Information-content analysis of aureole inversion methods: differential kernel versus normal

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It has recently been suggested that more satisfactory inversion results for the aerosol size distribution may be obtained if the scattered (aureole) data are first differentiated with respect to angle—the so-called differential-kernel method. Analytic eigenfunction theory provides an ideal framework for determining the relative information content of this method versus the standard approach. Our results, supported by the inversion of synthetic data sets, show the differential-kernel method to have significant advantages.

INTRODUCTION

The inversion of near-forward-scattered light—the solar aureole—is one of the two standard procedures for determining the atmospheric aerosol size distribution,[1–4] the other being the inversion of multispectral extinction data.[3–5] In a recent contribution to this technique, Trakhovsky and Shettle[6] have suggested that more satisfactory retrievals may be obtained if the experimental data are first differentiated—the so-called differential-kernel method. They have tested this idea by using a modified Twomey–Chahine algorithm[3,7,8] with subsequent smoothing of the inverted distributions.

While sample simulated inversions are one method of testing the usefulness of an inversion technique,[9] information content[8] is often of more direct use. Recently, two approaches to the question of the information content of remote-sensing experiments have been investigated: singular-function theory[10,11] and analytic eigenfunction theory.[12–14] Of these, singular-function theory[15] is the more powerful because of its wider applicability, although it is distinctly more difficult, numerically, to implement.[10]

Analytic eigenfunction theory is applicable only to product-type kernels[12] $K(x, y) = K(xy)$, such as occur in Laplace, Fourier, and Hankel transforms.[16] This requirement is satisfied in the case of the extinction kernel for both the exact Mie theory[17–19] and the anomalous diffraction approximation.[14,17] In the case of angular scattering the Mie kernel is not a product type,[17–19] although the various diffraction approximations are. For this reason, in this paper we will apply analytic eigenfunction theory to these diffraction kernels. After first showing from the eigenvalue spectra that we would expect a greater information content, and hence superior retrievals, for the differential-kernel method, we then confirm these expectations with a set of synthetic retrievals.

DIFFRACTION SCATTERING APPROXIMATIONS

For a polydispersion of spherical particles, with a size distribution function $n(r)$, the volume angular scattering coefficient $\beta(\theta)$ may be written as[6,20]

$$\beta(\theta) = k^{-2} \int_0^\infty n(r) i(r, \lambda, m, \theta) \mathrm{d}r, \tag{1}$$

where θ is the scattering angle, λ is the wavelength, $k = 2\pi/\lambda$, m is the refractive index of the particles, r is their radius, and i is the intensity distribution function (averaged over polarization states if appropriate). The connection between β and the intensity measured in any practical situation need not concern us here.

In the case of exact Mie theory, $i = (|S_1|^2 + |S_2|^2)/2$, where S_1 and S_2 are the amplitude scattering matrix elements[17–19] and, as indicated above, are functions of r and θ separately rather than the product $r\theta$ or something similar. (Note that λ and m are regarded as fixed parameters.)

For particles whose characteristic length is of the order of, or greater than, the wavelength λ, $i(\theta)$ is dominated by a peak in the near-forward direction (i.e., for small values of θ). This peak may be modeled, or derived on the basis of theoretical approximations, in a number of ways. These include Fraunhofer diffraction for large particles[6,17–19] and the Rayleigh–Gans (Born) approximation for so-called soft particles of moderate size.[17–19] [Note that these approximations are sometimes rescaled, in absolute magnitude, to some more accurate value of $S(0°)$.] Trakhovsky and Shettle[6] used the approximation

$$2\,\frac{S(0°)}{x^2} \cong \frac{1}{2}\, Q_{\mathrm{ext}} \cong \frac{1}{2}\,(2 + 2x^{-2/3}),$$

where Q_{ext} is the extinction efficiency[17–19] and $x = kr$. The final approximation is based on the asymptotic expansion by Nussenzveig and Wiscombe.[21] Higher accuracy was subsequently achieved[22] by using the leading terms of the asymptotic expansion for $S(0°)$.[23]

For Fraunhofer diffraction,[17]

$$S(\theta) = x^2 J_1(u)/u, \tag{2}$$

where $u = x \sin\theta$ and J_ν is the Bessel function of order ν.

