On the Shapes of Interstellar Grains: Modeling Extinction and Polarization by Spheroids and Continuous Distributions of Ellipsoids

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ABSTRACT

Although interstellar grains are known to be aspherical, their actual shapes remain poorly constrained. We assess whether three distributions of ellipsoidal shapes from the literature, employed principally for their convenient mathematical properties, are suitable for describing the shapes of interstellar grains. Randomly-selected shapes from each distribution are shown as illustrations. The often-used BHCDE distribution includes a very large fraction of extreme shapes: fully 10% of random draws have axial ratio $a_3/a_1 > 19.7$, and 5% have $a_3/a_1 > 33$. Of the three distributions considered, the CDE2 appears to be most realistic. For each of the three CDEs considered, we derive shape-averaged cross sections for extinction and polarization. Finally, we describe a method for “synthesizing” a dielectric function for an assumed shape or shape distribution if the actual absorption cross sections per grain volume are known from observations. This synthetic dielectric function predicts the wavelength dependence of polarization, which can then be compared to observations to constrain the grain shape.

Subject headings: dust, extinction, radiative transfer, infrared: ISM

1. Introduction

After many years of study, both the composition and the geometry (shape, porosity) of interstellar grains remain elusive. While meteorites can provide samples of presolar grains that were part of the interstellar grain population at the time of formation of the solar system, the surviving particles may not be representative, and the sampling techniques are biased toward large “stardust” grains with isotopic anomalies. Interstellar grains collide with interplanetary spacecraft, providing
some information on elemental composition, but the data are limited and generally involve vaporization of the impinging particle, leaving both mineralogy and preimpact morphology uncertain (e.g., Altobelli et al. 2016). The Stardust mission captured some particles relatively intact (Westphal et al. 2014a,b), but dynamical considerations argue against these particles having come from the interstellar medium (Silsbee & Draine 2016).

As a result, our knowledge of interstellar grains is based almost entirely on (1) evidence of elements that have been “depleted” from interstellar gas and incorporated into dust grains, and (2) observations of the interaction of electromagnetic waves with the interstellar grains – absorption, scattering, and emission.

Observations of absorption and scattering near X-ray absorption edges (e.g., Lee 2010; Pinto et al. 2013; Valencic & Smith 2013; Zeegers et al. 2017) can in principle provide chemical information, but X-ray spectra with very high energy resolution ($\lesssim 2$ eV) and high signal/noise ratio are required to reliably discriminate between different candidates. At this time interpretation of the X-ray spectra remains uncertain.

In the ultraviolet, the prominent extinction peak near 2175Å strongly suggests $sp^2$-bonded carbonaceous material (as in graphite or polycyclic aromatic hydrocarbons) but the absorbing material has not yet been definitively identified. In the infrared, a weak absorption feature at $3.4\mu m$ is generally accepted as being due to the aliphatic C-H stretching mode, but once again the actual hydrocarbon material remains conjectural.

Strong and broad absorption features near 10$\mu m$ and 18$\mu m$ are securely identified as arising from amorphous silicate material, but the composition and structure of this silicate are uncertain. However, elemental abundances and the strength of the feature imply that this amorphous silicate material accounts for $\sim 2/3$ of the total dust mass in the diffuse ISM.

In addition to not knowing the composition, we are also uncertain about the geometry (i.e., morphology) of the grains. Polarized extinction at optical wavelengths, polarization of the 10$\mu m$ feature, and polarized thermal emission from dust in the far-infrared and submm require that at least some interstellar grains be both appreciably nonspherical and aligned with the local magnetic field. However, it has been difficult to determine how nonspherical the grains are, as well as whether the grains are typically compact vs. highly porous.

The present work has two aims. The first goal is to discuss the optics of ellipsoidal particles in the “electric dipole” or “Rayleigh” limit. Continuous distributions of spheroidal or ellipsoidal shapes have been considered in some previous studies, but the discussions have been limited to absorption cross sections, with little said about the actual distribution of shapes. Here we explicitly discuss the distribution of shapes associated with three particular continuous distributions of ellipsoids (CDEs). We also derive the polarization cross sections for the CDEs when the grains are not randomly oriented.

The second aim is to present a method for using observational constraints on absorption at
long wavelengths, plus a prior estimate of the dielectric function at shorter wavelengths, to derive the complex dielectric function $\epsilon(\lambda)$ at long wavelengths $\lambda$. Absorption and polarization by grains both depend on the grain shape, or distribution of shapes. If we knew the dielectric function $\epsilon(\lambda)$, we could infer the actual grain shape by computing absorption vs. $\lambda$ for different assumed shape distributions, and seeing which assumed distribution agrees with observations. However, because the actual grain materials remain unknown, we don’t know $\epsilon(\lambda)$, and hence cannot use that approach to deduce the grain shape. However, if we have observations of both absorption and polarization, we can determine which shape distribution yields a dielectric function that is consistent with the observed absorption and polarization. We show here how this can be done.

The paper is organized as follows: absorption and polarization cross sections for ellipsoids in the long wavelength (Rayleigh) limit are reviewed in section 2. In section 3 we discuss the properties of three continuous distributions of ellipsoidal shapes – the BHCDE, ERCDE, and CDE2 distributions – and present images of shapes drawn randomly from each of these distributions. Analytic results for polarized absorption cross sections are presented in sections 4 and 5. Attenuation and polarization by a medium with partial grain alignment is discussed in section 6. The results obtained here apply only in the electric dipole limit, and the validity of this approximation is checked in section 7. In section 8 we discuss how the results obtained here can be employed, together with other constraints, to obtain a self-consistent dielectric function given observations of absorption as a function of wavelength. Our results are summarized in section 9. Certain technical results are collected in Appendices A–D.

2. Absorption in the Electric Dipole Limit

In the electric dipole limit (grain size $\ll$ wavelength $\lambda$), the interaction of a grain with an incident electromagnetic wave is fully characterized by the grain’s electric polarizability tensor (see, e.g., Draine & Lee 1984). Here we review the dependence of this polarizability tensor on the grain shape.

2.1. Ellipsoidal Grains

Consider an ellipsoidal grain with semimajor axes $a_1 \leq a_2 \leq a_3$ and volume $V = (4\pi/3)a_1a_2a_3$. Let $\hat{\mathbf{a}}_1, \hat{\mathbf{a}}_2, \hat{\mathbf{a}}_3$ be unit vectors along the three principal axes. We define an effective radius $a_{\text{eff}} \equiv (3V/4\pi)^{1/3} = (a_1a_2a_3)^{1/3}$.

The grain material is assumed to have an isotropic complex dielectric function $\epsilon(\lambda) = \epsilon_1 + i\epsilon_2$, where $\epsilon_1(\lambda)$ and $\epsilon_2(\lambda)$ are the real and imaginary parts of $\epsilon$, and $\lambda$ is the wavelength in vacuo. In the long-wavelength limit $a_3 \ll \lambda$, the electric polarizability tensor for radiation with $\mathbf{E} \parallel \hat{\mathbf{a}}_j$ is
\[ \alpha_{ij} = A_j V / 4\pi, \] where

\[ A_j(\epsilon) = \frac{\epsilon - 1}{1 + L_j(\epsilon - 1)} \] (1)

with \( L_j \) given by (see, e.g., Bohren & Huffman 1983)

\[ L_j = \frac{1}{2} \int_0^\infty \frac{dx}{y_j^2 + x} \left[ (y_1^2 + x)(y_2^2 + x)(y_3^2 + x) \right]^{1/2} \] (2)

\[ y_j \equiv \frac{a_j}{(a_1 a_2 a_3)^{1/3}}. \] (3)

The \( L_j \), referred to variously as “geometrical factors”, “shape factors”, or “depolarization factors”, are determined by the axial ratios \( a_1/a_3 \) and \( a_2/a_3 \). The \( L_j \) satisfy

\[ L_1 + L_2 + L_3 = 1. \] (4)

If \( a_1 \leq a_2 \leq a_3 \), then

\[ L_1 \geq L_2 \geq L_3. \] (5)

The absorption cross section for radiation with \( \mathbf{E} \parallel \hat{a}_j \) is simply

\[ C_{\text{abs}, j} = \frac{2\pi V}{\lambda} \text{Im}(A_j). \] (6)

After propagating a distance \( z \) through a medium with dust number density \( n_d \), a plane wave will undergo both attenuation (due to absorption) and a phase shift relative to propagation in vacuo. The phase shift (in radians) will be \( n_d C_{\text{pha}} z \), where

\[ C_{\text{pha}, j} = \frac{\pi V}{\lambda} \text{Re}(A_j). \] (7)

