Derivatives of the asymmetry parameter in `mie_derivs.pro`

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Abstract

Following from Grainger et al. (2004), here is the additional mathematics required to add the asymmetry parameter to the EODG `mie_derivs.pro` routine. The parameters are included as keywords, so that the additional computational overhead is only carried out if required.

1 Method

Following the notation from Grainger et al. (2004), the asymmetry parameter, g, is given by (Bohren and Huffman, 1983):

$$Q\text{sca}\ g = \frac{4}{x^2}\left[\sum_n^\infty \frac{n(n+2)}{n+1}\Re\left\{a_n a_{n+1}^* + b_n b_{n+1}^*\right\} + \sum_n^\infty \frac{2n+1}{n(n+1)}\Re\left\{a_n b_n^*\right\}\right]. \tag{1}$$

Taking the derivative wrt x, the size parameter, we obtain:

$$\begin{aligned}
\frac{\partial}{\partial x}\left[Q\text{sca}\ g\right] = {} & \frac{4}{x^2}\sum_n^\infty\left[\frac{n(n+2)}{n+1}\Re\left\{\frac{\partial a_n}{\partial x}a_{n+1}^* + a_n\frac{\partial a_{n+1}^*}{\partial x} + \frac{\partial b_n}{\partial x}b_{n+1}^* + b_n\frac{\partial b_{n+1}^*}{\partial x}\right\}\right. \\
& \left. + \frac{2n+1}{n(n+1)}\Re\left\{a_n\frac{\partial b_n^*}{\partial x} + \frac{\partial a_n}{\partial x}b_n^*\right\}\right] \\
& - \frac{8}{x^3}\left[\sum_n^\infty \frac{n(n+2)}{n+1}\Re\left\{a_n a_{n+1}^* + b_n b_{n+1}^*\right\} + \sum_n^\infty \frac{2n+1}{n(n+1)}\Re\left\{a_n b_n^*\right\}\right] \qquad (2) \\
= {} & \frac{4}{x^2}\sum_n^\infty\left[\frac{n(n+2)}{n+1}\Re\left\{\frac{\partial a_n}{\partial x}a_{n+1}^* + a_n\frac{\partial a_{n+1}^*}{\partial x} + \frac{\partial b_n}{\partial x}b_{n+1}^* + b_n\frac{\partial b_{n+1}^*}{\partial x}\right\}\right. \\
& \left. + \frac{2n+1}{n(n+1)}\Re\left\{a_n\frac{\partial b_n^*}{\partial x} + \frac{\partial a_n}{\partial x}b_n^*\right\}\right] - \frac{2}{x}\ g\ Q\text{sca}. \qquad (3)
\end{aligned}$$

Defining:

$$\xi_x = \sum_n^\infty\left[\frac{n(n+2)}{n+1}\Re\left\{\frac{\partial a_n}{\partial x}a_{n+1}^* + a_n\frac{\partial a_{n+1}^*}{\partial x} + \frac{\partial b_n}{\partial x}b_{n+1}^* + b_n\frac{\partial b_{n+1}^*}{\partial x}\right\} + \frac{2n+1}{n(n+1)}\Re\left\{a_n\frac{\partial b_n^*}{\partial x} + \frac{\partial a_n}{\partial x}b_n^*\right\}\right]. \tag{4}$$

we say

$$Q\text{sca}\ \frac{\partial g}{\partial x} + \frac{\partial Q\text{sca}}{\partial x}\ g = \frac{4}{x^2}\xi_x - \frac{2}{x}\ g\ Q\text{sca}, \tag{5}$$

leading to

$$\frac{\partial g}{\partial x} = \frac{1}{Q\text{sca}} \left[\frac{4}{x^2} \xi_x - g \left(\frac{2Q\text{sca}}{x} + \frac{\partial Q\text{sca}}{\partial x} \right) \right]. \tag{6}$$

Similarly, for the real and imaginary parts of refractive index, $m = m_r + im_i$, we define ξ_r and ξ_i:

$$\xi_r = \sum_n^\infty \left[\frac{n(n+2)}{n+1} \Re \left\{ \frac{\partial a_n}{\partial m_r} a^*_{n+1} + a_n \frac{\partial a^*_{n+1}}{\partial m_r} + \frac{\partial b_n}{\partial m_r} b^*_{n+1} + b_n \frac{\partial b^*_{n+1}}{\partial m_r} \right\} + \frac{2n+1}{n(n+1)} \Re \left\{ a_n \frac{\partial b^*_n}{\partial m_r} + \frac{\partial a_n}{\partial m_r} b^*_n \right\} \right]; \tag{7}$$

$$\xi_i = \sum_n^\infty \left[\frac{n(n+2)}{n+1} \Re \left\{ \frac{\partial a_n}{\partial m_i} a^*_{n+1} + a_n \frac{\partial a^*_{n+1}}{\partial m_i} + \frac{\partial b_n}{\partial m_i} b^*_{n+1} + b_n \frac{\partial b^*_{n+1}}{\partial m_i} \right\} + \frac{2n+1}{n(n+1)} \Re \left\{ a_n \frac{\partial b^*_n}{\partial m_i} + \frac{\partial a_n}{\partial m_i} b^*_n \right\} \right], \tag{8}$$

