Accuracy of the scalar approximation in computations of diffuse and coherent backscattering by discrete random media

Michael I. Mishchenko\textsuperscript{1,*} and Janna M. Dlugach\textsuperscript{2}

\textsuperscript{1}NASA Goddard Institute for Space Studies, 2880 Broadway, New York, New York 10025, USA
\textsuperscript{2}Main Astronomical Observatory of the National Academy of Sciences of Ukraine, 27 Zabolotny Street, 03680 Kyiv, Ukraine

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We use numerically exact computer simulations of multiple scattering in physically realistic models of sparse discrete random media to quantify the errors of the scalar approximation (SA) in computations of coherent backscattering (CB) assuming that the incident light is unpolarized. We show that while the SA errors in the diffuse backscattered intensity are often small, those in the CB enhancement factor can reach 25\% and often exceed 20\%. We attribute this to the fact that the computation of the enhancement factor involves all diagonal elements of the diffuse backscattering Stokes matrix rather than only its (1, 1) element. Therefore, the coherent enhancement of backscattered intensity appears to be the result of a complex interplay of various polarization effects involved in the process of multiple scattering. Thus our numerical data make a strong case against the use of the SA in theoretical computations of CB in the case of unpolarized incident light.

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I. INTRODUCTION

Although the (single) scattering of an electromagnetic wave by a particle is expressly described by the vector macroscopic Maxwell equations [1–4], the scalar approximation (SA) is widely used in theoretical treatments of multiple scattering by particulate media [5–24]. Usually this is done when the incident light is unpolarized and only the intensity of the scattered light is being analyzed. It is then expected that the effects of polarization are minimal and can largely be ignored. The case for using the SA appears to be especially compelling when the scattered light is also unpolarized. This can happen, for example, when the directions of incidence and scattering are normal to the boundary of a plane-parallel particulate medium.

The errors of the SA in radiative transfer computations of diffuse multiple scattering by sparse discrete random media have been studied comprehensively in [25–28]. However, a thorough numerical analysis of the scalar treatment of the effect of coherent backscattering (CB) [19,23] has never been published and is, therefore, the main objective of this paper.

The rigorous vector theory of multiple scattering in discrete random media is extremely complicated [20,27,29–33] and is not yet suitable for massive computations of the full angular profile of CB for a representative variety of physically realistic models. Therefore, we will restrict this paper to an analysis of SA errors in the amplitude of the CB intensity peak. In this case, one can exploit the result of [34,35] according to which all parameters of CB at the exact backscattering direction are rigorously expressed in terms of the solution of the vector radiative transfer equation (VRTE) provided that the scattering medium is composed of widely separated, randomly positioned particles [27,36]. The VRTE can be efficiently solved on computers with any desired degree of accuracy [27,37], thereby providing numerically exact values of the amplitude of the CB intensity peak [27,38–41].

II. BASIC FORMULAS

Let the discrete scattering medium be a homogeneous semi-infinite slab composed of sparsely and randomly distributed particles. The slab is illuminated by a quasimonochromatic parallel beam of light of infinite lateral extent incident in the direction of the unit vector \( \hat{n}_0 = (\theta_0, 0, \varphi_0) \), where \( \theta_0 \) is the corresponding zenith angle measured from the positive direction of the \( x \) axis, and \( \varphi_0 \) is the corresponding azimuth angle measured from the positive direction of the \( x \) axis in the clockwise sense when looking in the positive direction of the \( z \) axis (Fig. 1). The Stokes column vector has four Stokes parameters as its components: \( \mathbf{I} = [I, Q, U, V] \), where \( T \) stands for “transposed.” Let \( \mathbf{R}_n \) be the 4 × 4 Stokes reflection matrix for exactly the backscattering direction \( \hat{n}_b = (\theta = \pi - \theta_0, \varphi_0 = \pi) \). This matrix yields the specific...
cific Stokes column vector of the backscattered light as follows:

$$\mathbf{I}_b = \frac{1}{\pi} \mu_0 \mathbf{R}_b \mathbf{I}_0,$$

(1)

where $\mu_0 = -\cos \theta_b$ and $\mathbf{I}_0$ is the Stokes column vector of the incident beam. In what follows we will assume that the incident light is unpolarized and that $\mathbf{I}_0 = [1 \ 0 \ 0 \ 0]^T$. Under the simplifying assumption of a macroscopically isotropic and mirror-symmetric particulate medium, the backscattering matrix $\mathbf{R}_b$ has the following block-diagonal structure [27]:

$$\mathbf{R}_b = \begin{bmatrix} R_{b11} & R_{b12} & 0 & 0 \\ R_{b12} & R_{b22} & 0 & 0 \\ 0 & 0 & R_{b33} & R_{b34} \\ 0 & 0 & -R_{b34} & R_{b44} \end{bmatrix}.$$  

(2)

In accordance with the microphysical theory of coherent backscattering by sparse discrete random media [27], the backscattering Stokes matrix $\mathbf{R}_b$ can be decomposed as follows:

$$\mathbf{R}_b = \mathbf{R}_b^1 + \mathbf{R}_b^M + \mathbf{R}_b^C,$$

(3)

where $\mathbf{R}_b^1$ is the contribution of the first-order scattering, $\mathbf{R}_b^M$ is the diffuse component consisting of all the ladder terms of scattering orders $\geq 2$, and $\mathbf{R}_b^C$ is the cumulative contribution of all the cyclical terms. The matrices $\mathbf{R}_b^1$ and $\mathbf{R}_b^M$ can be found by solving the VRTE [27] using the numerically exact technique outlined in [39,42]. Then the matrix $\mathbf{R}_b^C$ can be determined from the following exact relation derived in [35]:

$$\mathbf{R}_b^C = \begin{bmatrix} R_{b11}^C & R_{b12}^C & 0 & 0 \\ R_{b12}^C & R_{b22}^C & 0 & 0 \\ 0 & 0 & R_{b33}^C & R_{b34}^M \\ 0 & 0 & -R_{b34} & R_{b44}^C \end{bmatrix},$$

(4)

where

$$R_{b11}^C = \frac{1}{2} (R_{b11}^M + R_{b22}^M - R_{b33}^M + R_{b44}^M),$$

(5)

$$R_{b22}^C = \frac{1}{2} (R_{b11}^M + R_{b22}^M + R_{b33}^M - R_{b44}^M),$$

(6)

$$R_{b33}^C = \frac{1}{2} (-R_{b11}^M + R_{b22}^M + R_{b33}^M + R_{b44}^M),$$

(7)

$$R_{b44}^C = \frac{1}{2} (R_{b11}^M + R_{b22}^M + R_{b33}^M + R_{b44}^M).$$

(8)

In the case of unpolarized incident light, the specific intensity reflected by the slab in the exact backscattering direction is given by

$$\bar{I}_b = \mu_0 R_{b11} = \mu_0 (R_{b11}^1 + R_{b11}^M + R_{b11}^C).$$

(9)

We can also write for the intensity of the surrounding diffuse background

$$\bar{I}_{bdiff} = \mu_0 (R_{b11}^M + R_{b11}^1).$$

(10)

Equations (9) and (10) can be used to define the enhancement factor as the ratio of the total specific intensity reflected in the exact backscattering direction to that of the diffuse background,

$$\xi_b = \frac{\bar{I}_b}{\bar{I}_{bdiff}} = \frac{R_{b11}^1 + R_{b11}^M + \frac{1}{2} (R_{b11}^M + R_{b22}^M - R_{b33}^M + R_{b44}^M)}{R_{b11}^M + R_{b11}^1}.$$

(11)

Importantly, the above formula for the enhancement factor corresponding to the case of unpolarized incident light involves all four diagonal elements of the diffuse multiple-scattering matrix $R_{b11}^M$ rather than only the $(1, 1)$ element. This makes Eq. (11) qualitatively different from the definition of the enhancement factor in the scalar approximation,

$$\tilde{\xi} = \frac{R_{b11}^1 + R_{b11}^M + R_{b11}^C}{R_{b11}^1 + R_{b11}^M} = 1 + \frac{R_{b11}^M}{R_{b11}^1 + R_{b11}^M},$$

(12)

where $R_{b11}^M$ and $R_{b11}^C$ are the single-scattering, diffuse multiple-scattering, and cyclical components of the scalar reflection coefficient. $R_{b11}^1$ and $R_{b11}^M$ can be found by solving the scalar radiative transfer equation.