For the Rayleigh–Gans approximation,[17]

$$S(\theta) = i(m - 1)(2\pi)^{1/2} x^3 J_{3/2}(u)/u^{3/2}, \tag{3}$$

where $u = 2x \sin \tfrac{1}{2}\theta$. If we now ignore the constant factors in Eq. (3), which are of the order of unity, we may write a general expression to include both:

$$S(\theta) = x^{\nu} J_{\nu}(x\theta)/\theta^{\nu}. \quad (4a)$$

Therefore

$$i(\theta) = x^{2\nu} J_{\nu}^{2}(x\theta)/\theta^{2\nu}. \quad (4b)$$

ν may take on the value of 1 or 3/2, and we have used the small-angle approximation for $\sin\theta$.

The main purpose of this paper is to compare the information content of a normal forward-scattering experiment with that of the differential-kernel method of Trakhovsky and Shettle.[6] Hence we must obtain the derivative of Eq. (4b), which becomes[16]

$$i' = -x^{2\nu+1} J_{\nu}(x\theta) J_{\nu+1}(x\theta)/\theta^{2\nu}. \quad (5)$$

ANALYTIC EIGENFUNCTION THEORY

Equation (1) may now be written as

$$\beta(\theta) = k^{-2} \int_0^{\infty} x^{2\nu} J_{\nu}^{2}(x\theta)\theta^{-2\nu} n(r)\mathrm{d}r, \quad (6)$$

which we can rewrite as

$$g(y) = \int_0^{\infty} K(yr) f(r)\mathrm{d}r, \quad (7)$$

where $y = k\theta$:

$$g(y) = k^{2-4\nu} y^{\alpha+2\nu} \beta(\theta), \quad (8a)$$

$$K(yr) = (yr)^{\alpha} J_{\nu}^{2}(yr), \quad (8b)$$

$$f(r) = r^{2\nu-\alpha} n(r). \quad (8c)$$

α is a free parameter, constrained only by the convergence criterion on the Mellin transform of K, as discussed below.

The equivalent expressions for the differential-kernel case are

$$\beta'(\theta) = -k^{-2} \int_0^{\infty} x^{2\nu+1} J_{\nu}(x\theta) J_{\nu+1}(x\theta) n(r)\mathrm{d}r, \quad (9)$$

$$g(y) = -k^{-4\nu} y^{\alpha+2\nu+1} \beta'(\theta), \quad (10a)$$

$$K(yr) = (yr)^{\alpha} J_{\nu}(yr) J_{\nu+1}(yr), \quad (10b)$$

$$f(r) = r^{2\nu-\alpha+1} n(r). \quad (10c)$$

Full details of analytic eigenfunction theory may be found in Refs. 13 and 14. However, a brief operational outline will prove useful. The final retrieval equation for the unknown function $f(r)$ may be written as

$$f(r) = r^{-1/2}\,\mathrm{Re} \int_0^{\omega_m} G(\omega) r^{-i\omega} \chi(\omega)/\lambda(\omega)\mathrm{d}\omega, \quad (11)$$

where

$$G(\omega) = \chi(\omega) \int_0^{\infty} g(y) y^{-1/2-i\omega}\mathrm{d}y,$$

$$\chi(\omega) = (\tilde{K}/\pi\lambda)^{1/2},$$

$$\lambda(\omega) = |\tilde{K}(1/2 + i\omega)|,$$

and

$$\tilde{K}\left(\frac{1}{2} + i\omega\right) = \int_0^{\infty} t^{-1/2+i\omega} K(t)\mathrm{d}t$$

is the Mellin transform of the kernel K. The final cutoff in Eq. (11), ω_m, is determined by the decay of the eigenvalue spectrum $\lambda(\omega)$. The free parameter α in the two kernels [Eqs. (8b) and (10b)] is confined by the requirement that $\tilde{K}$ be well defined. For the normal kernel, this requirement becomes

$$-2\nu - 1/2 < \alpha < 1/2, \quad (12a)$$

while, for the differential kernel, we have

$$-2\nu - 3/2 < \alpha < 1/2. \quad (12b)$$

The key to any expansion-type inversion is the decay of the eigenvalue spectrum $\lambda(\omega)$, which in this case is directly related to the Mellin transform of the kernel, $\tilde{K}$. For a simple analytic kernel, it is usually possible to find the transform in standard tabulations.[24] In the case of the normal kernel [Eq. (8b)] we find that

$$\tilde{K}\left(\frac{1}{2} + i\omega\right) = \frac{2^{\alpha-1/2+i\omega}\Gamma(1/2 - \alpha - i\omega)\Gamma(1/4 + \alpha/2 + \nu + i\omega/2)}{\Gamma^{2}(3/4 - \alpha/2 - i\omega/2)\Gamma(3/4 - \alpha/2 + \nu - i\omega/2)},$$

