Implications of Grain Size Distribution and Composition for the Correlation between Dust Extinction and Emissivity

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Abstract

We study the effect of variations in dust size distribution and composition on the correlation between the spectral shape of extinction (parameterized by $R_V$) and far-infrared dust emissivity (parameterized by the power-law index $\beta$). Starting from the size distribution models proposed by Weingartner & Draine, using the dust absorption and emission properties derived by Laor & Draine for carbonaceous and silicate grains, and by Li & Draine for polycyclic aromatic hydrocarbon grains, we calculate the extinction and compare it with the reddening vector derived by Schlafly et al. An optimizer and an Markov chain Monte Carlo method are used to explore the space of available parameters for the size distributions. We find that larger grains are correlated with high $R_V$. However, this trend is not enough to explain the emission-extinction correlation observed by Schlafly et al. For the $R_V - \beta$ correlation to arise, we need to impose explicit priors for the carbonaceous and silicate volume priors as functions of $R_V$. The results show that a composition with higher ratio of carbonaceous to silicate grains leads to higher $R_V$ and lower $\beta$. A relation between $E(B-V)/\tau_{353}$ and $R_V$ is apparent, with possible consequences for the recalibration of emission-based dust maps as a function of $R_V$.}

Unified Astronomy Thesaurus concepts: Interstellar dust extinction (837); Interstellar medium (847); Interstellar dust processes (838); Carbonaceous grains (201); Silicate grains (1456); Polycyclic aromatic hydrocarbons (1280); Interstellar scattering (854); Interstellar absorption (831)

1. Introduction

Dust is an important component of the interstellar medium, forming structures in the space between the stars in our galaxy. Dust is formed through the death process of stars, through supernovas or stellar winds. It is composed of elements that have formed in the stars, and it plays an important role in the further formation of complex molecules (Draine 2011).

Dust scatters and absorbs ultraviolet and visible light coming from the interstellar radiation field (ISRF) around it. The scattering and absorption together cause extinction of the ultraviolet and visible light. Past studies have aimed to characterize the wavelength dependencies of the extinction. Their work (Savage & Mathis 1979; Fitzpatrick 1999; Cardelli et al. 1989) used the parameter $R_V = A(V)/(A(B) - A(V))$ for characterizing extinction functions, based on the observation that one parameter would capture most of the variation in extinction across the sky.

This is a simplifying assumption that holds in certain wavelength regions and breaks down in the UV, where the complexity of the extinction has been shown to be too great for a single parameter (Peek & Schiminovich 2013). In this work, for the extinction we consider the wavelength range 0.4–4.5 $\mu$m, for which one parameter is sufficient to describe the variation in $R_V$, but see Section 2.2.2.

Dust grains are heated by absorption of the ambient radiation field and then radiate in the far-infrared and microwave. This emission is a major contributor to the foreground of the cosmic microwave background experiments. Reach et al. (1995) and Finkbeiner et al. (1999) made a comprehensive attempt using Far Infrared Absolute Spectrophotometer and Diffuse Infrared Background Experiment data to estimate what the contribution from dust is. This was used and improved by the Wilkinson Microwave Anisotropy Probe team (Bennett et al. 2003), followed by the Planck satellite (Planck Collaboration et al. 2014b).

Schlafly et al. (2016), hereafter S16, mapped the variation of the dust extinction curve toward different directions on the sky (using tens of thousands of stars), and found a correlation between $R_V$ and the far-infrared dust emissivity power law, $\beta$. The emissivity data was obtained from the Planck satellite (Planck Collaboration et al. 2016a). We will use the reddening law from S16 to constrain the dust. It is in good agreement with the commonly used Fitzpatrick (1999) reddening curve, including its variation about the mean. We use S16 because it provides error bars at each of 10 wavelengths providing an obvious way to compute a likelihood, whereas Fitzpatrick (1999) does not.