The axes \( \hat{a}_1, \hat{a}_2, \hat{a}_3 \) coincide with the principal axes of the moment of inertia tensor, with eigenvalues \( I_1 \geq I_2 \geq I_3 \). The absorption cross sections for \( \mathbf{E} \parallel \hat{a}_1 \) and \( \mathbf{E} \perp \hat{a}_1 \) are

\[ \begin{align*}
C_\parallel &\equiv C_{\text{abs}}(\mathbf{E} \parallel \hat{a}_1) = \frac{2\pi V}{\lambda} \text{Im}(A_1), \\
C_\perp &\equiv C_{\text{abs}}(\mathbf{E} \perp \hat{a}_1) = \frac{2\pi V}{\lambda} \text{Im} \left( \frac{A_2 + A_3}{2} \right),
\end{align*} \] (8) (9)

where the grains are assumed to be spinning or tumbling with \( \hat{a}_2 \) and \( \hat{a}_3 \) randomly-distributed in the plane \( \perp \) to \( \hat{a}_1 \). For randomly-oriented grains the absorption cross section is

\[ C_{\text{ran}} = \frac{C_\parallel + 2C_\perp}{3} = \frac{2\pi V}{\lambda} \text{Im}(A_1 + A_2 + A_3)/3. \] (10)

Interstellar grains are generally spinning rapidly, and it is appropriate to time-average over the tumbling of the grain. The direction of the grain axis \( \hat{a}_1 \) may be correlated with the angular momentum vector \( \mathbf{J} \); if the grains are in suprathermal rotation, \( \hat{a}_1 \) will tend to be aligned with \( \mathbf{J} \), as originally pointed out by Purcell (1979).
Consider the limiting case of spinning grains that are perfectly-aligned with $\hat{a}_1 \parallel \mathbf{J}$. For unpolarized radiation propagating with $\mathbf{K} \perp \mathbf{J}$, the polarization-averaged absorption cross section is

$$C_{\text{abs}} = \frac{C_\perp + C_\parallel}{2} = \frac{\pi V \text{Im}(A_2 + A_3 + 2A_1)}{2}. \quad (11)$$

The difference in absorption cross sections will produce linear polarization, characterized by the “polarization cross section”

$$C_{\text{pol}} = \frac{C_\perp - C_\parallel}{2} = \frac{\pi V \text{Im}(A_2 + A_3 - 2A_1)}{2}. \quad (12)$$

There will also be a phase shift between the two linear polarizations. We define

$$\Delta C_{\text{pha}} = C_{\text{pha},\perp} - C_{\text{pha},\parallel} = \frac{\pi V \text{Re}(A_2 + A_3 - 2A_1)}{2}. \quad (13)$$

After propagating a distance $z$ through a medium with dust number density $n_d$, the phase difference between the modes will be $n_d\Delta C_{\text{pha}}z$.

If the direction of grain alignment rotates along the direction of propagation, radiation that is initially unpolarized will develop circular polarization (Martin 1972, 1974). We define a “circular polarization efficiency factor”

$$Q_{\text{cpol}} \equiv \frac{C_{\text{pol}}}{\pi a^{2}_{\text{eff}}} \times \frac{\Delta C_{\text{pha}}}{\pi a^{2}_{\text{eff}}}. \quad (14)$$

If the rotation angle is small, and the percentage linear polarization is small, the circular polarization after propagating a pathlength $z$ is

$$\frac{V}{I} \propto Q_{\text{cpol}} \times (n_d\pi a^{2}_{\text{eff}}z)^2. \quad (15)$$

### 2.2. Spheroids

Prolate spheroids have $a_1 = a_2 < a_3$, and oblate spheroids have $a_1 < a_2 = a_3$. The “shape factors” $L_j$ are given by (van de Hulst 1957)

**prolate**: $L_3 = \frac{1 - e^2}{e^2} \left[ \frac{1}{2e} \ln \left( \frac{1 + e}{1 - e} \right) - 1 \right] < 1/3, \quad e^2 \equiv 1 - \left( \frac{a_1}{a_3} \right)^2 \quad (16)$

$$L_1 = L_2 = \frac{1 - L_3}{2} \quad (17)$$

**oblate**: $L_1 = \frac{1 + e^2}{e^2} \left[ 1 - \frac{1}{e} \arctan(e) \right] > 1/3, \quad e^2 \equiv \left( \frac{a_3}{a_1} \right)^2 - 1 \quad (18)$

$$L_2 = L_3 = \frac{1 - L_1}{2}. \quad (19)$$

A sphere has $(L_1, L_2, L_3) = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$; the prolate limit (needle-like) has $(L_1, L_2, L_3) = (\frac{1}{2}, \frac{1}{2}, 0)$; the oblate limit (disk-like) has $(L_1, L_2, L_3) = (1, 0, 0)$. 

3. Continuous Distributions of Ellipsoids

3.1. Shape Factors

![Graph showing the domain of allowed shape factors \((L_1, L_2)\). The shaded region is the domain where \(L_3 \leq L_2 \leq L_1\) (see text). Other regions, numbered 2-6, correspond to the other possible orderings of \(L_1, L_2, L_3\).](image)

Every ellipsoidal shape is uniquely specified by its triplet of depolarization factors \((L_1, L_2, L_3)\). Consider a population of ellipsoidal grains, each with the same volume \(V\), but with some continuous distribution of axial ratios – this is referred to as a “continuous distribution of ellipsoids” (CDE). Suppose that each grain has principal axes labelled 1,2,3 arbitrarily, and that \(G(\ell_1, \ell_2)d\ell_1d\ell_2\) is the fraction of the population with \(L_1 \in [\ell_1, \ell_1 + d\ell_1]\) and \(L_2 \in [\ell_2, \ell_2 + d\ell_2]\). The function \(G\) is non-negative (\(G \geq 0\)) and normalized: \(\int G(L_1, L_2)dL_2dL_2 = 1\) over the allowed \((L_1, L_2)\) domain. If labels 1,2,3 were assigned arbitrarily, the function \(G\) must satisfy symmetry requirements, including \(G(L_1, L_2) = G(L_2, L_1) = G(L_1, 1 - L_1 - L_2)\) but otherwise we have no a-priori knowledge of the function \(G\), other than expecting that very extreme axial ratios should be rare.

\[\text{Fig. 1.— The domain of allowed shape factors } (L_1, L_2). \text{ The shaded region is the domain where } L_3 \leq L_2 \leq L_1 \text{ (see text). Other regions, numbered 2-6, correspond to the other possible orderings of } L_1, L_2, L_3.\]

\[\text{\(^2\) One can also consider functions } G \text{ that do not satisfy these symmetry requirements, but in this case one must restrict discussion to only one of the six subregions in Figure \[\]\]}

Various distributions of shapes have been considered in the literature, including continuous distributions of spheroids (Treffers & Cohen 1974; Min et al. 2003), and continuous distributions of ellipsoids (CDEs). Bohren & Huffman (1983) gave a lucid introduction to CDEs in general, and presented a simple illustrative example, referred to here as the BHCDE. We discuss the BHCDE and two other distributions of ellipsoids that have been considered in the astrophysical literature.

1. BHCDE: The simplest functional form

\[
G(L_1, L_2) = 2 \quad \text{for } L_1 \geq 0, L_2 \geq 0, L_1 + L_2 \leq 1 \tag{20}
\]

is often considered; Bohren & Huffman (1983) present this as an example, and it has subsequently been applied by a number of authors (e.g., Rouleau & Martin 1991; Alexander & Ferguson 1994; Min et al. 2003, 2006; Sargent et al. 2006; Min et al. 2008; Rho et al. 2017). Because \( G(L_1, L_2) \) is independent of \( L_1 \) and \( L_2 \), it is sometimes asserted that “all shapes are equally probable” (Bohren & Huffman 1983) or “all shapes are equally weighted” (Sargent et al. 2006), seemingly suggesting that this is a “fair” sampling of ellipsoidal shapes. While it is correct that all ellipsoidal shapes are present, it is not clear how “all shapes are equally probable” is to be understood, given that shapes are not discrete and there is no commonly accepted metric for “shape space”. Furthermore, even if the depolarization factor \( L \) is taken as the relevant measure for shape, we will see below that the BHCDE distribution is not actually uniform in \( L \) (despite \( G \) being independent of \( L \)).

Although having the virtue of analytic simplicity, we will see below that the BHCDE distribution has an extreme representation of very elongated shapes, with \( L \to 0 \). We will argue that the BHCDE distribution seems unlikely to approximate grain shape distributions in nature, whether for desert sand or interstellar dust.

2. ERCDE: Zubko et al. (1996) proposed eliminating the most extreme shapes by truncating the distribution (20):

\[
G(L_1, L_2) = \frac{2}{(1 - 3L_{\text{min}})^2} \quad \text{for } L_1 \geq L_{\text{min}}, L_2 \geq L_{\text{min}}, L_1 + L_2 \leq 1 - L_{\text{min}} , \tag{21}
\]

referring to this as the “externally-restricted CDE” (ERCDE). \( L_{\text{min}} \) is a free parameter. While removing extreme shapes with \( L_j \to 0 \) or \( L_j \to 1 \) is desirable, the ERCDE distribution still seems unphysical, as we will see below. Note that if \( L_{\text{min}} \to 0 \), the ERCDE \( \to \) BHCDE.

3. CDE2: Ossenkopf et al. (1992) proposed the distribution

\[
G(L_1, L_2) = 120L_1L_2L_3 = 120L_1L_2(1 - L_1 - L_2) \quad \text{for } L_1 \geq 0, L_2 \geq 0, L_1 + L_2 \leq 1 , \tag{22}
\]

which has the desirable behavior \( G \to 0 \) for \( L_3 \to 0 \) and \( L_1 \to 1 \). This distribution was subsequently referred to as “CDE2” (Fabian et al. 2001; Sargent et al. 2006), and we shall so refer to it here.