and obtain the derivatives by:

$$\frac{\partial g}{\partial m_r} = \frac{1}{Q\text{sca}} \left[\frac{4}{x^2} \xi_r - g \frac{\partial Q\text{sca}}{\partial m_r} \right]; \tag{9}$$

$$\frac{\partial g}{\partial m_i} = \frac{1}{Q\text{sca}} \left[\frac{4}{x^2} \xi_i - g \frac{\partial Q\text{sca}}{\partial m_i} \right]. \tag{10}$$

During the execution of `mie_derivs.pro` , the calculations of ξ_x, ξ_r, and ξ_i are carried out iteratively as we ascend through values of n. At the end of the code, the final values are calculated using equations 6, 9, and 10.

2 Tests

A small number of tests have been carried out and appear to be fine. The calculations of g agree with those from `mie_single.pro` , and derivatives are sensible when plotted over variations in x, m_r, and m_i, as shown in Fig. 1.

References

Bohren, C. F. and D. R. Huffman, 1983: *Absorption and Scattering of Light by Small Particles*. Wiley-VCH, doi:10.1002/9783527618156.

Grainger, R. G., J. Lucas, G. E. Thomas, and G. B. Ewen, 2004: Calculation of Mie derivatives. *Applied Optics*, **43**(28):5386–5393, doi:10.1364/AO.43.005386.

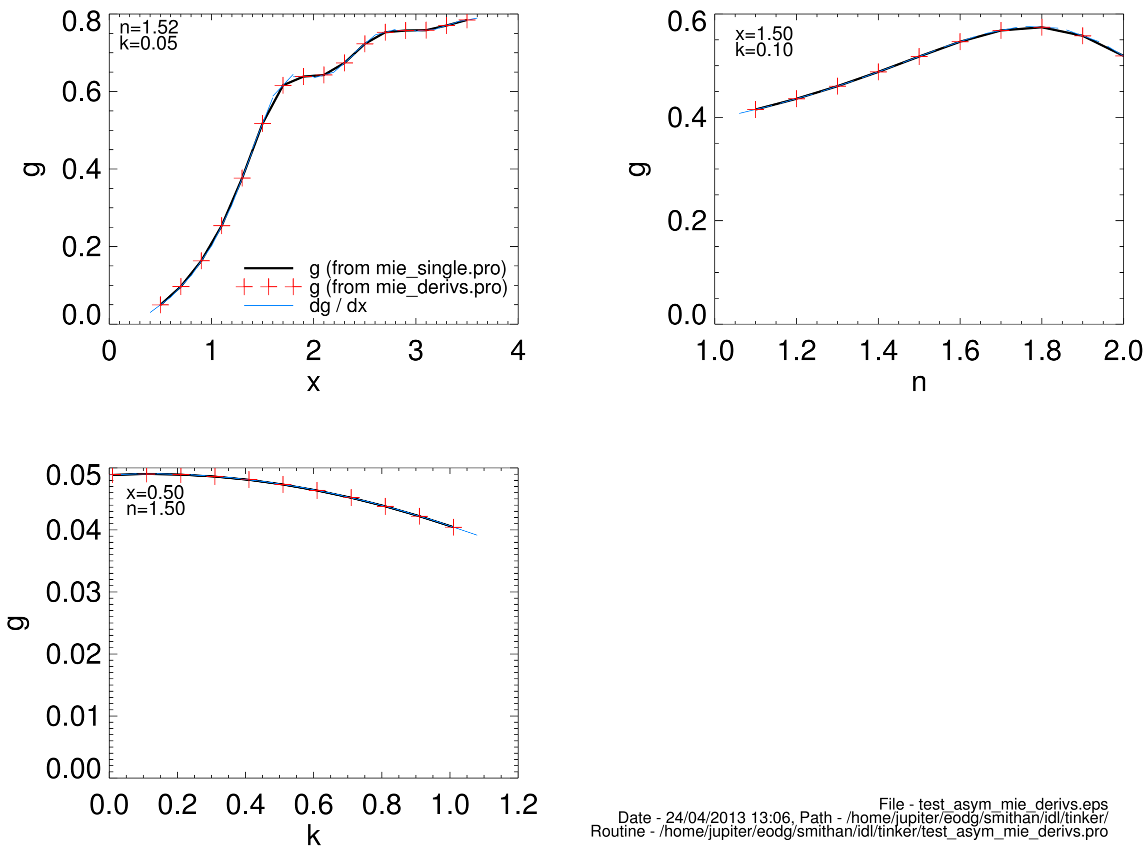

Figure 1: Tests of the derivatives calculated using `mie_derivs.pro`.