Our goal in this analysis is to see if variations in dust grain size distributions and composition can explain the observed correlation between $R_V$ and $\beta$. Weingartner & Draine (2001a, hereafter WD01) fit the size distributions using information for the volume of the grains, extinction $A(\lambda)$, and optical parameters of Laor & Draine (1993), under the assumption of spherical grains. In addition to this information, we take into account the $R_V - \beta$ relation found by S16, as well as their reddening law for values ranging between 0.5 and 4.5 $\mu$m (Figure 1). As a result, we can fit a size distribution with the new $R_V - \beta$ constraints and ask what drives the $R_V - \beta$ relation. We start from the parameters describing the size distribution of the grains of dust. The scope is to see if the variation in the 11 parameters of the proposed size distribution function can explain the observed correlation between $R_V$ and $\beta$. We can also explore the effect of a having dust grains exposed to different ISRF intensities.

In Section 2 we explain the modeling for the interstellar dust: its size distribution, composition, extinction, and emission. In Section 3 we summarize the optimizer and Markov chain...
normal size distributions for small radii is controlled by its amplitude positive (or negative at a c). In addition, in the function D(a), the sum of two log-normal size distributions for small radius is controlled by its amplitude bc, which represents the total carbon abundance per hydrogen nucleus in the log-normal population. Grains with radii smaller than 10^{-2} \mu m are modeled as PAHs.

**2. Modeling**

Our goal is to determine whether variations in the size distributions of the grains of dust can explain the correlation between R_V and \beta found in S16. We use models for the size distributions for different types of grains. Using these models together with models for the absorption and scattering cross sections of the grains, we are able to calculate the extinction.

Monte Carlo (MCMC) method used to constrain the dust size distributions to the reddening vector. Finally, we present our results in Section 4, and the conclusion in Section 5.

Also, together with emission cross section, and an ISRF we can compute an equilibrium temperature for each size and type of grain. Using that, we can predict the collective emission from any size distribution. As a result, we can use these models to study both absorption and emission of dust.

### 2.1. Properties of the Dust Grains

**Dust grain size distribution**—We use the models for the dust grain size distributions proposed by WD01 (for work leading up and related to this, see also Mathis et al. 1977; Greenberg 1978; Cardelli et al. 1989; Desert et al. 1990; Li & Greenberg 1997; Li & Draine 2001 and Jones et al. 2013 for the core-mantle model dust size distribution, and Wang et al. 2015 or the updated version of silicate-graphite model with the addition of a population of large, micron-sized dust grains). An alternative model for the size distribution has been proposed by Zubko et al. (2004), which can be explored in a future work.

In the WD01 model, the dust is modeled using two separate grain populations: silicate composition, and graphite (carbonaceous) composition. For the small carbonaceous grains (radii smaller than 10^{-2} \mu m), different optical coefficients are used, corresponding to neutral and ionized polycyclic aromatic hydrocarbons (PAHs). PAHs are structures made of hexagonal rings of carbon atoms with hydrogen atoms attached to the boundary. It is assumed that neutral and ionized PAHs each give half of the contribution of the PAHs. Other types of grains (such as oxides of silicon, magnetism, and iron, carbides, etc.) are not included.

The size distributions are modeled by Equations (1) and (2):

\[
\frac{1}{n_H} \frac{dn_{gr}(a)}{da} = D(a) + C \left( \frac{a}{a_1} \right)^\beta \times \begin{cases} 
1 + \beta a/a_1, & \beta > 0 \\
(1 - \beta a/a_1)^{-1}, & \beta < 0 
\end{cases} \\
\exp\left[-\left(\frac{a - a_1}{a_c}\right)^3\right], & a > a_1
\]

for silicate dust

\[
D(a) = \begin{cases} 
0, & \text{for carbonaceous/PAH dust} \\
2.04 \cdot 10^{-2} \frac{bC}{a} e^{-3.125(\ln(a/3.5 \text{ Å})^3) + 9.55 \cdot 10^{-6} \frac{bC}{a} e^{-3.125(\ln(a/30 \text{ Å})^3),} & a > a_1
\end{cases}
\]

for carbonaceous/PAH dust.
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The absorption optical coefficients for carbonaceous and silicate grains can be approximated with a power law for the wavelength range between 335 and 1000 µm. The power-law index has a different dependence on radius for each type of grain. In a collection of grains, carbonaceous grains can contribute higher $\beta$ than the silicate grains, leading to lower $\beta$ index for the entire collection.