while for the differential kernel [Eq. (10b)] we find that

$$\tilde{K}(1/2 + i\omega) = \frac{2^{\alpha-1/2+i\omega}\Gamma(1/2 - \alpha - i\omega)\Gamma(3/4 + \alpha/2 + \nu + i\omega/2)}{(1/4 - \alpha/2 - i\omega/2)\Gamma^{2}(1/4 - \alpha/2 - i\omega/2)\Gamma(5/4 - \alpha/2 + \nu - i\omega/2)}.$$

The asymptotic form of $\lambda(\omega)$ may then be found by using the asymptotic expansions of the gamma functions.[14,25] For both the normal and the differential kernels we find that

$$\lambda(\omega) \sim \omega^{\alpha-1}, \quad (13)$$

which is independent of ν, as well. This result shows clearly that we should choose as large a value of α as possible, which is consistent with relations (12); $\alpha = 0$ is the obvious choice.

In Fig. 1, we plot the normalized eigenvalues as functions of ω, for both the normal and differential kernels. We selected $\nu = 3/2$ and α values of 0, −1, and −2. Also shown is the eigenvalue spectrum for the best case for anomalous diffraction without the inclusion of *a priori* knowledge.[14] The plots of $\nu = 1$ were quite similar, although always below those for $\nu = 3/2$, especially for $\alpha = -1$ and $\alpha = -2$. This result is not entirely surprising, owing to the narrower range of α in this case [relations (12)].

By far the most interesting feature of Fig. 1 is the clear superiority of the differential kernel over the normal kernel. Despite identical asymptotic behavior, as is shown in relation (13), the differential-eigenvalue spectrum lies well above that of the normal kernel. The asymptotic expression such as relation (13) clearly does not always tell the whole story.

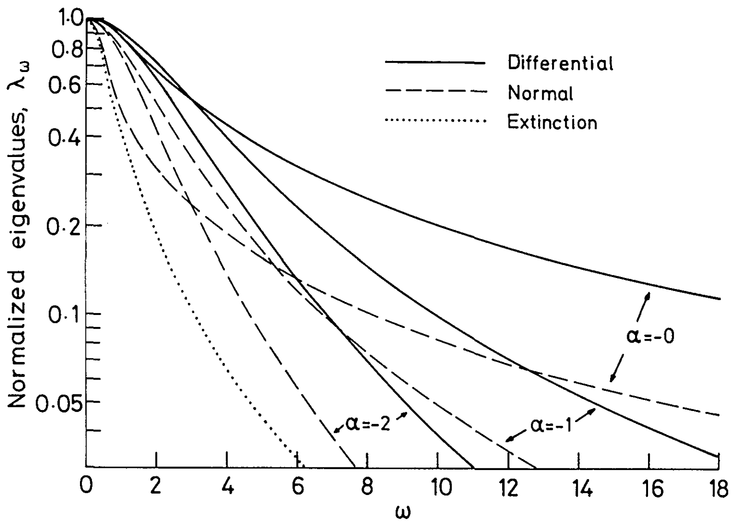

Fig. 1. Normalized eigenvalues for the normal and differential kernels for three values of α.

INVERSIONS

To confirm the results of our information content analysis, we have performed a series of inversions of synthetic data. In order to permit some comparison with our earlier research on the anomalous diffraction approximation,[14] we have used the same size distribution, namely,

$$n(r) = Ar^2e^{-br},$$

with $A = 10^6$ and $b = 20$. We assumed the Rayleigh–Gans approximation, i.e., $\nu = 3/2$, and chose $\alpha = 0$. Exact data were generated directly by integration of Eqs. (6) and (9) and then perturbed with random errors, uniformly distributed with a mean of 5% (i.e., the data points were multiplied by a random factor between 0.9 and 1.1). (Note that with the assumptions that we have made concerning measurement range, the actual measurement wavelength is not relevant.)

Figure 2 shows inversions in the case of the normal kernel, for two cutoffs ω_m of 4 and 6. The retrieval for $\omega_m = 4$ is reasonably satisfactory, while that for $\omega_m = 6$ shows considerable instability, particularly for small r.

Figure 3 shows two retrievals in the differential-kernel case, both for cutoffs of $\omega_m = 8$. Because differentiation of noisy data is known to increase that noise, our second inversion was performed for data perturbed with twice the amount of error. Even this retrieval is superior to both retrievals for the normal kernel.

