Vector spherical waves calculation procedure

Wednesday, May 19, 2021 10:52 AM

Equations are taken from:
Mishchenko, M.I., Travis, L.D., and Lacis, A.A. (2002). Scattering, absorption, and emission of light by small particles (Cambridge University Press).

Vector spherical waves ($\mathbf{M}$ and $\mathbf{N}$) are define as:

$$\begin{array}{c}\mathbf{M}_{mn}(kr,\vartheta,\varphi)\\ \mathrm{Rg}\mathbf{M}_{mn}(kr,\vartheta,\varphi)\end{array} = \gamma_{mn}\nabla\times\left(\mathbf{r}\begin{array}{c}\psi_{mn}(kr,\vartheta,\varphi)\\ \mathrm{Rg}\psi_{mn}(kr,\vartheta,\varphi)\end{array}\right)$$

$$= \gamma_{mn}\begin{array}{c}h_n^{(1)}(kr)\\ j_n(kr)\end{array}\mathbf{C}_{mn}(\vartheta,\varphi)$$

$$= \frac{1}{k}\nabla\times\begin{array}{c}\mathbf{N}_{mn}(kr,\vartheta,\varphi)\\ \mathrm{Rg}\mathbf{N}_{mn}(kr,\vartheta,\varphi)\end{array} \tag{C.14}$$

and

$$\begin{array}{c}\mathbf{N}_{mn}(kr,\vartheta,\varphi)\\ \mathrm{Rg}\mathbf{N}_{mn}(kr,\vartheta,\varphi)\end{array} = \frac{1}{k}\nabla\times\begin{array}{c}\mathbf{M}_{mn}(kr,\vartheta,\varphi)\\ \mathrm{Rg}\mathbf{M}_{mn}(kr,\vartheta,\varphi)\end{array}$$

$$= \gamma_{mn}\left\{\frac{n(n+1)}{kr}\begin{array}{c}h_n^{(1)}(kr)\\ j_n(kr)\end{array}\mathbf{P}_{mn}(\vartheta,\varphi) + \frac{1}{kr}\frac{\mathrm{d}}{\mathrm{d}(kr)}\left(kr\begin{array}{c}h_n^{(1)}(kr)\\ j_n(kr)\end{array}\right)\mathbf{B}_{mn}(\vartheta,\varphi)\right\}, \tag{C.15}$$

$\mathbf{B}_{mn}(\theta,\phi), \mathbf{C}_{mn}(\theta,\phi), \mathbf{P}_{mn}(\theta,\phi)$ are calculated from:
where

$$\mathbf{B}_{mn}(\vartheta,\varphi) = r\nabla[P_n^m(\cos\vartheta)\mathrm{e}^{\mathrm{i}m\varphi}]$$

$$= \left[\hat{\boldsymbol{\vartheta}}\frac{\mathrm{d}}{\mathrm{d}\vartheta}P_n^m(\cos\vartheta) + \hat{\boldsymbol{\varphi}}\frac{\mathrm{i}m}{\sin\vartheta}P_n^m(\cos\vartheta)\right]\mathrm{e}^{\mathrm{i}m\varphi}$$

$$= (-1)^m\sqrt{\frac{(n+m)!}{(n-m)!}}\,\mathbf{B}_{mn}(\vartheta)\mathrm{e}^{\mathrm{i}m\varphi}$$

$$= \hat{\mathbf{r}}\times\mathbf{C}_{mn}(\vartheta,\varphi), \tag{C.16}$$

$$\mathbf{C}_{mn}(\vartheta,\varphi) = \nabla\times[\mathbf{r}P_n^m(\cos\vartheta)\mathrm{e}^{\mathrm{i}m\varphi}]$$

$$= \left[\hat{\boldsymbol{\vartheta}}\frac{\mathrm{i}m}{\sin\vartheta}P_n^m(\cos\vartheta) - \hat{\boldsymbol{\varphi}}\frac{\mathrm{d}}{\mathrm{d}\vartheta}P_n^m(\cos\vartheta)\right]\mathrm{e}^{\mathrm{i}m\varphi}$$

$$= (-1)^m\sqrt{\frac{(n+m)!}{(n-m)!}}\,\mathbf{C}_{mn}(\vartheta)\mathrm{e}^{\mathrm{i}m\varphi}$$

$$= \mathbf{B}_{mn}(\vartheta,\varphi)\times\hat{\mathbf{r}}, \tag{C.17}$$

$$\mathbf{P}_{mn}(\vartheta,\varphi) = \hat{\mathbf{r}}P_n^m(\cos\vartheta)\mathrm{e}^{\mathrm{i}m\varphi}$$

$$= (-1)^m\sqrt{\frac{(n+m)!}{(n-m)!}}\,\mathbf{P}_{mn}(\vartheta)\mathrm{e}^{\mathrm{i}m\varphi}, \tag{C.18}$$