These equations are described by 11 parameters: five corresponding to the silicate population and six to the PAH and graphite (Figure 2).

Optical parameters of the dust grains—To calculate the emission and extinction of dust we need to know the optical properties of the grains of dust, such as the absorption and scattering coefficients. For silicates and graphite, we use the values derived by Laor & Draine (1993) and Draine & Lee (1984). For PAH-carbonaceous grains we use the properties obtained in Li & Draine (2001).3

The models contain 81 log-spaced radii between 10$^{-3}$ and 10 µm for silicates, 30 from 3.55 × 10$^{-4}$–10$^{-2}$ µm for PAHs, and 61 between 10$^{-2}$ and 10 µm for graphite.4

Laor & Draine (1993) model dust grains as solid spheres of radius $a$ with an absorption cross section at wavelength $\lambda$ of $C_{\text{abs}}(\lambda, a)$. They label the scattering cross section at wavelength $\lambda$ with $C_{\text{sca}}(\lambda, a)$ and the extinction cross section with $C_{\text{ext}}(\lambda, a) \equiv C_{\text{abs}}(\lambda, a) + C_{\text{sca}}(\lambda, a)$. The scattering and absorption efficiencies $Q_{\text{sca}}$ and $Q_{\text{abs}}$ are defined as:

$$Q_{\text{sca}}(\lambda, a) = \frac{C_{\text{sca}}(\lambda, a)}{\pi a^2}; \quad Q_{\text{abs}}(\lambda, a) = \frac{C_{\text{abs}}(\lambda, a)}{\pi a^2}. \quad (3)$$

The wavelength range for the optical parameters for all types of grains is 10$^{-3}$–1 mm. The graphite and silicate files have 241 log-spaced wavelength samples. For the PAH files, their wavelength array is five times more dense than the wavelength array from the graphite or silicate files, so we take only every fifth value, corresponding to exactly the same values as the sampling of the graphite and silicate files.

For the wavelength range between 335 and 1000 µm, we model the absorption using a power law, $Q_{\text{abs},\text{PAH}}(\lambda, a) = \tau(a) \cdot (\lambda/\lambda_0)^{-\beta(a)}$ (Appendix B). We are interested in looking at the absorption coefficient behavior for different compositions (Figure 3). What we notice is that carbonaceous and silicate grains show quite a different power-law index as a function of the radius. Thus, one can expect to control the resulting emissivity power-law index $\beta$ for a collection of dust grains by changing composition or size. We use the power-law fit of the absorption optical properties to extend them to 10$^3$ µm. This range is more in line with future cosmic microwave background (CMB) experiments such as Primordial Inflation Explorer (PIXIE; Kogut et al. 2011).

2.2. Extinction

2.2.1. Extinction Modeling

For a given collection of dust grains along the line of sight, we want to calculate the extinction $A$, defined as:

$$A(\lambda) = m_{\text{attenuated}} - m_0 = 2.5 \log_{10} \frac{F_{\lambda}^0}{F_{\lambda}^s}, \quad (4)$$

where $F_{\lambda}^0$, $m_{\text{attenuated}}$ are the dust attenuated observed flux and magnitude of the object, and $F_{\lambda}^s$, $m_0$ are the flux and magnitude that would have been observed if there would have been no attenuation from dust. Thus, extinction can be related to the optical depth $\tau(\lambda)$ by $A(\lambda) = (2.5 \log_{10} e) \tau(\lambda)$. The optical depth is created from the contributions of each grain along the line of sight. Let $i$ be the index of the grain type, referring to graphite, PAHs, or silicates. For grains of radius $a$ of type $i$, their impact on the optical depth can be expressed as the product of an effective extinction cross section $C_{\text{ext}, i}(\lambda, a)$ and the column density $N_i(a)$. Then, the optical depth given by a distribution of grains of different radius $a$ is given by

$$\tau(\lambda) = \sum_i \int \frac{dN_i}{da} C_{\text{ext}, i}(\lambda, a) da. \quad (5)$$

