (10) with $m\ge1$ and the $+$ sign has been given in Nijboer's 1942 thesis [9] as Eq. (2.31), where the proof uses methods from complex function theory. The two identities in Eq. (8) have been given in 1962 by Lukosz in [2], Anhang II, Eqs. (AII. 4a,b) for the case that $m\ge0$, using the monomial representation

$$R_n^{|m|}(\rho)=\sum_{s=0}^{\frac{1}{2}(n-|m|)}\binom{n-s}{\frac{1}{2}(n-|m|)}\binom{\frac{1}{2}(n-|m|)}{s}\rho^{n-2s}\tag{19}$$

of the radial polynomials. Lukosz writes $m\mp1$ instead of $|m\mp1|$ at the right-hand side of Eq. (8), which makes the result as presented by him somewhat doubtful in the case that $m=0$. The recursion

$$\frac{d}{d\rho}(R_n^{|m|}-R_{n-2}^{|m|})=n(R_{n-1}^{|m-1|}+R_{n-2}^{|m+1|}),\tag{20}$$

that follows from Eq. (8) by adding the $\pm$ cases has been presented for the case $m\ge0$ in 1976 by Noll in [5] as Eq. (13). Noll uses the integral representation

$$R_n^{|m|}(\rho)=(-1)^{\frac{n-m}{2}}\int_0^\infty J_{n+1}(t)J_m(\rho t)\mathrm{d}t,\qquad 0\le\rho<1,\tag{21}$$

also see [10], item 10.22.56, of the radial polynomials together with recursion formulas for Bessel functions and their derivatives. The two series equations in Eq. (10) have been presented for the case $m\ge0$ in 1987 by Braat [11] as Eqs. (10a) and (10b) using Nijboer's result [9] for Eqs. (2) and (31) for the $+$ case and an argument based on the monomial representation in Eq. (19) for the $-$ case (with a somewhat doubtful result for the case $m=0$). In Braat's forthcoming book, the two series identities in Eq. (10) are proved by establishing Eq. (8) via the integral result in Eq. (21) using recursions for Bessel functions and an induction step to go from Eqs. (8)–(10). The identities in Eqs. (17) and (18) have been given in 1999 by

Capozzoli [12] as Eqs. (10) and (12) for $m \geq 0$ and the versions of the circle polynomials with both the exponential and trigonometric dependence on ϑ (the case of $m = 0$ again being somewhat doubtful). The series representations in Eqs. (14) and (15) for normalized circle polynomials with trigonometric azimuthal dependence have been given in 2009 by the American National Standards Institute (ANSI) [13] as Eqs. (9) and (B8). A similar thing was done in 2014 by Stephenson [14] with Eqs. (30) and (31). Both ANSI and Stephenson base their derivation on the recursion in Eq. (20) that they ascribe to Noll.

3. ZERNIKE-BASED SOLUTION OF A BASIC PROBLEM IN WAVEFRONT SENSING

In this section, we consider the problem of estimating the Zernike coefficients of a wavefront function $W(\nu,\mu)$ from the Zernike coefficients of the first-order partial derivatives of W. At this point, we do not want to be more specific about how the latter coefficients have been obtained (e.g., analytically, semi-analytically or numerically, experimentally from matching on a set of sample points on the unit disk).

We start with the Zernike expansion of W,

$$W(\nu,\mu) = \sum_{m=-\infty}^{\infty} \sum_{n=|m|(2)\infty} \alpha_n^m Z_n^m(\nu,\mu), \tag{22}$$

with

$$\boldsymbol{\alpha} = (\alpha_n^m)_{\substack{m=-\infty,\ldots,\infty,\\ n=|m|(2)\infty}}, \tag{23}$$

an aggregate of unknown Zernike coefficients, and where $n = |m|(2)\infty$ denotes $n = |m|, |m|+2, \ldots$. When considering aggregates as in Eq. (23), it is sometimes convenient to set $\alpha_n^m = 0$ when $n < |m|$. We assume that empirical Zernike coefficients of $(\partial W/\partial\nu)$ and $(\partial W/\partial\mu)$ are available, and we let

$$\bar{\boldsymbol{\beta}}_\pm = ((\bar{\beta}_\pm)_n^m)_{\substack{m=-\infty,\ldots,\infty,\\ n=|m|(2)\infty}}, \tag{24}$$

be the aggregates of these empirical Zernike coefficients corresponding to $(\partial W/\partial\nu) \pm i(\partial W/\partial\mu)$. It is shown in Appendix A from Eq. (13) that the analytical aggregates $\boldsymbol{\beta}_\pm$ of Zernike coefficients of $(\partial W/\partial\nu) \pm i(\partial W/\partial\mu)$ are given in terms of the aggregate $\boldsymbol{\alpha}$ of Zernike coefficients of W by

$$\boldsymbol{\beta}_\pm = A_\pm\boldsymbol{\alpha} = \left(2(n+1)\sum\nolimits_{n'=n(2)\infty} \alpha_{n'+1}^{m\mp1}\right)_{\substack{m=-\infty,\ldots,\infty,\\ n=|m|(2)\infty}}. \tag{25}$$

In the matrix-vector notation just developed, we should therefore choose $\boldsymbol{\alpha}$ such that a best match occurs between $\bar{\boldsymbol{\beta}}_\pm$ of Eq. (24) and $A_\pm\boldsymbol{\alpha}$ of Eq. (25).

In the space ZC of aggregates $\boldsymbol{\gamma} = (\gamma_n^m)_{m=-\infty,\ldots,\infty,n=|m|(2)\infty}$ of Zernike coefficients, we take as inner product norm

$$\|\boldsymbol{\gamma}\|_{ZC}^2 = (\boldsymbol{\gamma},\boldsymbol{\gamma})_{ZC} = \sum_{m=-\infty}^{\infty} \sum_{n=|m|(2)\infty} \frac{|\gamma_n^m|^2}{2(n+1)}. \tag{26}$$