The distribution functions \( G(L_1, L_2) \) for these three CDEs are shown in Figure 2.
3.2. Shape Distributions

Because the optical properties of ellipsoids in the limit \( \alpha \ll \lambda \) are determined by \( L_1, L_2, \) and \( L_3 = 1 - L_1 - L_2, \) most discussions of CDEs have been concerned only with the distribution of \( L_j \) values, rather than the distributions of the ellipsoid axial ratios. However, it is of interest to examine the distributions of actual grain shapes that correspond to the BHCDE, ERCDE, and CDE2 distributions.

For a given set of axial ratios \( (a_2/a_1, a_3/a_1) \), the \( L_j \) values can be obtained by numerical quadrature (Bohren & Huffman 1983). Since there does not appear to be any direct way to invert Eq. (2) to obtain \( (a_2/a_1, a_3/a_1) \) from given \( (L_1, L_2) \), we have implemented a numerical procedure to find \( (a_2/a_1, a_3/a_1) \) corresponding to given \( (L_1, L_2) \). In Appendix D, we demonstrate that any solution found in this way is unique.

Table 1: Long/Short Axis Ratio \( a_3/a_1 \)

|        | BHCDE | ERCDE\(^b\) | CDE2 |
|--------|-------|-------------|------|
| mode\(^a\) | 3.26  | 3.27        | 2.24 |
| median | 4.58  | 3.35        | 2.73 |
| 25%    | 9.23  | 5.07        | 4.25 |
| 10%    | 19.7  | 6.97        | 6.72 |
| 5%     | 32.97 | 8.32        | 9.11 |
| 1%     | 98.49 | 10.92       | 17.11|

\(^a\) Maximum of \( dP/d\ln(a_3/a_1) \).

\(^b\) \( L_{\text{min}} = 0.05 \).

We continue to adopt the ordering \( a_1 \leq a_2 \leq a_3, L_1 \geq L_2 \geq L_3 \). We draw \( (L_1, L_2) \) values randomly according to the BHCDE, ERCDE, or CDE2 distributions, and for each \( (L_1, L_2) \) find the corresponding axial ratios \( (a_2/a_1, a_3/a_1) \). Figure 3 shows 20 examples selected randomly from each
Fig. 3.—20 randomly-selected ellipsoids drawn from the BHCDE, ERCDE, and CDE2 distributions. All examples have equal volume. 3 views are shown for each shape: viewed along the short axis $\hat{a}_1$ (top row), and along the $\hat{a}_3$ and $\hat{a}_2$ axes (2nd and 3rd rows). For each distribution the 20 random shapes are shown in order of increasing $a_3/a_1$ (left to right).

of these shape distributions. Figure 4a shows the distribution of long/short axial ratios $a_3/a_1$ for the BHCDE, ERCDE (with $L_{\text{min}} = 0.05$), and CDE2 distributions. Figure 4b shows the cumulative distribution function of axial ratios $a_3/a_1$, and Figure 5 shows the distributions of axial ratios for the BHCDE, ERCDE, and CDE2 distributions. Some characteristics of these shape distributions are listed in Table 1.

The BHCDE distribution has a very large fraction of extreme axial ratios – Figure 4b shows that 10% of the realizations have $a_3/a_1 > 19.7$, and 1% of the realizations have $a_3/a_1 > 98.5$. The actual shape distribution for interstellar grains is of course unknown, but it seems unlikely to include as large a fraction of extreme aspect ratios as the BHCDE distribution. The CDE2 (with $\sim$90% of the draws having $a_3/a_1 < 6.72$) or ERCDE (with $\sim$90% of the draws having $a_3/a_1 < 6.9$ for $L_{\text{min}} = 0.05$) may be more plausible shape distributions to consider for interstellar dust grains.
Fig. 4.— (a) Distribution of long/short axial ratio $a_3/a_1$ for three continuous distributions of ellipsoids. The ERCDE with $L_{\text{min}} = 0.05$ has a maximum allowed axial ratio $a_3/a_1 = 14$, but the CDE2 and BHCDE distributions both extend to infinite axial ratios. The BHCDE distribution has a much larger representation of extreme axial ratios. (b) Cumulative distribution functions. For the BHCDE distribution, 10% of the realizations have $a_3/a_1 > 19.7$, and 1% have $a_3/a_1 > 98.5$.

4. Polarization by CDEs

The observed polarization of starlight by dust, and of submm emission from dust, indicates that interstellar grains spin with their short axis tending to be aligned with the local magnetic field $\mathbf{B}$; this occurs because the grain’s angular momentum $\mathbf{J}$ aligns with the magnetic field, and the short axis of the grain aligns with $\mathbf{J}$. Rotation, nutation, and precession of $\mathbf{J}$ around $\mathbf{B}$ are all rapid. In order to discuss polarization by a population of partially-aligned grains, we require the distribution of depolarization factors separately for the short axis, and for the other two axes.

It is useful to restrict consideration to the ordering $0 \leq L_3 \leq L_2 \leq L_1 \leq 1$: for each ellipsoid, $j = 3$ corresponds to the long axis, $j = 1$ to the short axis, and $j = 2$ to the intermediate axis. Let $g_j(\ell)d\ell$ be the fraction of ellipsoids with $L_j \in [\ell, \ell + d\ell]$. The distribution functions $g_1, g_2, g_3$ can be obtained from $G$, as discussed in Appendix [A]. Figure 6 shows $g_1, g_2, g_3$ for the BHCDE, ERCDE, and CDE2 shape distributions.
Fig. 5.— Distributions of axial ratios $a_3/a_2$ and $a_2/a_1$ for the BHCDE, ERCDE ($L_{\text{min}} = 0.05$), and CDE2 shape distributions. Oblate spheroids have $a_3/a_2 = 1$, and prolate spheroids have $a_2/a_1 = 1$.

4.1. The BHCDE Distribution

Figure 6a shows the distribution functions $g_j$ for the BHCDE distribution. We see that $g_3(\ell)$ peaks at $\ell = 0$, corresponding to infinitely elongated needles: fully 10% of the ellipsoids have $L_3 < 0.0171$. Only very extreme shapes have such small values of $L_3$ – for example, a prolate spheroid with axial ratios 1:1:11.17 has $L_3 = 0.0171$. Another example with $L_3 = 0.0171$ would be an ellipsoid with axial ratios 1:4.72:22.3. It does not seem likely (to us) that interstellar grains will have such a large fraction of very elongated shapes.

4.2. The ERCDE Distribution

The ERCDE distribution is similar to the BHCDE distribution, except that cases with $L < L_{\text{min}}$ are excluded. Thus $L_{\text{min}}$ is a free parameter for the ERCDE distribution. The ERCDE distribution has $g_3$ peaking at $L_3 = L_{\text{min}}$. As an example, we consider $L_{\text{min}} = 0.05$ (see Figure 6c).

What shapes would correspond to the limiting cases $L_3 = L_{\text{min}}$? One example of a shape with $L_3 = 0.05$: a prolate spheroid with axial ratios 1:1:5.41 (with $L_1 = L_2 = 0.475$, $L_3 = 0.05$). Another example: an oblate spheroid with axial ratios 1:14.43:14.43 (with $L_1 = 0.9$, $L_2 = L_3 = 0.05$). A third example: an ellipsoid with axial ratios 1:2.965:8.79 (with $L_1 = 0.719$, $L_2 = 0.231$, $L_3 = 0.05$). Fully 10% of the ERCDE realizations with $L_{\text{min}} = 0.05$ have $L_3 < 0.06454$. Thus the ERCDE shape distribution also appears to overrepresent extreme shapes, unless $L_{\text{min}} \gtrsim 0.10$. The ERCDE shape distribution will be further discussed below.
4.3. The CDE2 Distribution

The distribution functions $g_j$ for the smooth CDE2 distribution are shown in Figure 6c. While the CDE2 does include extreme shapes, it has $g_3 \to 0$ for $L_3 \to 0$, and $g_1 \to 0$ for $L_1 \to 1$. 10% of the realizations have $L_3 < 0.06185$, so it is somewhat similar to the ERCDE with $L_{\text{min}} = 0.05$ in the representation of extreme shapes, although the CDE2 distribution function has the virtue of smoothness.

The mean values of the depolarization factors for the CDE2 distribution are $\langle L_1 \rangle = 0.5355$, $\langle L_2 \rangle = 0.3040$, and $\langle L_3 \rangle = 0.1605$, corresponding to an ellipsoid with axial ratios $1:1.664:2.716$. 
5. Absorption Cross Sections for the BHCDE, ERCDE and CDE2 Distributions

The shape-averaged absorption cross section associated with axis $j$ is

$$C_{\text{abs}}(E \parallel \hat{a}_j) = \frac{2\pi V}{\lambda} \text{Im}(\langle A_j \rangle) \quad (23)$$

$$\langle A_j \rangle \equiv \int A_j g_j(\ell) d\ell \quad , \quad (24)$$

where $A_j$ is given by Eq. (1).