The fraction of dust grains per radius becomes

$$\frac{dN_i(a)}{da} = \frac{d}{da} \int n_i(a, s) ds = \frac{d}{da} \int \left(\frac{n_i}{n_H}\right)(a, s)n_H(s)ds, \quad (6)$$

where $s$ is the path length along the direction of integration, $n_i$[grains cm$^{-3}$] is the number of dust particles of type $i$ per volume, $n_H$[atoms cm$^{-3}$] is the number of hydrogen atoms per volume, and $N_i$[atoms cm$^{-2}$] = $\int n_H(s)ds$ is the hydrogen column density. In this analysis we assume the dust to gas ratio is constant along the line of sight $s$. As a result,

$$\frac{dN_i(a)}{da} = \left(\int n_H(s)ds\right) \frac{1}{n_H} \frac{dn_i(a)}{da} = \frac{N_i}{n_H} \frac{dn_i(a)}{da}. \quad (7)$$

Using the fact that $da = ad \log a$, the optical depth can then be calculated as

$$\frac{\tau(\lambda)}{N_H} = \pi \sum_i \int \frac{1}{n_H} \frac{dn_i(a)}{da} Q_{\text{ext}, i}(\lambda, a)a^3d \log a. \quad (8)$$

3 The files that were used in this analysis can be found on Professor Bruce Draine’s website https://www.astro.princeton.edu/~draine/dust/dust.diel.html. The specific files are files Gra_81.gz, PAHion_30.gz, PAHneu_30.gz, and Sil_81.gz.

4 The file for graphite, Gra_81.gz, actually has 81 log-spaced radii between 10$^{-3}$ and 10 µm, but we use only the 61 between 10$^{-2}$ and 10 µm to complement the range of radius for the PAHs.
Wavelength and Frequency Values for the 10 Points Where We Compare the Modeled Extinction with the Extinction Data from the S16 Reddening Vector

| Filter | g | r | i | z | y |
|--------|---|---|---|---|---|
| $\lambda_{\mu m}$ | 0.503 | 0.6281 | 0.7572 | 0.8691 | 0.9636 |
| $\nu$(THz) | 595.8 | 477.3 | 395.9 | 344.9 | 311.1 |
| Filter | J | H | K | W1 | W2 |
| $\lambda_{\mu m}$ | 1.2377 | 1.6382 | 2.1510 | 3.2950 | 4.4809 |
| $\nu$(THz) | 242.2 | 183.0 | 139.4 | 90.98 | 66.90 |

The extinction $A_\lambda$ over the column density is

$$A_\lambda(\lambda) = \frac{(2.5 \log_{10} e) \pi}{N_H} \sum_i \int \frac{1}{n_H} \frac{dn_i(a)}{da} Q_{ext,i}(\lambda, a)a^3 d \log a.$$  

(9)

2.2.2. Extinction Data

S16 derived the dust extinction curve toward 37,000 stars in different directions across the sky. Using photometry from Pan-STARRS1 (Hodapp et al. 2004; Chambers et al. 2016), Two Micron All-Sky Survey (2MASS; Skrutskie et al. 2006) and the Wide-field Infrared Survey Explorer (WISE; Wright et al. 2010; Cutri et al. 2013), and spectra from the Apache Point Observatory Galactic Evolution Experiment survey (Eisenstein et al. 2011; Majewski et al. 2017), they performed a principal component analysis and found that the extinction function is well approximated by two principal components, called the vector $\mathbf{R}_0$ (constant across the directions in the sky) and a perturbation vector $\frac{d\mathbf{R}}{dx}$. Both $\mathbf{R}_0$ and $\frac{d\mathbf{R}}{dx}$ have norm 1. The extinction function can be expressed as

$$A_{Schlafly} = R_0 + x \frac{d\mathbf{R}}{dx},$$

(10)

where $x$ is a parameter that varies across the sky, with values between $0.4$ and $0.4$. Extinction laws are usually characterized by the parameter $R_V = \frac{A(V)}{A(B) - A(V)}$. However, since S16 did not have access to the distances to the stars, the absolute gray component of the extinction is not known. Instead, they approximate the $R_V$ parameter with $R'_V = 1.2 \frac{A(1.6) - A(2.2)}{A(1.6) - A(2.2)} - 1.18$. The parameter $x$ is related to $R'_V$ using Equation (11):

$$R'_V = 3.3 + 9.1x,$$

(11)

The intent was that $x = 0 (R'_V$ of $3.3$) corresponds to a mean reddening vector. However, this results in an $R'_V$ of $3.3$ at $h\nu > 13.6$ eV.