In the case of grazing incidence and/or a small single-scattering albedo $\tilde{\omega}$, the main contribution to the backscattered diffuse radiation comes from the singly scattered light. This means that in the limit $\mu_0 \rightarrow 0$ and/or with $\tilde{\omega} \rightarrow 0$, $R_{b11}^M$ decreases and ultimately vanishes in comparison with $R_{b11}^1$, which then implies that

$$\lim_{\mu_0 \rightarrow 0} \xi_b = \lim_{\tilde{\omega} \rightarrow 0} \tilde{\xi} = 1.$$ 

(13)

Analogously,

$$\lim_{\mu_0 \rightarrow 0} \tilde{\xi} = \lim_{\tilde{\omega} \rightarrow 0} \xi_b = 1.$$ 

(14)

### III. NUMERICAL RESULTS

The results of our extensive numerical computations are summarized in Figs. 2–5. The particles forming the semi-infinite scattering medium are assumed to be polydisperse spheres with a complex relative refractive index $m = m_R + i m_I$, where $i = \sqrt{-1}$. The dispersion of particle sizes is described by the simple gamma distribution.
The effective radius and effective variance of the size distribution are defined by

\[ r_{\text{eff}} = \frac{1}{\langle G \rangle} \int_0^\infty dr(r) r \pi r^2 = a \]  
\[ \nu_{\text{eff}} = \frac{1}{\langle G \rangle r_{\text{eff}}^2} \int_0^\infty dr(r)(r - r_{\text{eff}})^2 \pi r^2 = b, \]

respectively, where

\[ n(r) = \text{const} \times r^{(1-3b)/b} \exp\left(-\frac{r}{ab}\right), \quad b \in (0, 0.5). \]  
\[ \langle G \rangle = \int_0^\infty dr(r) \pi r^2 \]

\( \langle G \rangle \) is the average area of the geometrical projection per particle \( \langle G \rangle \). The results are shown for \( m_0 \in [0, 1] \); \( m_R = 1.2, 1.4, 1.6, 1.8, \) and 2; \( m_I = 0, 0.002, 0.01, \) and 0.3; \( \nu_{\text{eff}} = 0.2 \) and \( x_{\text{eff}} \) \( \in [0, 30] \), where \( x_{\text{eff}} = 2 \pi r_{\text{eff}} / \lambda \) is the dimensionless effective size parameter and \( \lambda \) is the wavelength of light in the non-absorbing medium surrounding the particles. The particle refractive index and effective size parameter ranges covered are quite broad and make our result representative of many situations encountered in practice.

Figures 2 and 4 show, respectively, the “vector” enhancement factor \( \zeta_f \) and the “vector” diffuse specific intensity \( I_{\text{diff}} \).
Figure 3 shows the percent error of the scalar approximation in the enhancement factor defined as
\[ \delta_\xi = \left| \frac{\xi_\text{approx} - \xi_\text{exact}}{\xi_\text{approx}} \right| \times 100\% , \]
while Fig. 5 shows the corresponding percent error in the diffuse specific intensity,
\[ \delta_\iota = \left| \frac{\iota_\text{approx} - \iota_\text{exact}}{\iota_\text{approx}} \right| \times 100\% . \]

IV. DISCUSSION AND CONCLUSIONS

The main traits of the enhancement factor \( \xi_\iota \) (Fig. 2) and the diffuse backscattered intensity \( \tilde{\iota}_b \) (Fig. 4) for polydisperse spherical particles have been analyzed in [27,38,39] and will not be discussed here. We only mention that the results shown in Fig. 2 satisfy the limits of Eq. (13) (note that the limit \( \tilde{\omega} \to 0 \) can be physically realized only for absorbing Rayleigh scatterers with \( x_{\text{eff}} \to 0 \)).