5.1. Randomly-Oriented Particles

For randomly-oriented particles, the absorption cross section is

$$C_{\text{ran}} = \frac{2\pi V}{\lambda} \text{Im} \left[ \frac{\langle A_1 \rangle + \langle A_2 \rangle + \langle A_3 \rangle}{3} \right] \quad . \quad (25)$$

Bohren & Huffman (1983) obtained the absorption cross section for randomly-oriented grains with the BHCDE shape distribution:

$$\frac{C_{\text{ran}}^{\text{BHCDE}}}{V} = \frac{4\pi}{\lambda} \text{Im} \left[ \left( \frac{1 + x}{x} \right) \ln \epsilon \right] \quad , \quad (26)$$

where $x \equiv \epsilon - 1$. For the ERCDE (Eq. (21)) the absorption cross section for randomly-oriented grains was obtained by Zubko et al. (1996):

$$\frac{C_{\text{ran}}^{\text{ERCDE}}}{V} = \frac{4\pi}{\lambda (1 - 3L_{\text{min}})^2} \text{Im} \left\{ \left( \frac{1}{x} + D \right) \ln \left[ \frac{1 + xD}{1 + xL_{\text{min}}} \right] \right\} \quad , \quad (27)$$

where $D \equiv 1 - 2L_{\text{min}}$. It is easily verified that this reduces to Eq. (26) for $L_{\text{min}} \rightarrow 0$.

For the CDE2 distribution (Eq. (22)) the absorption cross section for randomly-oriented ellipsoids was given by Fabian et al. (2001):

$$\frac{C_{\text{ran}}^{\text{CDE2}}}{V} = \frac{40\pi}{\lambda} \text{Im} \left[ \frac{1}{x^4} \left( -(1 + x)^3 \ln(1 + x) + x + \frac{5}{2} x^2 + \frac{11}{6} x^3 + \frac{1}{4} x^4 \right) \right] \quad . \quad (28)$$

5.2. Polarization Cross Sections for Aligned Particles

The polarization cross section (see Eq. [12]) is

$$C_{\text{pol}} \equiv \frac{\pi V}{\lambda} \text{Im} \left[ \frac{\langle A_2 \rangle + \langle A_3 \rangle - 2\langle A_1 \rangle}{2} \right] \quad . \quad (29)$$
For the BHCDE distribution, we find

$$C_{\text{BHCDE}} = \frac{C_{\text{pol}}}{V} = \frac{3\pi}{2\lambda} \text{Im} \left[ \frac{12}{x} \left( 1 + \frac{x}{2} \right) \ln \left( 1 + \frac{x}{2} \right) - \frac{9}{x} \left( 1 + \frac{x}{3} \right) \ln \left( 1 + \frac{x}{3} \right) - \frac{2}{x} \ln \left( 1 + x \right) \right]. \quad (30)$$

where $x \equiv \epsilon - 1$. For the ERCDE distribution we find

$$C_{\text{ERCDE}} = \frac{C_{\text{pol}}}{V} = \frac{3\pi}{2\lambda} \frac{1}{(1 - 3L_{\text{min}})^2} \text{Im} \left\{ 12 \left( \frac{1}{x} + B \right) \ln [1 + xB] - 9 \left( \frac{1}{x} + \frac{1}{3} \right) \ln \left[ 1 + \frac{x}{3} \right] - \left( \frac{1}{x} + D \right) \ln [1 + xL_{\text{min}}] - 2 \left( \frac{1}{x} + D \right) \ln [1 + xD] - (1 - 3L_{\text{min}}) \right\}. \quad (31)$$

$$B \equiv \frac{1}{2} - \frac{L_{\text{min}}}{2}, \quad D \equiv 1 - 2L_{\text{min}}. \quad (32)$$

See Appendix A for the derivation of Eq. (31). Eq. (30) is recovered by setting $L_{\text{min}} = 0$.

The polarization cross section for the CDE2 distribution is (see Appendix A):

$$C_{\text{CDE2}} = \frac{C_{\text{pol}}}{V} = \frac{30\pi}{\lambda} \text{Im} \left[ \frac{1}{x^4} \left( 3 \left( -9 - 3x + 3x^2 + x^3 \right) \ln \left( 1 + \frac{x}{3} \right) + 6 \left( 4 - 3x^2 - x^3 \right) \ln \left( 1 + \frac{x}{2} \right) + 2(1 + x)^3 \ln(1 + x) - 5x - \frac{1}{2}x^2 + \frac{7}{6}x^3 + \frac{11}{72}x^4 \right) \right]. \quad (33)$$

6. Polarized Absorption by Partially-Aligned Grains

An interstellar grain with angular momentum $\mathbf{J}$ will have a magnetic moment $\mu$ resulting from a combination of the Barnett effect (if the grain has unpaired electron spins), the Rowland effect (if the grain is charged), and ferromagnetism (if the grain contains magnetic material). If $|\mathbf{J} \times \mathbf{B}| \neq 0$, the $\mu \times \mathbf{B}_0$ torque will cause $\mathbf{J}$ to precess around $\mathbf{B}_0$. There are three distinct orientational issues:

1. The angle $\alpha$ between the grain’s principal axis of largest moment of inertia, $\hat{a}_1$, and the angular momentum $\mathbf{J}$ (alignment of the grain body with $\mathbf{J}$).

2. The angle $\beta$ between $\mathbf{J}$ and $\mathbf{B}_0$ (alignment of $\mathbf{J}$ with $\mathbf{B}_0$).

3 For ferromagnetic grains, the rotation-averaged effective magnetic moment $\langle \mu \rangle = \mathbf{J} \cdot \mu / J^2$. 


3. The angle $\gamma$ between $B_0$ and the plane of the sky.

Consider radiation propagating in the $\hat{z}$ direction, and suppose $B_0$ to be in the $\hat{y}$-$\hat{z}$ plane, making an angle $\gamma$ with the $\hat{y}$ axis. In the electric-dipole limit $a/\lambda \ll 1$, the mean absorption cross section and the polarization cross section sections for $x$- and $y$-polarized radiation can be written (see Appendix B)

$$\frac{C_x + C_y}{2} = C_{\text{ran}} - C_{\text{pol}} \Phi \left( \cos^2 \gamma - \frac{2}{3} \right)$$

(34)

$$\frac{C_x - C_y}{2} = C_{\text{pol}} \Phi \cos^2 \gamma$$

(35)

where (see Appendix B)

$$\Phi \equiv \frac{9}{4} \left( \langle \cos^2 \alpha \rangle - \frac{1}{3} \right) \left( \langle \cos^2 \beta \rangle - \frac{1}{3} \right)$$

(36)

is a generalization of the “polarization reduction factor” originally introduced by Greenberg (1968, p. 328) and Purcell & Spitzer (1971). Perfect alignment ($\langle \cos^2 \alpha \rangle = \langle \cos^2 \beta \rangle = 1$) has $\Phi = 1$; random orientation ($\langle \cos^2 \beta \rangle = 1/3$) results in $\Phi = 0$.

If $B_0$ is itself not perfectly uniform, Lee & Draine (1985) showed that $\cos^2 \gamma \rightarrow \cos^2 \gamma_0 \times \frac{1}{2} \left( \langle \cos^2 \delta \rangle - \frac{1}{3} \right)$ where $\gamma_0$ is now the angle between $\hat{y}$ and the (dust mass-weighted) mean magnetic field $\langle B_0 \rangle$, and $\delta$ is the angle between $\langle B_0 \rangle$ and the local $B_0$; $\langle \cos^2 \delta \rangle$ is the dust mass-weighted average of $\cos^2 \delta$ over the sightline. If we assume that $\alpha$, $\beta$ and $\delta$ vary independently, then the overall polarization reduction factor becomes

$$\Phi \equiv \frac{27}{8} \left( \langle \cos^2 \alpha \rangle - \frac{1}{3} \right) \left( \langle \cos^2 \beta \rangle - \frac{1}{3} \right) \left( \langle \cos^2 \delta \rangle - \frac{1}{3} \right)$$

(37)

Let $N_d$ be the column density of grains, an $C_x$ and $C_y$ be the average absorption cross section per grain for radiation polarized in the $\hat{x}$ and $\hat{y}$ directions. Let $\tau_x = N_d C_x$ and $\tau_y = N_d C_y$ be the optical depths for radiation polarized in the $\hat{x}$ and $\hat{y}$ directions. Initially unpolarized radiation will be attenuated and polarized as a result of linear dichroism (i.e., preferential attenuation of one linear polarization), with overall attenuation and fractional polarization

$$\frac{I}{I_0} = \frac{e^{-\tau_y} + e^{-\tau_x}}{2}$$

(38)

$$p = \frac{e^{-\tau_y} - e^{-\tau_x}}{e^{-\tau_y} + e^{-\tau_x}}$$

(39)

From (34) and (35) we can find the absorption cross section per grain volume $C_{\text{ran}}(\lambda)/V$ from the measured attenuation $I/I_0$ and polarization $p$ (see Appendix C) where $\rho$ is the grain mass density and $\Sigma$ is the surface density:

$$\frac{C_{\text{ran}}}{V} = \frac{\tau_0}{\Sigma/\rho} \left[ 1 + \frac{p}{\tau_0} \left( 1 - \frac{2}{3 \cos^2 \gamma} \right) - \frac{p^2}{2 \tau_0} - \frac{2 p^3}{3 \tau_0} \left( 1 - \frac{2}{3 \cos^2 \gamma} \right) + O \left( \frac{p^4}{\tau_0} \right) \right]$$

(40)

$$\tau_0 \equiv \ln \left( \frac{I_0}{I} \right).$$

(41)
7. Validity of the Electric Dipole Approximation

Fig. 7.— $\lambda(Q_{\text{ran}})/a_{\text{eff}}$, vs. wavelength $\lambda$, for $b/a = 2$ oblate silicate spheroids with $a_{\text{eff}} = 0.01, 0.1, 0.2, \text{and } 0.3 \mu m$. For $a_{\text{eff}} \leq 0.3 \mu m$, the electric dipole limit is an excellent approximation for $\lambda > 7 \mu m$.