The reddening vector is specified at the wavelengths/frequencies showed in Table 1. These wavelengths/frequencies have been obtained by S16 by weighting over the M-giant star spectrum and over the bandpass of the detectors. $\nu_{\text{mean},b} = \int S_\nu F_\nu d\nu$, where $S_\nu$ is the M-giant spectrum, $b$ represents the index of the band (g, r, i, ...), and $F_\nu$ represents the filter weight.

Li et al. (2014) found that the aliphatic 3.4 $\mu$m C-H stretch absorption band is seen in diffuse clouds, and absent in dense regions. Therefore, for lines of sight with larger $R_V$, the 3.4 $\mu$m extinction band is weaker or even absent. This raises the question of whether $R_V$-based Cardelli et al. (1989) parameterization is valid only at $\lambda < 3$ $\mu$m. However, within the range of $E(B - V)$ measured in S16, they did not see evidence for significant variation in $3.4$ $\mu$m W1 and $4.6$ $\mu$m W2 WISE (Wright et al. 2010) bands. Since in this work we employ the extinction laws of S16, the $R_V$ parameter is used.

2.3. Grain Equilibrium Temperature as a Function of Radius

To calculate the thermal radiation emitted by a collection of dust grains, we need to know the temperatures of the grains. The grains are exposed to the ambient radiation field. In this calculation, we take into account only radiative heating and ignore the collisional heating that would be provided to the grains in the situation when they are surrounded by gas. In the case of dense clouds, however, this can become a relevant contribution.

Interstellar radiation field—We follow Section 4 of Wein-gartner & Draine (2001b) and use the ISRF model of Mezger et al. (1982) and Mathis et al. (1983). The radiation field as a function of frequency (Figure 4) is

$$\nu d\nu = \begin{cases} 0, & h\nu > 13.6 \text{ eV} \\ 3.328 \times 10^{-9} \text{ erg cm}^{-3}(h\nu/eV)^{-4.4172}, & 11.2 < h\nu < 13.6 \text{ eV} \\ 8.463 \times 10^{-13} \text{ erg cm}^{-3}(h\nu/eV)^{-1}, & 9.26 < h\nu < 11.2 \text{ eV} \\ 2.055 \times 10^{-14} \text{ erg cm}^{-3}(h\nu/eV)^{0.6678}, & 5.04 < h\nu < 9.26 \text{ eV} \\ (4\pi\nu/c) \sum_{i=1}^{3} w_i B_\nu(T_i), & h\nu < 5.04 \text{ eV} \end{cases}$$

(12)



Table 1

| Filter | g | r | i | z | y |
|--------|---|---|---|---|---|
| $\lambda_{\mu m}$ | 0.503 | 0.6281 | 0.7572 | 0.8691 | 0.9636 |
| $\nu$(THz) | 595.8 | 477.3 | 395.9 | 344.9 | 311.1 |
| Filter | J | H | K | W1 | W2 |
| $\lambda_{\mu m}$ | 1.2377 | 1.6382 | 2.1510 | 3.2950 | 4.4809 |
| $\nu$(THz) | 242.2 | 183.0 | 139.4 | 90.98 | 66.90 |

Fitzpatrick’s (1999) $R_V$ of 3.1. Subsequently, in this analysis, we use the notation $R_V$ to refer to the $R'_V$ from S16.
we would want to modify the radiation field to account for inhomogeneities in the interstellar medium, where we can have areas that are hotter than others. For that, as an approximation, we will multiply the radiation field by a factor \( \chi_{\text{ISRF}} \) that varies from 0.5–2.

The thermal equilibrium equation—For each grain radius \( a \), we assume thermal equilibrium between the absorbed radiation and emitted radiation \( (P_{\text{in}} = P_{\text{out}}) \). Figure 5 We assume the grain is spherical and emits like a black body of unknown temperature \( T \), which we aim to determine. The absorbed radiation is assumed to come from the ISRF surrounding the grain sphere uniformly.