Note that in this pair of synthetic experiments we have generated our data by using the Rayleigh–Gans approximation and then inverted it by using the same formulation. Nature, of course, supplies us with data based on the Mie theory (at least for spherical particles), so that this formulation should be used to perform inversions. However, as indicated above, the Mie scattering kernel is unsuited to the analytic eigenfunction method. Nevertheless, we believe that the results presented in Figs. 2 and 3 give a good indication of the relative accuracy of Mie theory retrievals for the two types of kernel. (The use of the Rayleigh–Gans formulation to invert real Mie data is not recommended.)

DISCUSSION

It is not possible to plot the two sets of retrievals, i.e., for normal and differential kernels, on the same graph, as they are for different unknown functions, as can be seen from Eqs. (8c) and (10c). (While it would be possible to convert one functional form to the other by multiplying or dividing by r, there is little to be gained by doing so, as the resulting single graph would be too cluttered for easy comprehension.) Nevertheless it is clear from Figs. 2 and 3 that the differential-kernel method gave clearly superior inversions, even when a higher noise level was included in the data. This, of course, is entirely within our expectations based on the eigenvalue spectra of Fig. 1.

In their original paper, Trakhovsky and Shettle[6] produced inversions for $r^4n(r)$, based on Fraunhofer diffraction. These inversions correspond to α values of -2 and -1 for the normal and differential kernels, respectively. It is clear

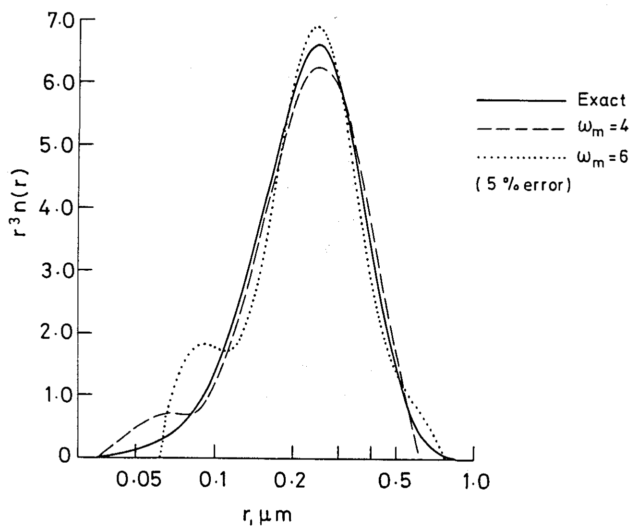

Fig. 2. Retrieved distribution for the normal-kernel method for two different cutoffs, ω_m.

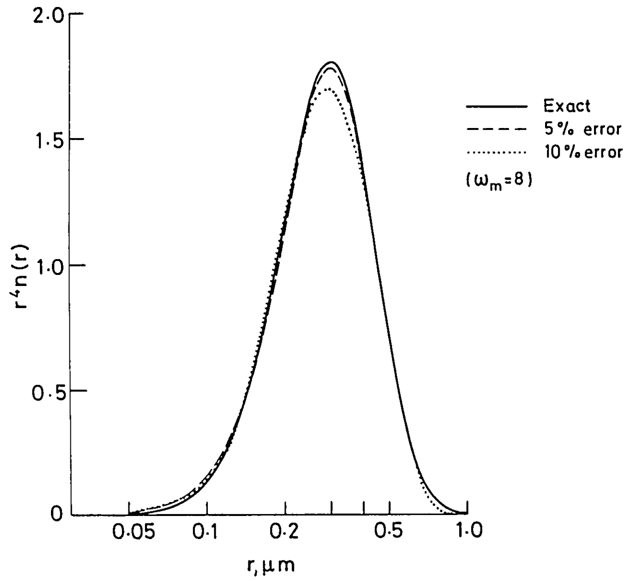

Fig. 3. Retrieved distribution for the differential-kernel method for two different error levels.

from Fig. 1, or from relation (13), that this choice is not optimal. Nevertheless it is not surprising that their calculations lead to superior retrievals for the differential-kernel case.

Bertero and Pike[13] have also applied analytic eigenfunction theory to Fraunhofer diffraction. They have also selected $\alpha = -2$, which is again less than optimal. Their approach is somewhat more formal than ours, and no specific inversions are provided. On the other hand, we have made no attempt to address such questions as resolution limits and would direct interested readers to their paper for a valuable discussion.