The preceding discussion has assumed that the extinction by spheroidal or ellipsoidal dust grains can be treated in the electric dipole limit, with extinction cross sections given by Eq. (1–6). This approximation is valid for $a_{\text{eff}}/\lambda \ll 1$, and gives an extinction cross section per volume $C_{\text{ext}}/V$ that is independent of size.

Figure 7 shows the extinction cross section per volume $C_{\text{ran}}/V$ for randomly-oriented oblate spheroids with axial ratio $b/a = 2$ and the dielectric function of “astronomical silicate” (Draine & Hensley 2017). Results are shown for selected radii. The cross sections were calculated using the spheroid code developed by Voshchinnikov & Parafonov (1993).

At short wavelengths, the absorption calculated in the electric dipole limit is not a good approximation for the extinction, because (1) scattering becomes important and (2) the electric field within the ellipsoidal grain ceases to be spatially uniform when $a_{\text{eff}}/\lambda$ is no longer small. However, for the grain sizes $a_{\text{eff}} \lesssim 0.3 \mu m$ that are thought to account for the bulk of interstellar silicates, Figure 7 shows that the electric dipole approximation is quite accurate for $\lambda \gtrsim 7 \mu m$.

\footnote{For silicate feature absorption/volume $[\Delta C_{\text{abs}}/V]_9, \tau_{\mu m} = 9000 \text{ cm}^{-1}$ and providing a fraction $f_8 = 0.2$ of the interstellar extinction at 8$\mu m$.}
8. Self-Consistent Dielectric Functions Derived from Infrared Absorption

Suppose that we have an estimate for the dielectric function $\epsilon(\lambda)$ of the grain material at short wavelengths $\lambda < \lambda_1$, and have observational knowledge of the extinction $\tau(\lambda)$ at infrared wavelengths $\lambda > \lambda_1$, from which we can estimate the absorption cross section per grain volume $C_{\text{ran}}/V$ for randomly-oriented grains (see Appendix C). This applies to the silicate material in the ISM, where we have constraints on the absorption cross section in the neighborhood of the strong absorption features at 9.7$\mu$m and 18$\mu$m. Here we show how one can use the observed $C_{\text{ran}}^{(\text{obs})}/V$ to obtain the complex dielectric function $\epsilon(\lambda)$ at infrared wavelengths. We will apply this to interstellar silicates in a following paper (Draine & Hensley 2017).

We will assume that at wavelengths $\lambda > \lambda_1$ the grains have $a \ll \lambda$, so that we can employ the electric dipole approximation (10) to relate $C_{\text{ran}}/V$ to the complex dielectric function. We must, of course, make an assumption about the grain shape, or distribution of grain shapes. For spheres, spheroids, ellipsoids, or the CDEs discussed in this paper, we have analytic expressions relating $C_{\text{ran}}/V$ to the dielectric function $\epsilon(\lambda)$; the analytic result enables efficient iterative algorithms to be applied to solve the system of equations.

The dielectric function must satisfy the Kramers-Kronig relations (Landau et al. 1993). We suppose that we start with a dielectric function $\epsilon^0(\lambda)$ that is reasonably accurate at $\lambda < \lambda_1$. We extend the imaginary part of $\epsilon^0$ to long wavelengths in a smooth way:

$$\epsilon^0_2(\lambda) = \epsilon^0_2(\lambda_1) \times \left( \frac{\lambda_1}{\lambda} \right) ,$$

and obtain (by numerical integration) the real part $\epsilon^0_1(\lambda)$ at all wavelengths using the Kramers-Kronig relation (Landau et al. 1993):

$$\epsilon^0_1(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{x \epsilon^0_2(x)}{x^2 - \omega^2} dx ,$$

where $P$ indicates that the “principal value” of the singular integral is to be taken. The actual behavior of $\epsilon^0_2(\lambda > 1\mu\text{m})$ is unimportant, because we will adjust the total absorption as required to reproduce $C_{\text{ran}}^{(\text{obs})}/V$ at $\lambda > \lambda_1$. We accomplish this by adding additional absorption in the form of $N$ Lorentz oscillators, each with resonant frequency $\omega_{0k}$, dimensionless damping parameter $\gamma_k$, and dimensionless strength $S_k$:

$$\epsilon(\omega) = \epsilon^{(0)}(\omega) + \sum_{k=1}^N S_k \left[ 1 - \left( \frac{\omega}{\omega_{0k}} \right)^2 - i \frac{\omega}{\omega_{0k}} \gamma_k \right]^{-1} .$$

Because $\epsilon^{(0)}(\omega)$ and each of the Lorentz oscillators separately satisfy the Kramers-Kronig relations, $\epsilon(\omega)$ given by eq. (44) will satisfy the Kramers-Kronig relations for any $\{\omega_{0k}, \gamma_k, S_k\}$.

Let $\lambda_1 = 2\pi c/\omega_{01} = 1\mu\text{m}$ and $\lambda_N = 2\pi c/\omega_{0N} = 5\text{ cm}$. We distribute the Lorentz oscillators between $\lambda_1$ and $\lambda_N > \lambda_1$ according to some smooth prescription, with dimensionless damping
parameter $\gamma_k$:

\[
\begin{align*}
\gamma_1 &= C \times \left( \frac{\lambda_2}{\lambda_1} - 1 \right) \\
\gamma_k &= C \times \left( \frac{\lambda_k}{\lambda_{k-1}} - 1 \right) \quad \text{for } 2 \leq k \leq N.
\end{align*}
\] (45)

For $\gamma \ll 1$, each resonance contributes $\text{Im}(\epsilon)$ with a FWHM $(\delta \omega)_k \approx \gamma \omega_{0k}$. We want $\gamma_k$ to be small but not too small: to represent a smooth function, we want $(\delta \omega)_k$ to be large compared to $\omega_{0,k+1} - \omega_{0k}$. This is accomplished by setting $C \approx 5\text{–}10$.

To find the self-consistent solution, we try to iteratively adjust the $S_k$ to solve the $N$ simultaneous equations

\[
Y_k \equiv \left[ \frac{\lambda C_{\text{ran}}^{(\text{model})}}{V} \right] \lambda_k - \left[ \frac{\lambda C_{\text{ran}}^{(\text{obs})}}{V} \right] \lambda_k = 0, \quad k = 1, ..., N. \quad \text{(47)}
\]

In a separate study [Draine & Hensley 2017] this procedure is applied to obtain $\epsilon(\lambda)$ for the material in the silicate-bearing interstellar grains. For each trial shape and porosity, a dielectric function is obtained that reproduces the assumed extinction vs. $\lambda$, and the polarization cross section $C_{\text{pol}}(\lambda)$ is predicted. By comparing the predicted polarization profile to the observed polarization profile of the $10\mu$m silicate feature, we are able to select the shape and porosity that is in best agreement with observation.

We remark here that the problem does not always have a solution: if the “observed” $\lambda C_{\text{ran}}^{(\text{obs})}/V$ is too large, there may not be any dielectric function $\epsilon(\lambda)$ that can reproduce the assumed $\lambda C_{\text{ran}}^{(\text{obs})}/V$ for the assumed grain shape. Because of the Kramers-Kronig relations, all wavelengths matter: strong absorption at one wavelength will imply a large $\epsilon_1$ at longer wavelengths, limiting the ability of the grain to absorb at those wavelengths. [Draine & Hensley 2017] find that this limits the strength of the $9.7\mu$m interstellar silicate feature to be $\Delta C_{\text{ran}}(9.7\mu m)/V \lesssim 1.0 \times 10^4 \text{ cm}^{-1}$, or opacity $\Delta \kappa(9.7\mu m) \lesssim 2800 \text{ cm}^2 \text{ g}^{-1}$.

9. Summary

The principal results of this study are as follows:

1. We discuss the distributions of ellipsoidal shapes that correspond to three previously-proposed continuous distributions of ellipsoids (CDEs). Twenty randomly-selected shapes from each distribution (Figure 3) serve to illustrate the three distributions.

2. The often-used CDE discussed by [Bohren & Huffman 1983] (here referred to as the BHCDE distribution) includes what appears to be an unrealistically large fraction of extremely elongated or extremely flattened shapes.
3. The CDE2 distribution proposed by [Ossenkopf et al. (1992)] includes a much smaller fraction of extreme shapes, and seems more realistic as a model for distributions of grains shapes.