The thermal equilibrium equation for one dust grain of size \( a \) is thus

\[
\int_{0}^{\infty} Q_{\text{abs}}(\lambda, a) \pi a^2 \chi_{\text{ISRF}} n_{\text{ISRF}}(\lambda) d\lambda
= \int_{0}^{\infty} Q_{\text{abs}}(\lambda, a) \pi a^2 \frac{4\pi}{c} B_\lambda(T) d\lambda.
\]

The integral in Equation (13) is taken over the wavelength range from \( 10^{-3} \) to 10 mm, using the extension shown in Appendix B. We obtain the equilibrium temperatures for four types of grains for different radii (Figure 6).

This method of calculation for the equilibrium temperature assumes that at each radius for each type of grain there is a single temperature. This approximation breaks down as the radius of the grain becomes small enough. A grain stays at an equilibrium temperature if no one photon it absorbs or emits carries enough energy to perturb the temperature much. Big grains have a thermal energy much larger than one photon. But small grains do not: a single photon with several eV carries more energy than the entire thermal energy of the grain, and the emission and absorption of a single quanta can create temperature spikes. In our calculation, we are considering grains as small as 3.55 Å; especially for grains smaller than \( 10^{-2} \) \( \mu \)m (like the PAHs), in a future study, there can be a benefit from replacing the approximation with a different method where one considers a temperature distribution for each radius size, as done in the work of Draine & Li (2001). However, in this work we are mainly interested in long wavelength emission where \( B_\nu(T) = B_\nu(T_\text{eq}) \).

In addition to the grain size and type, the variation of the ISRF throughout the ISM leads to variations in temperature. To reproduce this effect, we allow the ISRF multiplier parameter \( \chi_{\text{ISRF}} \) to vary between 0.5 and 2, and calculate the equilibrium temperature for the range (Figure 7).

2.4. Modeling Emission

2.4.1. Calculating the Emission Intensity from a Collection of Grains

The emissivity (power radiated per unit volume per unit frequency per unit solid angle) coming from a collection of grains is defined as

\[
j_\nu = \sum_i \int da \frac{dn_i}{da} C_{\text{abs},i}(\nu, a) B_\nu(T_{\text{eq}}(a)),
\]

where \( i \) is the index for carbonaceous, silicate, and PAH grains. The spectral intensity \( I_\nu \) is defined as the emissivity integrated along the line of sight \( s \):

\[
I_\nu = \int j_\nu ds = \int \left( \frac{j_\nu}{n_{\text{HI}}} \right) n_{\text{HI}}(s) ds.
\]

Since \( \frac{n_{\text{HI}}}{n_{\text{HI}}} \) is assumed to be constant along the line of sight, \( \frac{j_\nu}{n_{\text{HI}}} \) becomes constant along the line of sight as well. Using \( N_{\text{HI}} = \int n_{\text{HI}}(s) ds \), we obtain

\[
I_\nu = \frac{j_\nu}{n_{\text{HI}}} \int n_{\text{HI}}(s) ds = \frac{j_\nu}{n_{\text{HI}}} N_{\text{HI}}
= n_{\text{HI}} \sum_i \int da \frac{1}{n_{\text{HI}}} \frac{dn_i}{da} C_{\text{abs},i}(\nu, a) B_\nu(T_{\text{eq}}(a)).
\]
used in the optically thin limit. The power law parameterized by $\beta$ models the dependence of the emission cross section with frequency. The fit for the three parameters in Equation (17) is performed using data from four photometric bands: 353, 545, and 857 GHz from Planck, and 3000 GHz (100 $\mu$m) from IRAS (Beichman et al. 1988; Schlegel et al. 1998). Because these are the bandpasses the Planck Collaboration et al. (2014a) used in their analysis, to compare to their results, we evaluate the intensity at the same four bandpasses. We use the weighting given in Appendix B/Table 1 of Planck Collaboration et al. (2014a), and the corresponding response functions.5

3. Methods

The goal of this work is to explore the space of WD01 grain size distributions to find those that are consistent with our prior knowledge about dust, including:

1. the shape of the reddening curve and its variation with $R_V$,
2. the amount of reddening per H atom, and
3. the abundance of metals (C, Si, etc.) per H atom required to make dust.