This inner product is consistent with the normalization condition

$$\iint_{\nu^2+\mu^2\leq1} |Z_n^m(\nu,\mu)|^2 \mathrm{d}\nu\mathrm{d}\mu = \frac{\pi}{(n+1)} \tag{27}$$

of the circle polynomials. Thus, we choose $\boldsymbol{\alpha} \in ZC$ such that

$$\|A\alpha - \bar{\boldsymbol{\beta}}\|_{ZC^2}^2 = \|A_+\boldsymbol{\alpha} - \bar{\boldsymbol{\beta}}_+\|_{ZC}^2 + \|A_-\boldsymbol{\alpha} - \bar{\boldsymbol{\beta}}_-\|_{ZC}^2 \tag{28}$$

is minimal. Here, we have set in a symbolic matrix notation

$$A = \begin{bmatrix} A_+ \\ A_- \end{bmatrix}; \quad A\alpha = \begin{bmatrix} A_+\boldsymbol{\alpha} \\ A_-\boldsymbol{\alpha} \end{bmatrix} \in ZC^2, \quad \bar{\boldsymbol{\beta}} = \begin{bmatrix} \bar{\boldsymbol{\beta}}_+ \\ \bar{\boldsymbol{\beta}}_- \end{bmatrix} \in ZC^2 \tag{29}$$

and $\|\boldsymbol{\gamma}\|_{ZC^2} = \|\boldsymbol{\gamma}_+\|_{ZC}^2 + \|\boldsymbol{\gamma}_-\|_{ZC}^2$ is the inner product norm for $\boldsymbol{\gamma} = [\begin{smallmatrix}\gamma_+\\ \gamma_-\end{smallmatrix}] \in ZC^2$.

The least-squares α is found by the usual linear algebra methods of generalized inverses as

$$\hat{\boldsymbol{\alpha}} = (A^H A)^{-1} A^H \bar{\boldsymbol{\beta}}, \tag{30}$$

where A^H is the adjoint of the operator A in Eq. (29), relative to the inner product $(,)_{ZC^2}$ in ZC^2. The operator A^H is computed in Appendix A as

$$A^H\boldsymbol{\delta} = A_+^H\boldsymbol{\delta}_+ + A_-^H\boldsymbol{\delta}_-, \qquad \boldsymbol{\delta} = \begin{bmatrix} \boldsymbol{\delta}_+ \\ \boldsymbol{\delta}_- \end{bmatrix} \in ZC^2 \tag{31}$$

with

$$A_\pm^H\boldsymbol{\gamma} = \left(2(n+1)\sum\nolimits_{n'=|m|(2)n} \gamma_{n'-1}^{m\pm1}\right)_{\substack{m=-\infty,\ldots,\infty,\\ n=|m|(2)\infty}}, \quad \boldsymbol{\gamma} \in ZC. \tag{32}$$

The operator $A^H A$ is computed in Appendix A as

$$A^H A\boldsymbol{\gamma} = \left(4(n+1)\sum\nolimits_{n'=|m|(2)\infty} B_{n\wedge n'}^m \gamma_{n'}^m\right)_{\substack{m=-\infty,\ldots,\infty,\\ n=|m|(2)\infty}}, \quad \boldsymbol{\gamma} \in ZC, \tag{33}$$

where

$$n \wedge n' = \min(n, n') \tag{34}$$

and, for $n'' = |m|(2)\infty$,

$$B_{n''}^m = |m| + \frac{1}{2}(n'' - |m|)(n'' + |m| + 2). \tag{35}$$

Thus, $\hat{\boldsymbol{\alpha}}$ is found by solving

$$A^H A\alpha = A^H \bar{\boldsymbol{\beta}}. \tag{36}$$

It follows from Eqs. (31) and (32) that

$$(A^H\bar{\boldsymbol{\beta}})_n^m = 2(n+1) \sum_{n'=|m|(2)n} ((\bar{\beta}_+)_{n'-1}^{m+1} + (\bar{\beta}_-)_{n'-1}^{m-1}), \tag{37}$$

and so, by Eq. (33) we should find the α's from

$$\sum_{n'=|m|(2)\infty} B_{n\wedge n'}^m \alpha_{n'}^m = \psi_n^m, \qquad n = |m|(2)\infty, \tag{38}$$

where we have set

$$\psi_n^m = \sum_{n'=|m|(2)n} \frac{1}{2}((\bar{\beta}_+)_{n'-1}^{m+1} + (\bar{\beta}_-)_{n'-1}^{m-1}), \tag{39}$$

and where the B's are given by Eqs. (34) and (35). Note that $B_0^0 = \psi_0^0 = 0$, and so Eq. (38) with $m = n = 0$ leaves α_0^0 undetermined. Also note that Eq. (38) allows solving $\alpha_{n'}^m$ per separate m.

The linear system in Eq. (38) is considered for finite $I = 0, 1, \ldots,$ and assumes the particular simple form

$$\sum_{j=0}^{I} M_{ij} x_j = c_i, \qquad i = 0, 1, \ldots, I, \tag{40}$$

where M is an $(I+1) \times (I+1)$ matrix of the form

$$M = (b_{\min(i,j)})_{i,j=0,1,\ldots,I}. \tag{41}$$

The right-hand side $\mathbf{c} = (c_i)_{i=0,1,\ldots,I}$ of Eq. (40) has the form

$$\mathbf{c} = L_1 \mathbf{d}, \tag{42}$$

where [see Eqs. (38) and (39)]

$$\mathbf{d} = (d_k)_{k=0,1,\ldots,I} = (\varphi_{|m|+2k}^m)_{k=0,1,\ldots,I}, \tag{43}$$

with

$$\varphi_{n'}^m = \frac{1}{2}(\bar{\beta}_+)_{n'-1}^{m+1} + \frac{1}{2}(\bar{\beta}_-)_{n'-1}^{m-1}, \tag{44}$$

and L_1 is the $(I+1) \times (I+1)$ lower triangular matrix with all entries 1 on and below the main diagonal. This L_1 is the inverse L^{-1} of the lower triangular, bidiagonal matrix L considered in Eq. (B1). Thus, the required solution $\mathbf{x} = (x_j)_{j=0,1,\ldots,I}$ is given as

$$\mathbf{x} = M^{-1} L_1 \mathbf{d} = (LM)^{-1} \mathbf{d}. \tag{45}$$

In Appendix B it is shown that

$$(LM)^{-1} = \begin{bmatrix} a_0 & -a_1 & 0 & & 0 \\ 0 & a_1 & -a_2 & & \\ & & & & \\ & & & a_{I-1} & -a_I \\ 0 & & & 0 & a_I \end{bmatrix} \tag{46}$$

(upper triangular, bidiagonal $(I+1) \times (I+1)$ matrix with $a_0, a_1, \ldots, a_I$ on the main diagonal and $-a_1, -a_2, \ldots, -a_I$ on the first upper codiagonal), where

$$a_j = \frac{1}{b_j - b_{j-1}}, \qquad j = 0, 1, \ldots, I, \tag{47}$$

with b_j from Eq. (41) and where we have set $b_{-1} = 0$. Thus, we get

$$x_j = a_j d_j - a_{j+1} d_{j+1}, \qquad j = 0, 1, \ldots, I-1; \qquad x_I = a_I d_I. \tag{48}$$

In the present case, we have

$$b_j = B_{|m|+2j}^m = |m| + 2j(|m| + j + 1), \qquad j = 0, 1, \ldots, I, \tag{49}$$

and so we get

$$a_0 = \frac{1}{|m|}; \qquad a_j = \frac{1}{2(|m| + 2j)}, \qquad j = 1, 2, \ldots, I. \tag{50}$$

For the case $m = 0$, we have $b_0 = B_0^0 = 0$, and one should delete the first row and column of the M-matrix in Eq. (41) and solve for $x_1, x_2, \ldots, x_I$.