Symmetry relations that may speed the code:

$$\mathbf{B}_{-mn}(\vartheta,\varphi) = (-1)^m \frac{(n-m)!}{(n+m)!}\mathbf{B}^*_{mn}(\vartheta,\varphi), \tag{C.27}$$

and analogous relations hold for $\mathbf{C}_{mn}(\vartheta,\varphi)$ and $\mathbf{P}_{mn}(\vartheta,\varphi)$. The regular vector spherical wave functions obey a similar symmetry relation:

$$\mathrm{Rg}\mathbf{M}_{-mn}(kr,\vartheta,\varphi) = (-1)^m \mathrm{Rg}\mathbf{M}^*_{mn}(kr,\vartheta,\varphi), \tag{C.28}$$

and analogous relations again hold for $\mathrm{Rg}\mathbf{N}$ and $\mathrm{Rg}\mathbf{L}$.

$\mathbf{B}_{mn}(\theta), \mathbf{C}_{mn}(\theta), \mathbf{P}_{mn}(\theta)$ are calculated from:

$$\mathbf{B}_{mn}(\vartheta) = \hat{\boldsymbol{\vartheta}}\frac{\mathrm{d}}{\mathrm{d}\vartheta}d^n_{0m}(\vartheta) + \hat{\boldsymbol{\varphi}}\frac{\mathrm{i}m}{\sin\vartheta}d^n_{0m}(\vartheta)$$

$$= \hat{\boldsymbol{\vartheta}}\tau_{mn}(\vartheta) + \hat{\boldsymbol{\varphi}}\mathrm{i}\pi_{mn}(\vartheta), \tag{C.19}$$

$$\mathbf{C}_{mn}(\vartheta) = \hat{\boldsymbol{\vartheta}}\frac{\mathrm{i}m}{\sin\vartheta}d^n_{0m}(\vartheta) - \hat{\boldsymbol{\varphi}}\frac{\mathrm{d}}{\mathrm{d}\vartheta}d^n_{0m}(\vartheta)$$

$$= \hat{\boldsymbol{\vartheta}}\mathrm{i}\pi_{mn}(\vartheta) - \hat{\boldsymbol{\varphi}}\tau_{mn}(\vartheta), \tag{C.20}$$

$$\mathbf{P}_{mn}(\vartheta) = \hat{\mathbf{r}}d^n_{0m}(\vartheta), \tag{C.21}$$

$$\gamma_{mn} = \left[\frac{(2n+1)(n-m)!}{4\pi n(n+1)(n+m)!}\right]^{1/2}. \tag{C.22}$$

In Eqs. (C.19) and (C.20),

$$\pi_{mn}(\vartheta) = \frac{m}{\sin\vartheta}d^n_{0m}(\vartheta),$$

$$\tau_{mn}(\vartheta) = \frac{\mathrm{d}}{\mathrm{d}\vartheta}d^n_{0m}(\vartheta).$$

d^n_{nm} are the Wigner d-functions. They can be calculated using one of two methods:

<u>Method 1: Direct calculation</u>

For now, this one works with auto-differentiation. It is slower and not as stable as calculation using recurrence.

$$d^s_{mn}(\vartheta) = \sqrt{(s+m)!(s-m)!(s+n)!(s-n)!}$$

$$\times\sum_k (-1)^k \frac{(\cos\frac{1}{2}\vartheta)^{2s-2k+m-n}(\sin\frac{1}{2}\vartheta)^{2k-m+n}}{k!(s+m-k)!(s-n-k)!(n-m+k)!}, \tag{B.1}$$

The summation index k runs from

$k_{min} = \max(0, m-n)$

$k_{max} = \min(s+m, s-n)$

If $k_{min} > k_{max}$, then $d^n_{nm} = 0$

$\frac{d(d^n_{nm})}{d\theta}$ can be calculated from:

$$\frac{\mathrm{d}}{\mathrm{d}\vartheta}d^s_{mn}(\vartheta) = \frac{m-n\cos\vartheta}{\sin\vartheta}d^s_{mn}(\vartheta) + \sqrt{(s+n)(s-n+1)}\,d^s_{mn-1}(\vartheta)$$

$$= -\frac{m-n\cos\vartheta}{\sin\vartheta}d^s_{mn}(\vartheta) - \sqrt{(s-n)(s+n+1)}\,d^s_{mn+1}(\vartheta). \tag{B.25}$$