4. For each of the CDEs, we obtain the distribution functions $g_j(L_j)$ for the geometric factors $L_1, L_2, L_3$.

5. In the electric dipole limit $a/\lambda \ll 1$, we obtain absorption and polarization cross sections for partially-aligned ellipsoidal grains with the three proposed CDEs.

6. We present a method for obtaining a self-consistent dielectric function consistent with an assumed absorption opacity and an assumed distribution of shapes.

We thank Eric Stansifer and Chris Wright for helpful discussions. This work was supported in part by NSF grant AST-1408723, and carried out in part at the Jet Propulsion Laboratory, California Institute of Technology, under a contract with the National Aeronautics and Space Administration.

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A. Polarization Cross Sections for Grain Populations with Continuously-Distributed Ellipticities

A.1. General Considerations

Consider a population of ellipsoids with a distribution of depolarization factors \((L_1, L_2, L_3)\). Because \(L_3 = 1 - L_1 - L_2\), the ellipsoid shape is fully-determined by \((L_1, L_2)\), which must lie in the triangular region bounded by \(L_1 = 0, L_2 = 0,\) and \(L_1 + L_2 = 1\), as shown in Figure 1.

The distribution of shapes can be characterized by the distribution of \(L\) values. Because \(L_3 = 1 - L_1 - L_2\), the shape is fully determined by the doublet \((L_1, L_2)\). Let \(dP = G(L_1, L_2)dL_1dL_2\) be the probability that \(L_1 \in (L_1 + dL_1), L_2 \in (L_2 + dL_2),\) with \(L_3 = 1 - L_1 - L_2\). The function \(G(L_1, L_2)\) fully determines the shape distribution (i.e., the distribution of axial ratios). If \(G\) is to apply to the full triangular region in Figure 1, then (because labelling of axes 1, 2, 3 is arbitrary), \(G\) must depend symmetrically on \(L_1, L_2, L_3\):

\[
G(L_1, L_2) = G(L_2, L_1) = G(L_1, 1 - L_1 - L_2) \quad \text{for all allowed} \ L_1, L_2 .
\] (A1)

The region of allowed \((L_1, L_2)\) can be divided into 6 triangular subregions of equal area, shown in Figure 1 corresponding to the six possible orderings of \(L_1, L_2, L_3\): (1) \(L_3 \leq L_2 \leq L_1\), (2) \(L_2 \leq L_1 \leq L_3\), (3) \(L_1 \leq L_3 \leq L_2\), (4) \(L_2 \leq L_3 \leq L_1\), (5) \(L_3 \leq L_1 \leq L_2\), and (6) \(L_1 \leq L_2 \leq L_3\).

For clarity, we fix the order of the \(L\) values: we choose the ordering \(0 \leq L_3 \leq L_2 \leq L_1 \leq 1\), corresponding to region 1 (shaded) in Figure 1. Then \(L_1\) is for \(E\) parallel to the principal axis of largest moment of inertia (the “short axis”), and \(L_3\) is for \(E\) along the principal axis of smallest moment of inertia (the “long axis”).

This preprint was prepared with the AAS LATEX macros v5.2.
Within subregion 1, let $g_j(L_j)dL_j$ be the probability that $L_j \in (L_j, L_j + dL_j)$:

$$
g_1(L_1) = \begin{cases} 
0 & \text{for } 0 < L_1 < 1/3 \\
6 \int_{(1-L_1)/2}^{L_1} G(L_1, L_2) dL_2 & \text{for } 1/3 < L_1 < 1/2 \\
6 \int_{1-2L_2}^{1-L_1} G(L_1, L_2) dL_1 & \text{for } 1/2 < L_1 < 1
\end{cases}
$$

$$
g_2(L_2) = \begin{cases} 
0 & \text{for } 0 < L_2 < 1/3 \\
6 \int_{L_2}^{1-L_2} G(L_1, L_2) dL_1 & \text{for } 1/3 < L_2 < 1/2 \\
12L_2 & \text{for } 1/2 < L_2
\end{cases}
$$

$$
g_3(L_3) = \begin{cases} 
3 \int_{0}^{1-3L_3} G((1 - L_3 + z)/2, (1 - L_3 - z)/2) dz & \text{for } 0 < L_3 < 1/3 \\
6(1 - 3L_3) & \text{for } 1/3 < L_3 < 1/2 \\
0 & \text{for } 1/2 < L_3
\end{cases}
$$

(A2)

where we have introduced $z \equiv (L_1 - L_2)$ for evaluation of $g_3$. The factor of six in (A2) appears because we assume the normalization $\int G dL_1 dL_2 = 1$ over the full triangular region, hence $\int G dL_1 dL_2 = 1/6$ over region 1. It can be verified that

$$
\int_0^1 g_j(L_j) dL_j = 1 \quad \text{for } j = 1, 2, 3 .
$$

(A3)

For distributions of ellipsoidal shapes, we require

$$
\langle A_j \rangle = \int \frac{(\epsilon - 1)}{1 + L_j(\epsilon - 1)} g_j(L_j) dL_j .
$$

(A4)

### A.2. BHCDE

The simplest CDE is the uniform distribution

$$
G(L_1, L_2) = 2 \quad \text{for } 0 \leq L_1 + L_2 \leq 1 ,
$$

(A5)

which obviously satisfies the symmetry condition (A1). This example was discussed by Bohren & Huffman (1983); we refer to (A5) as the BHCDE. For this case we have

$$
g_1 = \begin{cases} 
0 & \text{for } L_1 < 1/3 \\
18(L_1 - \frac{1}{3}) & \text{for } \frac{1}{3} \leq L_1 \leq \frac{1}{2} \\
6(1 - L_1) & \text{for } \frac{1}{2} \leq L_1 \leq 1
\end{cases}
$$

$$
g_2 = \begin{cases} 
12L_2 & \text{for } 0 \leq L_2 \leq \frac{1}{3} \\
12(1 - 2L_2) & \text{for } \frac{1}{3} \leq L_2 \leq \frac{1}{2} \\
0 & \text{for } \frac{1}{2} \leq L_2
\end{cases}
$$

$$
g_3 = \begin{cases} 
6(1 - 3L_3) & \text{for } 0 \leq L_3 \leq \frac{1}{3} \\
0 & \text{for } \frac{1}{3} \leq L_3
\end{cases}
$$

(A6)
Distributions $g_1, g_2,$ and $g_3$ are shown in Figure 6a. Then

$$
\langle A_1 \rangle = \frac{6}{x} \left( (1 + x) \ln \left( \frac{1 + x}{1 + x/2} \right) - 3 \left( 1 + \frac{x}{3} \right) \ln \left( \frac{1 + x/2}{1 + x/3} \right) \right) \quad (A7)
$$

$$
\langle A_2 \rangle = \frac{12}{x} \left( 2 \left( 1 + \frac{x}{2} \right) \ln \left( \frac{1 + x/2}{1 + x/3} \right) - \ln (1 + x/3) \right) \quad (A8)
$$

$$
\langle A_3 \rangle = 18 \left( \frac{1}{3} \ln (1 + x/3) - \frac{1}{3} \right) \quad . \quad (A9)
$$

![Fig. 8.— The shaded area is the ERCDE locus with depolarization factors $L_1 \geq L_2 \geq L_3 \geq L_{\text{min}}$ (see text).](image)

### A.3. ERCDE

The BHCDE includes shapes that are infinitely elongated ($L_j \to 0$) and infinitely flattened ($L_j \to 1$). Zubko et al. (1996) proposed to exclude the most extreme shapes by imposing the restriction $L_j \geq L_{\text{min}}$, where $0 \leq L_{\text{min}} \leq 1/3$, giving what Zubko et al. refer to as the “externally restricted distribution of ellipsoids” (ERCDE):

$$
G(L_1, L_2) = \frac{2}{(1 - 3L_{\text{min}})^2} \quad \text{for} \quad L_{\text{min}} \leq L_1, L_{\text{min}} \leq L_2, (L_1 + L_2) \leq 1 - 2L_{\text{min}} . \quad (A10)
$$
With $L_{\text{min}} = 0$ one obtains the original BHCDE; with $L_{\text{min}} \to 1/3$ one obtains spheres. The domain in the $L_1-L_2$ plane is shown in Fig. 8.