With d_j given in Eq. (43) and a_j given in Eq. (50), we can then write the solution of the finitized Eq. (38) as

$$\hat{\alpha}_n^m = C_n^m \varphi_n^m - C_{n+2}^m \varphi_{n+2}^m, \qquad n = |m|(2)(|m| + I - 2), \tag{51}$$

$$\hat{\alpha}_{|m|+2I}^m = C_{|m|+2I}^m \varphi_{|m|+2I}^m, \tag{52}$$

where φ_n^m are given by Eq. (44) and

$$C_{|m|}^m = \frac{1}{|m|}, \qquad n = |m|; \qquad C_n^m = \frac{1}{2n}, \qquad n = (|m| + 2)(2)(|m| + 2I). \tag{53}$$

In Eq. (51), we consider $n = 2(2)(I-2)$ in the case that $m = 0$.

It is important to note that the finitization to linear systems of order $(I+1) \times (I+1)$ has virtually no influence on the computed $\hat{\alpha}_n^m$, except for the validity range $n = |m|(2)(|m| + 2I - 2)$.

It is relatively straightforward to check that Eqs. (51) and (53) yield $\alpha_n^m = \delta_{mm_1}\delta_{nn_1}$ when $W = Z_{n_1}^{m_1}$ and the partial derivative data $\bar{\boldsymbol{\beta}}_\pm$ are perfect (integer n_1, m_1 with $n_1 - |m_1|$ even and non-negative, and $0 < n_1 \le |m_1| + 2I - 2$).

Observe that $\hat{\alpha}_n^m$ in Eq. (51) is a linear combination of the four numbers $(\bar{\beta}_\pm)_{n'}^{m\pm1}$ with $n' = n-1$, $n+1$.

4. ZERNIKE EXPANSION OF THE LAPLACIAN AND THE INVERSE LAPLACIAN OF CIRCLE POLYNOMIALS

Higher-order partial derivatives of wavefront functions occur in various places in the optics literature on wavefront reconstruction and ophthalmics. In [15], wavefront reconstruction from defocused images in an astronomical setting is considered, and conservation of the intensity flux requires studying Jacobians of transformations that involve the second-order partial derivatives of the aberration. In [8], a detailed study is made of the action of the Laplacian on the linear space $\mathcal{Z}_{N+2}$ spanned by the circle polynomials with a degree not exceeding $N+2$ as a mapping into $\mathcal{Z}_N$ in connection with the transport-of-intensity equation. In particular, one is interested in solving the Neumann problem of finding $\varphi \in \mathcal{Z}_{N+2}$ from $-\Delta\varphi = f \in \mathcal{Z}_N$ with $\partial_{\mathbf{n}}\varphi = \psi$ on the boundary of the disk. Such a problem is also considered, with boundary function $\psi = 0$, in [16]. The Neumann problem in question has been considered as a classical object in mathematical physics in Section 2 of [8], and a motivation for why the Zernike-based solution is sought after is given in the beginning of Subsection 3.A in [8]. Finally, in [13], one is in principle interested in the partial derivatives of the circle polynomials of all orders in order to study the effect of decentration of the optical system. Here, one aims at obtaining a Zernike expansion of a displaced wavefront function $W(\nu+\nu_0,\mu+\mu_0)$ from such an expansion of $W(\nu,\mu)$ by Taylor expansion.

In this section, we concentrate on the Laplacians of the circle polynomials, and we show that for integers n and m such that $n-|m|$ is even and non-negative

$$\left(\frac{\partial^2}{\partial\nu^2}+\frac{\partial^2}{\partial\mu^2}\right)Z_n^m = 4\sum_{t=0}^{\frac{1}{2}(n-|m|)-1}(n-1-2t)(n-t)(t+1)Z_{n-2-2t}^m. \tag{54}$$

From this formula, many of the observations made in [8] are verified instantly. Similar, but somewhat more complicated, series expressions can be shown to hold for the three second-order partial derivatives of Z_n^m separately.

To show Eq. (54), we observe that

$$\frac{\partial^2}{\partial\nu^2}+\frac{\partial^2}{\partial\mu^2} = \left(\frac{\partial}{\partial\nu}+i\frac{\partial}{\partial\mu}\right)\left(\frac{\partial}{\partial\nu}-i\frac{\partial}{\partial\mu}\right), \tag{55}$$

and so, we get from Eq. (13) with summation upper limits $(1/2)(n-1-|m\pm 1|)$ that

$$\begin{aligned}\left(\frac{\partial^2}{\partial\nu^2}+\frac{\partial^2}{\partial\mu^2}\right)Z_n^m &= 2\sum_{l=0}^{\frac{n-1-|m-1|}{2}}(n-2l)\left(\frac{\partial}{\partial\nu}+i\frac{\partial}{\partial\mu}\right)Z_{n-1-2l}^{m-1}\\ &= 2\sum_{l=0}^{\frac{n-1-|m-1|}{2}}\sum_{k=1}^{\frac{n-1-2l-1-|m-1+1|}{2}}2(n-1-2l-2k)Z_{n-1-2l-1-2k}^{m-1+1}\\ &= 4\sum_{l=0}^{\frac{n-1-|m-1|}{2}}\sum_{k=0}^{\frac{n-2l-2-|m|}{2}}(n-2l)(n-1-2l-2k)Z_{n-2-2l-2k}^m.\end{aligned} \tag{56}$$

We must now carefully rearrange the double series on the last line of Eq. (56). First, we have

$$\frac{n-1-|m-1|}{2} = \begin{cases}\frac{1}{2}(n-|m|), & m\geq 1,\\ \frac{1}{2}(n-|m|)-1, & m\leq 0.\end{cases} \tag{57}$$