Symmetry relations may speed up the code:

$$d^s_{mn}(\vartheta) = (-1)^{m-n} d^s_{-m,-n}(\vartheta) = (-1)^{m-n} d^s_{nm}(\vartheta) = d^s_{-n,-m}(\vartheta), \tag{B.5}$$

$$d^s_{mn}(-\vartheta) = (-1)^{m-n} d^s_{mn}(\vartheta) = d^s_{nm}(\vartheta), \qquad d^s_{mn}(0) = \delta_{mn}, \tag{B.6}$$

$$d^s_{mn}(\pi-\vartheta) = (-1)^{s-n} d^s_{-mn}(\vartheta) = (-1)^{s+m} d^s_{m,-n}(\vartheta), \qquad d^s_{mn}(\pi) = (-1)^{s-n}\delta_{-mn}, \tag{B.7}$$

Method 2: using recurrence

$$s_{\min} = \max(|m|, |n|).$$

Recurrence relation over s:

$$d^{s+1}_{mn}(\vartheta) = \frac{1}{s\sqrt{(s+1)^2-m^2}\sqrt{(s+1)^2-n^2}}\{(2s+1)[s(s+1)x-mn]d^s_{mn}(\vartheta)$$
$$-(s+1)\sqrt{s^2-m^2}\sqrt{s^2-n^2}\, d^{s-1}_{mn}(\vartheta)\}, \qquad s \ge s_{\min}. \tag{B.22}$$

Initial values:

$$d^{s_{\min}-1}_{mn}(\vartheta) = 0, \tag{B.23}$$

$$d^{s_{\min}}_{mn}(\vartheta) = \xi_{mn} 2^{-s_{\min}} \left[\frac{(2s_{\min})!}{(|m-n|)!(|m+n|)!}\right]^{1/2} (1-x)^{|m-n|/2}(1+x)^{|m+n|/2}, \tag{B.24}$$

$$\xi_{mn} = \begin{cases} 1 & \text{for } n \ge m, \\ (-1)^{m-n} & \text{for } n < m. \end{cases} \tag{B.16}$$

Denoting $x = \cos\vartheta$

If $m = n = 0$

$$d^s_{00}(\vartheta) = P_s(x). \tag{B.27}$$

If $n = 0$

$$d^s_{m0}(\vartheta) = \sqrt{\frac{(s-m)!}{(s+m)!}}\, P^m_s(x), \tag{B.28}$$

P_s is the Legendre polynomils and P^m_s are the associated Legendre functions:

$$P^m_l(x) = (-1)^m (1-x^2)^{m/2} \frac{d^m}{dx^m} P_l(x), \quad P_l(x) = \frac{1}{2^l l!}\frac{d^l}{dx^l}(x^2-1)^l \tag{A.3}$$

Associated

https://en.wikipedia.org/wiki/Associated_Legendre_polynomials#Recurrence_formula

$$P^\ell_\ell(x) = (-1)^\ell (2\ell-1)!!(1-x^2)^{(\ell/2)}$$

$$P^\ell_{\ell+1}(x) = x(2\ell+1)P^\ell_\ell(x)$$

$$(\ell-m+1)P^m_{\ell+1}(x) = (2\ell+1)xP^m_\ell(x) - (\ell+m)P^m_{\ell-1}(x)$$

Remember that for P^m_n, $0 \le m \le n$

Derivative of Wigner-d using the recurrence relation over s:

$$\frac{d}{d\vartheta} d^s_{mn}(\vartheta) = \frac{1}{\sin\vartheta}\left[-\frac{(s+1)\sqrt{(s^2-m^2)(s^2-n^2)}}{s(2s+1)} d^{s-1}_{mn}(\vartheta)\right.$$
$$\left. -\frac{mn}{s(s+1)} d^s_{mn}(\vartheta) + \frac{s\sqrt{(s+1)^2-m^2}\sqrt{(s+1)^2-n^2}}{(s+1)(2s+1)} d^{s+1}_{mn}(\vartheta)\right]. \tag{B.26}$$