The results depicted in Fig. 5 confirm the main conclusions of [25–28] and show that in the case of a moderately absorbing discrete random medium, the errors of the scalar approximation in the diffuse specific intensity are maximal for Rayleigh or quasi-Rayleigh particles and rapidly decrease with increasing \( x_{\text{eff}} \). Our computations (not shown here) also indicate that the sign of the difference \( R_{b11}^1 + R_{b11}^M - R_b^1 - R_b^M \) is always positive whenever \( \delta_\iota > 1\% \), which means that the scalar approximation tends to underestimate the backscattered diffuse specific intensity. Figure 5 implies that...
in most cases $\delta_t$ does not exceed a few percent, which makes the scalar approximation quite applicable given the typical accuracy of laboratory and remote-sensing photometers.

In contrast, the errors of the scalar approximation in the CB enhancement factor can be quite significant (cf. [43]) and often exceed 20% (Fig. 3). The errors are especially large for nonabsorbing particles (the left-hand column of Fig. 3) and can reach 25%. Increasing absorption suppresses multiple scattering, thereby making both $\zeta_t$ and $\zeta$ closer to unity and resulting in smaller $\delta_t$. The same, obviously, happens in the limit $\mu_0 \to 0$. Large nonabsorbing spherical particles with $m_R=1.8$ and 2 develop a strong backscattering peak in the single-scattering phase function (see, e.g., Fig. 9.22 in [3]).

As a consequence, $I_{\text{diff}}$ strongly increases, whereas $\zeta_t$, $\zeta$, and $\delta_t$ decrease. The case of $m_R=1.6$ in Fig. 3 appears to be especially interesting in that the SA errors for $m_l=0$ and 0.002 become size-parameter-independent for $x_{\text{eff}} > 10$. Also our computations show that in most cases the ratio $(\zeta_t - \zeta_t)/\zeta_t$ is negative, with the exception of particles with $m_R=1.2$ and 1.4, $m_l=0.3$, and $x_{\text{eff}}<3$, for which it becomes slightly positive. This means that the scalar approximation tends to overestimate the enhancement factor.

The SA errors in the CB enhancement factor for the case of unpolarized light are so large that one should exercise extreme caution when using this approximation. We would even submit that this approximation should not be used at all. This conclusion should have significant practical ramifications, especially in passive planetary and terrestrial remote sensing since the natural sunlight is essentially unpolarized.
It is not immediately obvious to us why the SA errors in the CB enhancement factor are so large whereas those in the backscattered diffuse intensity are often much smaller. Again, Eq. (11) shows that the rigorous computation of \( \xi_f \) involves all the diagonal elements of the matrix \( R^M \), thereby making the CB enhancement factor the result of a complex interplay of various polarization effects involved in the process of multiple scattering. One instructive manifestation of this complexity is the somewhat counterintuitive fact that \( \xi_f \) reaches maximal values for moderately absorbing \( m_I = 0.01 \) rather than for nonabsorbing \( m_I = 0 \) particles (Fig. 2).

Our final comment concerns potential packing density effects. The above numerical results have been obtained under the assumption that the discrete random medium is sparse and is composed of widely separated particles \([27,34]\), whereas many real media (such as particulate surfaces and liquid particle suspensions) may consist of rather densely packed scatterers. However, comparisons of low-density theoretical results and actual laboratory data \([34]\) as well as recent exact numerical computations of multiple scattering by densely packed random particle groups \([44]\) suggest that the main conclusions of this paper should remain valid even when the particle packing density deviates from zero significantly.

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ACCURACY OF THE SCALAR APPROXIMATION IN...