In the case that $m\geq 1$ and $l=(1/2)(n-|m|)$, the summation over k in the last line of Eq. (56) is empty, and so we can delete the term with $l=(1/2)(n-|m|)$. Hence, in all cases

$$\left(\frac{\partial^2}{\partial\nu^2}+\frac{\partial^2}{\partial\mu^2}\right)Z_n^m = 4\sum_{l=0}^{p-1}\sum_{k=0}^{p-1-l}(n-2l)(n-1-2l-2k)Z_{n-2-2l-2k}^m, \tag{58}$$

where we have set $p=(1/2)(n-|m|)$. The summation in Eq. (58) can be written as

$$\begin{aligned}4\sum_{t=0}^{p-1}\sum_{l,k\geq 0;l+k=t}(n-2l)(n-1-2t)Z_{n-2-2t}^m\\ = 4\sum_{t=0}^{p-1}(n-1-2t)Z_{n-2-2t}^m S_{nt},\end{aligned} \tag{59}$$

where

$$S_{nt} = \sum_{l,k\geq 0;l+k=t}(n-2l) = \sum_{l=0}^{t}(n-2l) = (n-t)(t+1), \tag{60}$$

and we arrive at the result of Eq. (54). In the third column of Table 1, we display ΔZ_n^m for $m\geq 0$ and $n\leq 6$.

With the notation introduced in Eq. (12), we can write Eq. (54) concisely as

$$\Delta Z_n^m = \sum_{s=|m|(2)(n-2)}(s+1)(n+s+2)(n-s)Z_s^m. \tag{61}$$

We next consider, as in [8], for a given integer $N\geq 0$, the Neumann problem

$$-\Delta\varphi = f, \qquad \partial_{\mathbf{n}}\varphi = \psi, \tag{62}$$

where f belongs to the linear space Z_N spanned by all circle polynomials of degree $\leq N$, and $\psi=\psi(\vartheta)$ is a periodic function of degree $\leq N+2$ (and thus a linear combination of $\exp[im\vartheta]$, integer m, $|m|\leq N+2$).

We let $\mathcal{Z}_N^m$ and $\mathcal{Z}_{N+2}^m$, for integer m with $|m|\leq N$, be the spaces spanned by the circle polynomials of azimuthal order m and of degree $\leq N$ and $N+2$, respectively. It is seen from Eq. (61) that Δ maps $\mathcal{Z}_{N+2}^m$ into $\mathcal{Z}_N^m$ and that $\Delta Z_{|m|}^m=0$. Furthermore, the matrix B^m of Δ, when choosing in $\mathcal{Z}_N^m$ and $\mathcal{Z}_{N+2}^m$ the orthogonal basis of circle polynomials of azimuthal

Table 1. Equations (54) and (68) for Z_n^m with $m\geq 0$, $n\leq 6$

m	n	ΔZ_n^m	$\Delta^{-1}Z_n^m$
0	0	0	$\frac{1}{8}Z_2^0$
0	2	$8Z_0^0$	$\frac{-1}{16}Z_2^0+\frac{1}{48}Z_4^0$
0	4	$48Z_2^0+24Z_0^0$	$\frac{1}{80}Z_2^0-\frac{1}{48}Z_4^0+\frac{1}{120}Z_6^0$
0	6	$120Z_4^0+120Z_2^0+48Z_0^0$	$\frac{1}{168}Z_4^0-\frac{1}{96}Z_6^0+\frac{1}{224}Z_8^0$
1	1	0	$\frac{1}{24}Z_3^1$
1	3	$24Z_1^1$	$\frac{-1}{30}Z_3^1+\frac{1}{80}Z_5^1$
1	5	$80Z_3^1+64Z_1^1$	$\frac{1}{120}Z_3^1-\frac{1}{70}Z_5^1+\frac{1}{168}Z_7^1$
2	2	0	$\frac{1}{48}Z_4^2$
2	4	$48Z_2^2$	$\frac{-1}{48}Z_4^2+\frac{1}{120}Z_6^2$
2	6	$120Z_4^2+120Z_2^2$	$\frac{1}{168}Z_4^2-\frac{1}{96}Z_6^2+\frac{1}{224}Z_8^2$
3	3	0	$\frac{1}{80}Z_5^3$
3	5	$80Z_3^3$	$\frac{-1}{70}Z_5^3+\frac{1}{168}Z_7^3$
4	4	0	$\frac{1}{120}Z_6^4$
4	6	$120Z_4^4$	$\frac{-1}{96}Z_6^4+\frac{1}{224}Z_8^4$
5	5	0	$\frac{1}{168}Z_7^5$
6	6	0	$\frac{1}{224}Z_8^6$

order m and degree $\le N$ and $N+2$, respectively, is lower triangular. The matrix elements B_{ns}^m are given by

$$B_{ns}^m = \begin{cases} (s+1)(n+s+2)(n-s), & s = |m|(2)(n-2), \\ 0, & s = n(2)N_m, \end{cases} \tag{63}$$

where

$$N_m = |m| + 2\lfloor \frac{1}{2}(N-|m|) \rfloor \tag{64}$$

so that $N_m = N$ or $N-1$ according to whether N and $|m|$ have the same or opposite parity. Observing that $B_{n,n-2} \neq 0$, it follows that the functions ΔZ_n^m, $n = (|m|+2)(2)(N_m+2)$ are independent, and so Δ maps $\mathcal{Z}_{N+2}^m$ onto $\mathcal{Z}_N^m$.

For solving $-\Delta\varphi = f$ [see Eq. (62)], we develop f as

$$f = \sum_{m=-N}^{N} \sum_{n'=|m|(2)N_m} \alpha_{n'}^m Z_{n'}^m. \tag{65}$$

It is seen that the basic problem is to solve β_n^m for a given m, $|m| \le N$, and a given $n' = |m|(2)N_m$ from the linear equations

$$\Delta\left(\sum_{n=(|m|+2)(2)(N_m+2)} \beta_n^m Z_n^m \right) = Z_{n'}^m. \tag{66}$$

In terms of the matrix elements B_{ns}^m in Eq. (63), Eq. (66) can be written as

$$\sum_{n=s(2)N_m} B_{n+2,s}^m \beta_{n+2}^m = \delta_{sn}, \qquad s = |m|(2)N_m. \tag{67}$$

It is shown in Appendix B that the linear system in Eq. (67) can be solved explicitly, with the result

$$Z_{n'}^m = \Delta\left[\frac{1}{4(n'+2)(n'+1)} Z_{n'+2}^m - \frac{1}{2n'(n'+2)} Z_{n'}^m + \frac{1}{4n'(n'+1)} Z_{n'-2}^m \right], \tag{68}$$

where we recall that $\Delta Z_n^m = 0$ when $n \le |m|$. The result of Eq. (68) is illustrated in the fourth column of Table 1 for Z_n^m with $m \ge 0$ and $n \le 6$.