Zubko et al. (1996) obtained $\langle A_1 + A_2 + A_3 \rangle$ for randomly-oriented grains with the ERCDE distribution. Discussion of aligned grains requires the absorption per volume for grains aligned with the electric fields along their principal axes. The ERCDE has

\[
g_1 = \begin{cases} 
  0 & \text{for } L_1 < \frac{1}{3} \\
  \frac{18}{(1-3L_{\text{min}})^2} (L_1 - \frac{1}{3}) & \text{for } \frac{1}{3} \leq L_1 \leq \frac{1-L_{\text{min}}}{2} \\
  \frac{6}{(1-3L_{\text{min}})^2} (1 - L_1 - 2L_{\text{min}}) & \text{for } \frac{1-L_{\text{min}}}{2} \leq L_1 \leq 1 - 2L_{\text{min}} \\
  0 & \text{for } 1 - 2L_{\text{min}} \leq L_1 
\end{cases}
\]

\[
g_2 = \begin{cases} 
  0 & \text{for } L_2 < L_{\text{min}} \\
  \frac{12}{(1-3L_{\text{min}})^2} (L_2 - L_{\text{min}}) & \text{for } L_{\text{min}} \leq L_2 \leq \frac{1}{3} \\
  \frac{12}{(1-3L_{\text{min}})^2} (1 - L_{\text{min}} - 2L_2) & \text{for } \frac{1}{3} \leq L_2 \leq \frac{(1-L_{\text{min}})}{2} \\
  0 & \text{for } \frac{(1-L_{\text{min}})}{2} \leq L_2 
\end{cases}
\]  

\[
g_3 = \begin{cases} 
  0 & \text{for } L_3 \leq L_{\text{min}} \\
  \frac{6}{(1-3L_{\text{min}})^2} (1 - 3L_3) & \text{for } L_{\text{min}} \leq L_3 \leq \frac{1}{3} \\
  0 & \text{for } \frac{1}{3} \leq L_3 
\end{cases}
\]

Distributions $g_1$, $g_2$, and $g_3$ are shown in Figure 6 for $L_{\text{min}} = 0.05$. It is convenient to define

\[
B \equiv \frac{1}{2} - L_{\text{min}}/2 \\
D \equiv \frac{1}{2} - 2L_{\text{min}} \\
x \equiv \epsilon - 1
\]

We obtain

\[
\langle A_1 \rangle = \frac{6}{(1-3L_{\text{min}})^2} \left\{ \left( \frac{1}{x} + D \right) \ln \left[ \frac{1+xD}{1+xB} \right] - 3 \left( \frac{1}{x} + \frac{1}{3} \right) \ln \left[ \frac{1+xB}{1+x/3} \right] \right\} 
\]

\[
\langle A_2 \rangle = \frac{12}{(1-3L_{\text{min}})^2} \left\{ 2 \left( \frac{1}{x} + B \right) \ln \left[ \frac{1+xB}{1+x/3} \right] - \left( \frac{1}{x} + L_{\text{min}} \right) \ln \left[ \frac{1+x/3}{1+xL_{\text{min}}} \right] \right\} 
\]

\[
\langle A_3 \rangle = \frac{18}{(1-3L_{\text{min}})^2} \left\{ \left( \frac{1}{x} + \frac{1}{3} \right) \ln \left[ \frac{1+x/3}{1+xL_{\text{min}}} \right] - \frac{1}{3} \right\} 
\]

\[
\frac{\langle A_1 + A_2 + A_3 \rangle}{3} = \frac{2}{(1-3L_{\text{min}})^2} \left\{ \left( \frac{1}{x} + \frac{1}{3} \right) \ln \left[ \frac{1+x/3}{1+xL_{\text{min}}} \right] - \frac{1}{3} \right\} 
\]

A.4. CDE2

Ossenkopf et al. (1992) proposed the distribution

\[
G(L_1, L_2) = 120L_1L_2L_3
\]
This satisfies the symmetry requirement (A1), and has the desirable property that $G \to 0$ for $L_j \to 0$. We find

\[
\begin{align*}
\langle A_1 \rangle &= \frac{60V}{x^4} \left[ (9 + 3x - 3x^2 - x^3) \ln \left(1 + \frac{x}{3}\right) + (-8 + 6x^2 + 2x^3) \ln \left(1 + \frac{x}{2}\right) \right. \\
&\quad \left. + (-1 - 3x - 3x^2 - x^3) \ln (1 + x) + 2x + x^2 + \frac{2}{9} x^3 + \frac{7}{216} x^4 \right] \quad \text{(A21)} \\
\langle A_2 \rangle &= \frac{60V}{x^4} \left[ (-18 - 6x + 6x^2 + 2x^3) \ln \left(1 + \frac{x}{3}\right) + (8 - 6x^2 - 2x^3) \ln \left(1 + \frac{x}{2}\right) \right. \\
&\quad \left. + 2x + 2x^2 + \frac{5}{9} x^3 + \frac{13}{216} x^4 \right] \quad \text{(A22)} \\
\langle A_3 \rangle &= \frac{60V}{x^4} \left[ (9 + 3x - 3x^2 - x^3) \ln \left(1 + \frac{x}{3}\right) - 3x - \frac{1}{2} x^2 + \frac{19}{18} x^3 + \frac{17}{108} x^4 \right] \quad \text{(A23)} \\
\frac{\langle A_1 + A_2 + A_3 \rangle}{3} &= \frac{20V}{x^4} \left[ -(1 + x)^3 \ln (1 + x) + x + \frac{5}{2} x^2 + \frac{11}{6} x^3 + \frac{1}{4} x^4 \right] \quad \text{(A24)}
\end{align*}
\]

where $x \equiv \epsilon - 1$.

**B. Orientation-Averaged Cross Sections for Partially-Aligned Grains**

Consider radiation propagating along the $\hat{z}$ axis. Let the local magnetic field be in the $\hat{y} - \hat{z}$ plane, with $\gamma$ = the angle between $\mathbf{B}$ and the plane-of-the-sky: $\hat{\mathbf{B}} = \hat{y} \cos \gamma + \hat{z} \sin \gamma$.

Let $\mathbf{J}$ be a unit vector in the direction of the grain’s angular momentum. Let $\beta$ be the angle between $\mathbf{J}$ and $\hat{\mathbf{B}}$. If $\beta > 0$, the grain’s magnetic moment will cause $\mathbf{J}$ to precess around $\hat{\mathbf{B}}$, and we may write

\[
\hat{\mathbf{J}} = \hat{\mathbf{B}} \cos \beta + \hat{\mathbf{x}} \sin \beta \cos \phi_1 + (\hat{\mathbf{x}} \times \hat{\mathbf{B}}) \sin \beta \sin \phi_1 \quad \text{(B1)}
\]

\[
= \hat{\mathbf{x}} \sin \beta \cos \phi_1 + \hat{\mathbf{y}} (\cos \beta \cos \gamma - \sin \beta \sin \gamma \sin \phi_1) + \hat{\mathbf{z}} \cos \beta \sin \gamma + \sin \beta \cos \gamma \sin \phi_1 \quad \text{(B2)}
\]
with $\phi$ varying from 0 to $2\pi$ over one precession period. Observations of starlight polarization indicate that there is systematic alignment of $\mathbf{J}$ with $\mathbf{B}$, i.e., $\langle \cos^2 \beta \rangle > 1/3$, with the alignment presumed to result from some combination of paramagnetic dissipation \cite{Davis:1951}, superparamagnetic dissipation \cite{Jones:1967}, ferromagnetic dissipation \cite{Draine:2013} or starlight torques \cite{Draine:1997,Weingartner:2003,Loang:2009a,Loang:2009b}.

On short time scales the grain spins and nutates with fixed $\mathbf{J}$ according to the dynamics of rigid bodies \cite[see, e.g.,]{Weingartner:2003}. Let $\mathbf{a}_1$ be the principal axis of largest moment of inertia, and let $\alpha$ be the angle between $\mathbf{J}$ and $\mathbf{a}_1$. At constant $J$ and kinetic energy $E_{\text{rot}}$ the grain will tumble: $\mathbf{a}$ will nutate around $\mathbf{J}$. If the grain is triaxial, the angle $\alpha$ does not remain constant during the nutation, but will have some time-averaged value of $\langle \cos^2 \alpha \rangle$.

For fixed $J$, the kinetic energy of the grain is minimized if $\alpha = 0$ ($\cos^2 \alpha = 1$). If the direction of $\mathbf{a}$ is uncorrelated with $\mathbf{J}$, then $\langle \cos^2 \alpha \rangle = 1/3$. Thus we expect dissipation in the grain to result in $\langle \cos^2 \alpha \rangle > 1/3$. Suprathermally rotating grains, with rotational kinetic energy $E_{\text{rot}} \gg kT_{\text{grain}}$, are expected to have $\cos^2 \alpha \approx 1$ as the result of dissipation associated with viscoelasticity \cite{Purcell:1979} or the even greater dissipation associated with the Barnett effect \cite{Lazarian:1997} and nuclear spin relaxation \cite{Lazarian:1999}.