Our results show clearly that, even allowing for the increased noise level involved, the differential-kernel method does provide distinctly superior retrievals to the normal method, as indicated by Trakhovsky and Shettle.[6] For optimal results, however, Eqs. (8c) and (10c) indicate that the most appropriate retrievals in the two cases should actually be made for different forms of the unknown function.

REFERENCES

1. A. E. S. Green, A. Deepak, and B. J. Lipofsky, "Interpretation of the Sun's aureole based on atmospheric aerosol models," Appl. Opt. **10**, 1263–1279 (1971).
2. J. T. Twitty, "The inversion of aureole measurements to derive aerosol size distributions," J. Atmos. Sci. **32**, 584–591 (1975).
3. A. Deepak, ed., *Inversion Methods in Atmospheric Remote Sounding* (Academic, New York, 1977).
4. D. Deirmendjian, "A survey of light scattering techniques used in the remote monitoring of atmospheric aerosols," Rev. Geophys. Space Phys. **18**, 341–360 (1980).
5. M. D. King, D. M. Byrne, B. M. Herman, and J. A. Reagan, "Aerosol size distributions obtained by inversion of spectral optical depth measurements," J. Atmos. Sci. **35**, 2153–2167 (1978).
6. E. Trakhovsky and E. P. Shettle, "Improved inversion procedure for the retrieval of aerosol size distributions using aureole measurements," J. Opt. Soc. Am. A **2**, 2054–2061 (1985).
7. M. T. Chahine, "Inversion problems in radiative transfer: determination of atmospheric parameters," J. Atmos. Sci. **27**, 960–967 (1970).
8. S. Twomey, *Introduction to the Mathematics of Inversion in Remote Sensing and Indirect Measurements* (American Elsevier, New York, 1977).
9. N. Wolfson, J. H. Joseph, and Y. Mekler, "Comparative study of inversion techniques. Part I: accuracy and stability," J. Appl. Meteorol. **18**, 543–555 (1979).
10. G. Viera and M. A. Box, "Information content analysis of aerosol remote sensing experiments using singular function theory. 1: Extinction measurements," Appl. Opt. **26**, 1312–1327 (1987).
11. G. Viera and M. A. Box, "Information content analysis of aerosol remote sensing experiments using singular function theory. 2: Scattering measurements," Appl. Opt. **27**, 3262–3274 (1988).
12. J. G. McWhirter and E. R. Pike, "On the numerical inversion of the Laplace transform and similar Fredholm integral equations of the first kind," J. Phys. A **11**, 1729–1745 (1978).
13. M. Bertero and E. R. Pike, "Particle size distributions from Fraunhofer diffraction. I. An analytic eigenfunction approach," Opt. Acta **30**, 1043–1049 (1983).
14. G. Viera and M. A. Box, "Information content analysis of aerosol remote sensing experiments using an analytic eigenfunction theory: anomalous diffraction approximation," Appl. Opt. **24**, 4525–4533 (1985).
15. F. Smithies, *Integral Equations* (Cambridge U. Press, London, 1958).
16. G. Arfken, *Mathematical Methods for Physicists* (Academic, New York, 1970).
17. H. C. van de Hulst, *Light Scattering by Small Particles* (Dover, New York, 1981).
18. M. Kerker, *The Scattering of Light, and Other Electromagnetic Radiation* (Academic, New York, 1969).
19. C. F. Bohren and D. R. Huffman, *Absorption and Scattering of Light by Small Particles* (Wiley, New York, 1983).
20. E. J. McCartney, *Optics of the Atmosphere* (Wiley, New York, 1976).
21. H. M. Nussenzveig and W. J. Wiscombe, "Efficiency factors in Mie scattering," Phys. Rev. Lett. **45**, 1490–1494 (1980).
22. E. P. Shettle, U.S. Air Force Geophysics Laboratory, Hanscom Air Force Base, Bedford, Massachusetts 01731 (personal communication).
23. P. Attard, M. A. Box, G. Bryant, and B. H. J. McKellar, "Asymptotic behavior of the Mie scattering amplitude," J. Opt. Soc. Am. A **3**, 256–258 (1986).
24. I. S. Gradshteyn and I. W. Ryzhik, *Tables of Integrals, Series and Products* (Academic, New York, 1965).
25. M. Abramowitz and I. A. Stegun, eds., *Handbook of Mathematical Functions* (Dover, New York, 1965).