Having solved the problem in Eq. (66), and therefore, by linear combination with f as in Eq. (65), the problem $-\Delta\varphi = f \in \mathcal{Z}_N$, the boundary condition $\partial_{\mathbf{n}}\varphi = \psi$ [see Eq. (62)] remains to be satisfied. This problem can be solved in the same manner as was done in [8], pp. 1936–1937, where a linear combination of $Z_{|m|}^m$, $m = -N, \ldots, N$, was used to satisfy this boundary condition. To this end, it is useful to note that

$$\begin{aligned} \partial_{\mathbf{n}}[Z_n^m(\rho,\vartheta)] &= (R_n^{|m|})'(1)\exp[im\vartheta] \\ &= \frac{1}{2}(n(n+2)-m^2)\exp[im\vartheta], \end{aligned} \tag{69}$$

so that $\partial_{\mathbf{n}}[Z_m^m(\rho,\vartheta)] = |m|\exp[im\vartheta]$. Thus, the solution φ_0 of $-\Delta\varphi_0 = f$, not comprising any $Z_{|m|}^m$, has computable Fourier coefficients of its normal derivative $\partial_{\mathbf{n}}\varphi_0 = \psi_0$, and the coefficients c_m of $Z_{|m|}^m$ in the full φ should be chosen such that $|m|c_m$ equals the mth Fourier coefficient of $\psi - \psi_0$.

5. CONCLUSION

We have given a review of the results concerning the first-order Cartesian derivatives of the Zernike circle polynomials. By choosing the version of the circle polynomials with exponential azimuthal dependence and by proper combination of the two first-order partial derivatives, the results have been brought into a concise form. This form allows a convenient formulation and solution of a basic problem in wavefront sensing in which the Zernike coefficients of the wavefront function are to be estimated from the Zernike coefficients of the first-order Cartesian derivatives. It has been shown that the matrix inversion required for solving the ensuing least-squares problem can be done analytically. The preferred version of the circle polynomials together with proper combination of the first-order derivatives also leads to a concise result for the Laplacians of the circle polynomials. This concise result has been used to find an explicit formula for the inverse Laplacian of any circle polynomial. This yields a concise solution of the Neumann problem, which occurs when studying the transport-of-intensity equation on spaces of circle polynomials with a radial degree not exceeding a fixed number.

APPENDIX A: PROOFS OF THE PROPERTIES OF $A_\pm$ IN SECTION 3

In this appendix, we prove the results on the operators $A_\pm$ and A used in Section 3. We start with the proof of Eq. (25) that expresses the aggregate of Zernike expansion coefficients $\boldsymbol{\beta}_\pm$ of $(\partial W/\partial\nu) \pm i(\partial W/\partial\mu)$ in terms of the corresponding aggregate $\boldsymbol{\alpha}$ of W [see Eq. (22)]. With integer m_1, n_1, such that $n_1 - |m_1|$ is even and non-negative, we shall verify Eq. (25) directly for the case that $W = Z_{n_1}^{m_1}$ so that $\alpha_n^m = \delta_{m_1 m}\delta_{n_1 n}$. The identity to be verified is

$$\frac{\partial W}{\partial\nu} \pm i\frac{\partial W}{\partial\mu} = 2\sum_{m=-\infty}^{\infty} \sum_{n=|m|(2)\infty} (n+1)\left(\sum_{n'=n(2)\infty} \alpha_{n'+1}^{m\mp 1} \right) Z_n^m. \tag{A1}$$

With $\alpha_n^m = \delta_{m_1 m}\delta_{n_1 n}$, it is seen that in the series over m in Eq. (A1) only the term m with $m \mp 1 = m_1$ is nonvanishing, and so we should only consider

$$2\sum_{n=|m_1\pm 1|(2)\infty} \left(\sum_{n'=n(2)\infty} (n+1)\alpha_{n'+1}^{m_1} \right) Z_n^{m_1\pm 1}. \tag{A2}$$

With $n = |m_1 \pm 1|(2)\infty$, we have

$$\sum_{n'=n(2)\infty} \alpha_{n'+1}^{m_1} = \begin{cases} 1, & n+1 \le n_1, \\ 0, & \text{otherwise}. \end{cases} \tag{A3}$$

Hence, the expression in Eq. (A2) equals

$$2\sum_{n=|m_1\pm1|(2)(n_1-1)}(n+1)Z_n^{m_1\pm1}=2\sum_{n=(|m_1\pm1|+1)(2)n_1}nZ_{n-1}^{m_1\pm1}$$
$$=2\sum_{l=0}^{\frac{1}{2}(n_1-1-|m_1\pm1|)}(n_1-2l)Z_{n_1-1-2l}^{m_1\pm1}=\left(\frac{\partial}{\partial\nu}\pm i\frac{\partial}{\partial\mu}\right)Z_{n_1}^{m_1} \tag{A4}$$

according to Eq. (13) with summation of nonzero terms only. This shows Eq. (25) for the case that $W=Z_{n_1}^{m_1}$, and the general case follows from this by linear superposition of terms $Z_{n_1}^{m_1}$ in W with integers m_1 and n_1 such that $n_1-|m_1|$ is even and non-negative.