After averaging over precession and nutation,

\begin{align}
\langle (\mathbf{a}_1 \cdot \mathbf{x})^2 \rangle &= \frac{1}{3} - \frac{3}{4} \left( \langle \cos^2 \alpha \rangle - \frac{1}{3} \right) \left( \cos^2 \beta - \frac{1}{3} \right) \\
\langle (\mathbf{a}_1 \cdot \mathbf{y})^2 \rangle &= \frac{1}{3} + \frac{9}{4} \left( \langle \cos^2 \alpha \rangle - \frac{1}{3} \right) \left( \cos^2 \beta - \frac{1}{3} \right) \left( \cos^2 \gamma - \frac{1}{3} \right) \\
\langle (\mathbf{a}_2 \cdot \mathbf{x})^2 \rangle &= \langle (\mathbf{a}_3 \cdot \mathbf{x})^2 \rangle = \frac{1}{3} + \frac{3}{8} \left( \langle \cos^2 \alpha \rangle - \frac{1}{3} \right) \left( \langle \cos^2 \beta \rangle - \frac{1}{3} \right) \\
\langle (\mathbf{a}_2 \cdot \mathbf{y})^2 \rangle &= \langle (\mathbf{a}_3 \cdot \mathbf{y})^2 \rangle = \frac{1}{3} - \frac{9}{8} \left( \langle \cos^2 \alpha \rangle - \frac{1}{3} \right) \left( \cos^2 \beta - \frac{1}{3} \right) \left( \cos^2 \gamma - \frac{1}{3} \right) .
\end{align}
The cross sections for radiation polarized in the \( \hat{x} \) and \( \hat{y} \) directions are

\[
C_x = C_{\text{ran}} + \frac{2}{3} C_{\text{pol}} \Phi \tag{B7}
\]

\[
C_y = C_{\text{ran}} - 2 C_{\text{pol}} \Phi \left( \cos^2 \gamma - \frac{1}{3} \right) \tag{B8}
\]

\[
\frac{C_x + C_y}{2} = C_{\text{ran}} - C_{\text{pol}} \Phi \left( \cos^2 \gamma - \frac{2}{3} \right) \tag{B9}
\]

\[
\frac{C_x - C_y}{2} = C_{\text{pol}} \Phi \cos^2 \gamma \tag{B10}
\]

\[
C_{\text{ran}} \equiv \frac{1}{3} \left[ C_{\text{abs}}(E \parallel \hat{a}_1) + C_{\text{abs}}(E \parallel \hat{a}_2) + C_{\text{abs}}(E \parallel \hat{a}_3) \right] \tag{B11}
\]

\[
C_{\text{pol}} \equiv \frac{1}{4} \left[ C_{\text{abs}}(E \parallel \hat{a}_2) + C_{\text{abs}}(E \parallel \hat{a}_3) - 2 C_{\text{abs}}(E \parallel \hat{a}_1) \right] \tag{B12}
\]

\[
\Phi \equiv \frac{9}{4} \left( \langle \cos^2 \alpha \rangle - \frac{1}{3} \right) \left( \cos^2 \beta - \frac{1}{3} \right). \tag{B13}
\]

C. Estimating \( C_{\text{ran}} \) from Observations

Suppose that the attenuation \( I/I_0 \) is known, where the intensity \( I(\lambda) \) is summed over both polarization modes, and the unattenuated radiation \( I_0 \) is unpolarized. The fractional polarization \( p(\lambda) \) is also measured. Let \( \hat{z} \) be the direction of propagation, and \( \hat{y} \) be the polarization direction. If \( N \) is the total column density of grains, we seek to determine the cross section \( C_{\text{ran}}(\lambda) \) for randomly-oriented grains. Define

\[
\bar{\tau} \equiv \frac{\tau_x + \tau_y}{2} \tag{C1}
\]

\[
\tau_p \equiv \frac{\tau_x - \tau_y}{2} \tag{C2}
\]

\[
\frac{I}{I_0} = \frac{e^{-\tau_x} + e^{-\tau_y}}{2} \tag{C3}
\]

\[
= e^{-\tau_p} \left[ 1 - \frac{1}{2} \tau_p^2 + O(\tau_p^4) \right] \tag{C4}
\]
\[
p = \frac{e^{-\tau_y} - e^{-\tau_x}}{2I/I_0} \quad (C5)
\]

\[
= \tau_p \left[ \frac{1 + \frac{1}{2} \tau_p^2 + O(\tau_p^4)}{1 - \frac{1}{2} \tau_p^2 + O(\tau_p^4)} \right] = \tau_p \left[ 1 + \frac{2}{3} \tau_p^2 + O(\tau_p^4) \right] \quad (C6)
\]

\[
\tau_p \approx p - \frac{2}{3} p^3 + O(p^5) \quad (C7)
\]

\[
\bar{\tau} = \ln(I_0/I) + \ln \left[ 1 - \frac{1}{2} \tau_p^2 + O(\tau_p^4) \right] \quad (C8)
\]

\[
\approx \ln(I_0/I) - \frac{1}{2} \tau_p^2 + O(\tau_p^4) \quad (C9)
\]

\[
\approx \ln(I_0/I) - \frac{1}{2} p^2 + O(p^4) \quad . \quad (C10)
\]

From (B9, B12) we have

\[
\bar{\tau} = N \left[ C_{\text{ran}} - C_{\text{pol}} \Phi (\cos^2 \gamma - \frac{2}{3}) \right] \quad (C11)
\]

\[
= NC_{\text{ran}} - \tau_p \left( 1 - \frac{2}{3 \cos^2 \gamma} \right) \quad (C12)
\]

\[
C_{\text{ran}} = \frac{1}{N} \left[ \ln \left( \frac{I_0}{I} \right) + p \left( 1 - \frac{2}{3 \cos^2 \gamma} \right) - \frac{1}{2} p^2 - \frac{2}{3} p^3 \left( 1 - \frac{2}{3 \cos^2 \gamma} \right) + O(p^4) \right] \quad . \quad (C13)
\]

If the polarization fraction \( p \ll 1 \), we may approximate \( C_{\text{ran}} \approx (1/N) \ln(I_0/I) \). For finite \( p \ll 1 \), we can correct for the alignment if \( p \) is measured and \( \cos^2 \gamma \) can be estimated.

\section*{D. Proof of Uniqueness}

For an ellipsoid with semi-major axes \( a_1 \leq a_2 \leq a_3 \), the corresponding shape factors \( L_1 \geq L_2 \geq L_3 \) are given by Eq. (23). While we do not offer a proof that there is an \((a_2/a_1, a_3/a_1)\) corresponding to every possible \((L_1, L_2, L_3)\), we have implemented a numerical procedure that always returns a solution. In this note, we demonstrate that this solution is unique.

Suppose that \((a_2/a_1, a_3/a_1)\) corresponds to the desired \((L_1, L_2, L_3)\). Without loss of generality, let \( a_1 = 1 \). We may then rewrite

\[
L_j = \frac{a_2 a_3}{2} \int_0^\infty \frac{dx}{\left( a_j^2 + x \right) \left[ (1 + x) (a_2^2 + x) (a_3^2 + x) \right]^{1/2}} \quad . \quad (D1)
\]
Computing the derivatives

\[ \frac{\partial L_1}{\partial a_2} = \frac{1}{2} \int_0^\infty \frac{a_3 x dx}{(1 + x)^{3/2} (a_2^2 + x)^{3/2} (a_3^2 + x)^{1/2}} \]

\[ \frac{\partial L_1}{\partial a_3} = \frac{1}{2} \int_0^\infty \frac{a_2 x dx}{(1 + x)^{3/2} (a_2^2 + x)^{1/2} (a_3^2 + x)^{3/2}} \]

\[ \frac{\partial L_2}{\partial a_3} = \frac{1}{2} \int_0^\infty \frac{a_2 x dx}{(1 + x)^{1/2} (a_2^2 + x)^{3/2} (a_3^2 + x)^{3/2}} \]

\[ \frac{\partial L_3}{\partial a_2} = \frac{1}{2} \int_0^\infty \frac{a_3 x dx}{(1 + x)^{1/2} (a_2^2 + x)^{3/2} (a_3^2 + x)^{3/2}} \]

we see that the integrands are positive definite for all \(a_2, a_3\), and \(x\). Therefore,

\[ \frac{\partial L_1}{\partial a_2} > 0 \]

\[ \frac{\partial L_1}{\partial a_3} > 0 \]

\[ \frac{\partial L_2}{\partial a_3} > 0 \]

\[ \frac{\partial L_3}{\partial a_2} > 0 \]

Because the \(L_j\) sum to one, it must be true that

\[ \frac{\partial L_1}{\partial a_2} + \frac{\partial L_2}{\partial a_2} + \frac{\partial L_3}{\partial a_2} = 0 \]

\[ \frac{\partial L_1}{\partial a_3} + \frac{\partial L_2}{\partial a_3} + \frac{\partial L_3}{\partial a_3} = 0 \]

and so

\[ \frac{\partial L_2}{\partial a_2} < 0 \]

\[ \frac{\partial L_3}{\partial a_3} < 0 \]

Assume that there are two sets of axial ratios \((a_2, a_3)\) and \((a'_2, a'_3)\) which yield the same \((L_1, L_2, L_3)\). We will proceed by starting from \((a_2, a_3)\) and adjusting the axial ratios one at a time to the values \((a'_2, a'_3)\). We will show that it is impossible to make a nonzero adjustment and return back to the original \((L_1, L_2, L_3)\). Note that since \(1 \leq a_2 \leq a_3\) by construction, \(L_1 \geq L_2 \geq L_3\) and thus permutations of the \(L_j\) are excluded.

If \(a_2 > a'_2\), we can first decrease \(a_2\) until it is equal to \(a'_2\). From the relations above, doing so decreases \(L_1\), increases \(L_2\), and decreases \(L_3\). To return the \(L_j\) to their original values, adjusting \(a_3\) must increase \(L_1\), decrease \(L_2\), and increase \(L_3\). However, decreasing \(a_3\) decreases \(L_1\) while
increasing \( a_3 \) increases \( L_2 \), and so the desired adjustment is not possible. An analogous argument holds for \( a_2 < a'_2 \).

Therefore, \((a_2, a_3)\) is the \textit{unique} set of axial ratios corresponding to \((L_1, L_2, L_3)\).