We shall now compute A^H and A^HA as required in Eq. (30) for the least squares α. With $\boldsymbol{\gamma}$, $\boldsymbol{\delta}\in ZC^2$, written as

$$\boldsymbol{\gamma}=\begin{bmatrix}\boldsymbol{\gamma}_+\\ \boldsymbol{\gamma}_-\end{bmatrix},\qquad \boldsymbol{\delta}=\begin{bmatrix}\boldsymbol{\delta}_+\\ \boldsymbol{\delta}_-\end{bmatrix}, \tag{A5}$$

where $\boldsymbol{\gamma}_\pm$, $\boldsymbol{\delta}_\pm\in ZC$, and with the notation of Eq. (29), we have

$$(A\boldsymbol{\gamma},\boldsymbol{\delta})_{ZC^2}=(A_+\boldsymbol{\gamma}_+,\boldsymbol{\delta}_+)_{ZC}+(A_-\boldsymbol{\gamma}_-,\boldsymbol{\delta}_-)_{ZC}$$
$$=(\boldsymbol{\gamma}_+,A_+^H\boldsymbol{\delta}_+)_{ZC}+(\boldsymbol{\gamma}_-,A_-^H\boldsymbol{\delta}_-)_{ZC}=(\boldsymbol{\gamma},A^H\boldsymbol{\delta})_{ZC^2}, \tag{A6}$$

where $A_\pm^H$ are the adjoints of $A_\pm$ and

$$A^H\boldsymbol{\delta}=A_+^H\boldsymbol{\delta}_++A_-^H\boldsymbol{\delta}_-. \tag{A7}$$

We therefore need to determine $A_\pm^H$.

As to the $+$ case, we have for $\boldsymbol{\alpha}\in ZC$ by Eq. (25)

$$A_+\boldsymbol{\alpha}=\left(2(n+1)\textstyle\sum_{n'=n(2)\infty}\alpha_{n'+1}^{m-1}\right)_{\substack{m=-\infty,\dots,\infty,\\ n=|m|(2)\infty}}. \tag{A8}$$

Hence, with the definition of the inner product in ZC [see Eq. (26)], we have for α, $\boldsymbol{\beta}\in ZC$ that

$$(A_+\boldsymbol{\alpha},\boldsymbol{\beta})_{ZC}=\sum_{m=-\infty}^{\infty}\sum_{n=|m|(2)\infty}\frac{(A^+\boldsymbol{\alpha})_n^m(\beta_n^m)^*}{2(n+1)}$$
$$=\sum_{m=-\infty}^{\infty}\left(\sum_{n=|m|(2)\infty}\left(\sum_{n'=n(2)\infty}\alpha_{n'+1}^{m-1}\right)(\beta_n^m)^*\right)$$
$$=\sum_{m=-\infty}^{\infty}\left(\sum_{n'=|m|(2)\infty}\sum_{n=|m|(2)n'}\alpha_{n'+1}^{m-1}(\beta_n^m)^*\right)$$
$$=\sum_{m=-\infty}^{\infty}\left(\sum_{n'=(|m+1|+1)(2)\infty}\sum_{n=|m+1|(2)(n'-1)}\alpha_{n'}^m(\beta_n^{m+1})^*\right). \tag{A9}$$

Now $|m+1|=m+1$ when $m=0,1,\dots$ and $|m+1|=|m|-1$ when $m=-1,-2,\dots$, and so

$$(A_+\boldsymbol{\alpha},\boldsymbol{\beta})_{ZC}=\sum_{m=0}^{\infty}\left(\sum_{n'=(m+2)(2)\infty}\sum_{n=(m+1)(2)(n'-1)}\alpha_{n'}^m(\beta_n^{m+1})^*\right)$$
$$+\sum_{m=-\infty}^{-1}\left(\sum_{n'=|m|(2)\infty}\sum_{n=(|m|-1)(2)(n'-1)}\alpha_{n'}^m(\beta_n^{m+1})^*\right)$$
$$=\sum_{m=0}^{\infty}\left(\sum_{n'=(m+2)(2)\infty}\sum_{n=(m+2)(2)n'}\alpha_{n'}^m(\beta_{n-1}^{m+1})^*\right)$$
$$+\sum_{m=-\infty}^{-1}\left(\sum_{n'=|m|(2)\infty}\sum_{n=|m|(2)n'}\alpha_{n'}^m(\beta_{n-1}^{m+1})^*\right). \tag{A10}$$

The terms β_{n-1}^{m+1} with $n=m$ in the first triple series in the last member of Eq. (A10) vanish, and so we can extend the n-summation range in this triple series to $m(2)n'$. In doing so, and subsequently extending the n'-summation range to $m(2)\infty$ in this same triple series, we get

$$(A_+\boldsymbol{\alpha},\boldsymbol{\beta})_{ZC}=\sum_{m=0}^{\infty}\left(\sum_{n'=m(2)\infty}\sum_{n=m(2)n'}\alpha_{n'}^m(\beta_{n-1}^{m+1})^*\right)$$
$$+\sum_{m=-\infty}^{-1}\left(\sum_{n'=|m|(2)\infty}\sum_{n=|m|(2)n'}\alpha_{n'}^m(\beta_{n-1}^{m+1})^*\right)$$
$$=\sum_{m=-\infty}^{\infty}\left(\sum_{n'=|m|(2)\infty}\sum_{n=|m|(2)n'}\alpha_{n'}^m(\beta_{n-1}^{m+1})^*\right). \tag{A11}$$

Next, interchanging the summation indices n' and n in the last line of Eq. (A11), and throwing in a factor $2(n+1)/2(n+1)$, we get

$$(A_+\boldsymbol{\alpha},\boldsymbol{\beta})_{ZC}=\sum_{m=-\infty}^{\infty}\left(\sum_{n=|m|(2)\infty}\frac{\alpha_n^m(2(n+1)\sum_{n'=|m|(2)n}\beta_{n'-1}^{m+1})^*}{2(n+1)}\right)$$
$$=(\boldsymbol{\alpha},A_+^H\boldsymbol{\beta})_{ZC}, \tag{A12}$$

where

$$A_+^H\boldsymbol{\beta}=\left(2(n+1)\textstyle\sum_{n'=|m|(2)n}\beta_{n'-1}^{m+1}\right)_{\substack{m=-\infty,\dots,\infty\\ n=|m|(2)\infty}}. \tag{A13}$$

In an entirely similar fashion, we compute

$$(A_-\boldsymbol{\alpha},\boldsymbol{\beta})_{ZC}=(\boldsymbol{\alpha},A_-^H\boldsymbol{\beta})_{ZC}, \tag{A14}$$

where

$$A_-^H\boldsymbol{\beta}=\left(2(n+1)\textstyle\sum_{n'=|m|(2)\infty}\beta_{n'-1}^{m-1}\right)_{\substack{m=-\infty,\dots,\infty,\\ n=|m|(2)\infty}}. \tag{A15}$$

We finally compute $A^HA=A_+^HA_++A_-^HA$. Thus, for $\boldsymbol{\gamma}\in ZC$, we have from Eq. (32) that

$$(A_+^HA_+\boldsymbol{\gamma})_n^m=2(n+1)\sum_{n'=|m|(2)n}(A_+\boldsymbol{\gamma})_{n'-1}^{m+1}, \tag{A16}$$

when m, n are integers and $n=|m|(2)\infty$. Now for $n'-1=|m+1|(2)\infty$, we have from Eq. (25) that

$$(A_+\gamma)^{m+1}_{n'-1} = 2(n'+1-1)\sum_{n''=(n'-1)(2)\infty}\gamma^{(m+1)-1}_{n''+1} = 2n'\sum_{n''=n'(2)\infty}\gamma^m_{n''}. \tag{A17}$$

Hence,

$$(A_+^H A_+\gamma)^m_n = 2(n+1)\sum_{\substack{n'=|m|(2)n,\\ n'-1\geq|m+1|}} 2n'\sum_{n''=n'(2)\infty}\gamma^m_{n''}. \tag{A18}$$

In a similar fashion

$$(A_-^H A_-\gamma)^m_n = 2(n+1)\sum_{\substack{n'=|m|(2)n\\ n'-1\geq|m-1|}} 2n'\sum_{n''=n'(2)\infty}\gamma^m_{n''}. \tag{A19}$$

As to the conditions $n'-1\geq|m+1|$, $n'-1\geq|m-1|$ that appear in the summations in Eqs. (A18) and (A19), we note that

$$|m+1| = \begin{cases}|m|+1, & m\geq 0\\ |m|-1, & m<0\end{cases},\qquad |m-1| = \begin{cases}|m|-1, & m>0\\ |m|+1, & m\leq 0.\end{cases} \tag{A20}$$

Hence, we have $n'=(|m|+2)(2)n$ when $m\geq 0$ and $n'=|m|(2)n$ when $m<0$ in Eq. (A18), and $n'=|m|(2)n$ when $m>0$ and $n'=(|m|+2)(2)n$ when $m\leq 0$ in Eq. (A19). Therefore,

$$\begin{aligned}(A^H A\gamma)^m_n &= (A_+^H A_+\gamma)^m_n + (A_-^H A_-\gamma)^m_n\\ &= 4(n+1)\sum_{n'=|m|(2)n}\ \sum_{n''=n'(2)\infty} n'\varepsilon_{n'-|m|}\gamma^m_{n''},\end{aligned} \tag{A21}$$

where $\varepsilon_k=1$ when $k=0$ and $\varepsilon_k=2$ when $k=2,4,\ldots$ (Neumann's symbol). The formula in Eq. (A21) is also valid for $m=0$, for $n'\varepsilon_{n'-|m|}\gamma^m_{n''}$ vanishes when $n'=|m|=0$.

We rearrange the result of Eq. (A21) further as

$$(A^H A\gamma)^m_n = 4(n+1)\sum_{n''=|m|(2)\infty}\gamma^m_{n''}\sum_{n'=|m|(2)(n''\wedge n)} n'\varepsilon_{n'-|m|}, \tag{A22}$$

where $k\wedge l$ is short-hand notation for $\min(k,l)$. Finally, for $n'''=|m|(2)\infty$, we have

$$\sum_{n'=|m|(2)n'''} n'\varepsilon_{n'-|m|} = |m| + \frac{1}{2}(n'''-|m|)(n'''+|m|+2), \tag{A23}$$

and the result of Eq. (33) follows from Eqs. (A22) and (A23) upon changing n'' into n' in $\gamma^m_{n''}$ and n' into n''' in $\sum_{n'}$ in Eq. (A22) and using Eq. (A23) with $n'''=n'\wedge n=n\wedge n'$.

APPENDIX B: INVERSION OF SOME SPECIAL MATRICES

We shall first show that $(LM)^{-1}$ is given by Eq. (46), where L is the $(I+1)\times(I+1)$ lower triangular matrix

$$L = \begin{bmatrix}1 & 0 & 0 & & 0\\ -1 & 1 & 0 & & 0\\ 0 & & & -1 & 1\end{bmatrix} \tag{B1}$$

(bidiagonal matrix with 1's on the main diagonal and -1's on the first lower codiagonal), and

$$M = (b_{\min(i,j)})_{i,j=0,1,\ldots,I} = \begin{bmatrix}b_0 & b_0 & b_0 & \cdots & b_0\\ b_0 & b_1 & b_1 & \cdots & b_1\\ b_0 & b_1 & b_2 & \cdots & b_2\\ \vdots & & & & \vdots\\ b_0 & b_1 & b_2 & \cdots & b_I\end{bmatrix}. \tag{B2}$$

We have

$$LM = \begin{bmatrix}b_0 & b_0 & b_0 & & b_0\\ 0 & b_1-b_0 & b_1-b_0 & & b_1-b_0\\ & & & b_{I-1}-b_{I-2} & b_{I-1}-b_{I-2}\\ 0 & & & 0 & b_I-b_{I-1}\end{bmatrix} \tag{B3}$$

(upper triangular matrix with $(LM)_{ij}=b_i-b_{i-1}$, $j=i,i+1,\ldots,I$ for $i=0,1,\ldots,I$ and b_{-1} defined 0). Next, when U is the $(I+1)\times(I+1)$ upper triangular matrix

$$U = \begin{bmatrix}1 & c_0 & 0 & & 0\\ 0 & 1 & c_1 & & \\ & & & 1 & c_{I-1}\\ 0 & & & 0 & 1\end{bmatrix},\qquad c_i = -\frac{b_i-b_{i-1}}{b_{i+1}-b_i}, \tag{B4}$$

(bidiagonal matrix with 1's on the main diagonal and c_i, $i=0,1,\ldots,I-1$ on the first upper codiagonal), we have

$$ULM = \begin{bmatrix}b_0-b_{-1} & 0 & & 0\\ 0 & b_1-b_0 & & \\ & & & 0\\ 0 & & 0 & b_I-b_{I-1}\end{bmatrix} = D \tag{B5}$$

(diagonal matrix with diagonal elements b_i-b_{i-1}, $i=0,1,\ldots,I$). Therefore, $D^{-1}ULM=I$, and Eq. (46) follows on computing $D^{-1}U$ from Eqs. (B4) and (B5).

We next determine the inverse of the matrix

$$(B^m_{n+2,s})_{s,n=|m|(2)N_m} \tag{B6}$$

that occurs in Eq. (67), also see Eq. (63). With

$$s=|m|+2u,\qquad n=|m|+2k,\qquad u,k=0,1,\ldots,K, \tag{B7}$$

where we have set $K=(1/2)(N_m-|m|)$, the matrix in Eq. (B6) assumes the form

$$C=(C_{uk})_{u,k=0,1,\ldots,K}, \tag{B8}$$

where

$$C_{uk} = \begin{cases}4(|m|+2u+1)(|m|+k+u+2)(k+1-u), & k\geq u,\\ 0, & k<u,\end{cases} \tag{B9}$$

for integer u,k, with $0\leq u,k\leq K$. Thus, $C=D_1E$, where D_1 is the $(K+1)\times(K+1)$ diagonal matrix with diagonal elements $8(|m|+2u+1)$, $u=0,1,\ldots,K$, and E is the upper triangular matrix with entries

$$E_{uk} = \frac{1}{2}(|m| + k + u + 2)(k + 1 - u) = \sum_{j=u}^{k} \left(\frac{1}{2}|m| + j + 1\right) \tag{B10}$$

for $0 \le u \le k \le K$. Setting $d_j = (1/2)|m| + j + 1$ for $j = 0, 1, \ldots, K$, and letting U_1, U_2 the two bidiagonal upper triangular matrices, given by

$$\begin{bmatrix} 1 & -1 & 0 & & 0 \\ 0 & 1 & -1 & & \\ & & & 1 & -1 \\ 0 & & & 0 & 1 \end{bmatrix}, \quad \begin{bmatrix} 1 & -d_0/d_1 & 0 & & 0 \\ 0 & 1 & -d_1/d_2 & & \\ & & & 1 & -d_{K-1}/d_K \\ 0 & & & 0 & 1 \end{bmatrix} \tag{B11}$$

respectively, it is seen that

$$U_2(U_1 E) = U_2 \begin{bmatrix} d_0 & d_0 & & d_0 \\ 0 & d_1 & & d_1 \\ 0 & & 0 & d_K \end{bmatrix} = \begin{bmatrix} d_0 & 0 & & 0 \\ 0 & d_1 & & \\ & & & 0 \\ 0 & & 0 & d_K \end{bmatrix} = D_2. \tag{B12}$$

Therefore, from $E = D_1^{-1} C$ and Eq. (B12) we get

$$C^{-1} = D_2^{-1} U_2 U_1 D_1^{-1}. \tag{B13}$$

Finally, we compute $U_2 U_1$ from Eq. (B11) as the upper triangular matrix with 1's on the main diagonal, $-1 - d_u/d_{u+1}$, $u = 0, 1, \ldots, K-1$ on the first upper codiagonal, d_u/d_{u+1}, $u = 0, 1, \ldots, K-2$ on the second upper codiagonal, and 0 elsewhere. Hence, with the definitions of D_1 and D_2 as given, we have that C^{-1} is an upper triangular tridiagonal matrix whose nonzero entries are given for $k, k' = 0, 1, \ldots, K$ by

$$(C^{-1})_{kk'} = \frac{(U_2 U_1)_{kk'}}{4(|m| + 2k + 2)(|m| + 2k' + 1)} = \begin{cases} \frac{1}{4(|m|+2k+2)(|m|+2k+1)}, & k = k', \\ \frac{-1}{2(|m|+2k+2)(|m|+2k+4)}, & k = k' - 1, \\ \frac{1}{4(|m|+2k+4)(|m|+2k+5)}, & k = k' - 2. \end{cases} \tag{B14}$$

From this the result of Eq. (68) can be obtained by restoring the index $n' = |m| + 2k$.

ACKNOWLEDGMENTS

It is a pleasure to thank Professor J. Braat for his constant interest and feedback during the development of the results of this paper, in addition to providing technical assistance of various sorts. Furthermore, a comment of Professor R. Aarts, which yielded an enhancement of the results in Section 3, is appreciated.

REFERENCES

1. H. H. Hopkins, "Canonical pupil coordinates in geometrical and diffraction image theory," Jpn. J. Appl. Phys. **3**, 31 (1964).
2. W. Lukosz, "Der Einfluss der Aberrationen auf die optische Übertragungsfunktion bei Kleinen Orts-Frequenzen," Opt. Acta **10**, 1–19 (1963).
3. M. Born and E. Wolf, *Principles of Optics* (Cambridge University, 1999).
4. B. C. Platt and R. Shack, "History and principles of Shack–Hartmann wavefront sensing," J. Refract. Surg. **17**, 573–577 (2001).
5. R. J. Noll, "Zernike polynomials and atmospheric turbulence," J. Opt. Soc. Am. **66**, 207–211 (1976).
6. F. Roddier, "Curvature sensing and compensation: a new concept in adaptive optics," Appl. Opt. **27**, 1223–1225 (1988).
7. J. J. M. Braat, S. van Haver, A. J. E. M. Janssen, and P. Dirksen, "Assessment of optical systems by means of point-spread functions," in *Progress in Optics*, E. Wolf, ed. (Elsevier, 2008), Vol. **51**, pp. 349–468.
8. T. E. Gureyev, A. Roberts, and K. A. Nugent, "Phase retrieval with the transport-of-intensity equation: matrix solution with use of Zernike polynomials," J. Opt. Soc. Am. A **12**, 1932–1941 (1995).
9. B. R. A. Nijboer, "The diffraction theory of aberrations," Ph.D. dissertation (Rijksuniversiteit Groningen, 1942).
10. F. W. J. Olver, D. W. Lozier, R. F. Boisvert, and C. W. Clark, *Handbook of Mathematical Functions* (Cambridge University, 2010).
11. J. Braat, "Polynomial expansion of severely aberrated wave fronts," J. Opt. Soc. Am. A **4**, 643–650 (1987).
12. A. Capozzoli, "On a new recursive formula for Zernike polynomials first order derivatives," Atti della Fondazione Giorgio Ronchi **54**, 767–774 (1999).
13. ANSI Z80.28–2009, "Ophthalmics: methods of reporting optical aberrations of eyes," American National Standards Institute, 2009.
14. P. C. L. Stephenson, "Recursive relations for the Cartesian derivatives of the Zernike polynomials," J. Opt. Soc. Am. A **31**, 708–715 (2014).
15. C. Roddier and F. Roddier, "Wave-front reconstruction from defocused images and the testing of ground-based optical telescopes," J. Opt. Soc. Am. A **10**, 2277–2287 (1993).
16. S. Bará, S. Ríos, and E. Acosta, "Integral evaluation of the modal phase coefficients in curvature sensing: Albrecht's cubatures," J. Opt. Soc. Am. A **13**, 1467–1474 (1996).