For each sample from the WD01 parameter space, we compute the emission spectrum expected for dust in a reference radiation field, and fit the $\tau$, $\beta$, and $T$ parameters of an MBB as described in Section 2.4. Combining the emission and extinction for each sample, we can study the relation between the $R_V$ and $\beta$ parameters.

To perform our analysis, we create a reference extinction function, constrain the gray component of the extinction, normalize to physical values of extinction per column density of hydrogen ($A(I)/N_H$), impose physical boundaries on the parameters, and keep the total mass per H atom of the grain distributions within an expected range.

An MCMC-like algorithm is used to explore the available space for the size distribution parameters. However, MCMCs are not an optimization technique, and they can take a long time to converge on the points of high likelihood. To help the solver converge, an optimizer is run to obtain an initial guess for the MCMC. A possible downside is that by doing this, a region of the parameter space might remain unexplored.

Using the posterior points from the MCMC analysis we create the emissivity corresponding to the Planck bandpass filters and perform an MBB fit as described in section Section 2.4.

Using the data for extinction and emissivity, we explore the relation between the $R_V$ and $\beta$ parameters.

Creating the reference extinction functions—S16 focused on the shape of the reddening curve by using the relative extinction in 10 bands. Their work does not inform us about the gray component (which could not be measured without knowing the distance to each star) or the overall amplitude per H atom (which they did not measure). Therefore our first step is to establish a “target” reddening curve by setting an additive

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5 The spectral index data can be found in the file HFI_CompMap_Termal_DustModel_2048_R1.20.fits at https://irsa.ipac.caltech.edu/data/Planck/release_1/all-sky-maps/preview/HFI_CompMap_TermalDustModel_2048_R1.20/index.html. We select the directions in the sky to reproduce the same analysis done by S16, whose data is available at https://dataverse.harvard.edu/dataset.xhtml?persistentId=doi:10.7910/DVN/WMA5KJ. The HEALPIX binning used was NSIDE = 64.

6 The Planck filter files can be found on the website http://pla.esac.esa.int/ in the section called “Software, Beams, and Instrument Model”. At the time of this paper, Planck has 3 releases HFI_RIMO_R1.10.fits (2013), HFI_RIMO_R2.00.fits (2015), HFI_RIMO_R2.00.fits (2016). We use HFI_RIMO_R1.10 fits because it was the one used for the data release from the Planck Collaboration et al. (2014a). For IRAS, the filter files can be found on the website https://irsa.ipac.caltech.edu/IRASdocs/expmap/ch2/tabC5.html.
and multiplicative term to fix these degrees of freedom. The condition that \( A(H)/A(K) = 1.55 \) (Indebetouw et al. 2005) constrains the additive term as follows: we define \( A'_{\text{Schlafly}} = A_{\text{Schlafly}} + C_{\text{Schlafly}} \) with \( A_{\text{Schlafly}} = R_0 + x \frac{dR}{dx} \)

\[
A_{\text{Schlafly}}(H) + C_{\text{Schlafly}} = 1.55 = r
\]

\[
A_{\text{Schlafly}}(K) + C_{\text{Schlafly}}
\]

\[
A_{\text{Schlafly}}(H) + C_{\text{Schlafly}} = A_{\text{Schlafly}}(K)r + C_{\text{Schlafly}}r
\]

\[
C_{\text{Schlafly}} = \frac{A_{\text{Schlafly}}(H) - A_{\text{Schlafly}}(K)r}{r - 1}
\]

\[
A'_{\text{Schlafly}} = A_{\text{Schlafly}} + C_{\text{Schlafly}}.
\]

Fixing the gray component creates degeneracy between \( A(H) \) and \( A(K) \). To maintain the correct number of degrees of freedom, we remove the \( H \) band from the \( A \) vectors and therefore from the covariance matrix and the \( \Delta \chi^2 \) calculation. \( A(H) \) is determined by the other parameters and is no longer independent, so it can be ignored in the calculation and recovered at the end.

Having fixed the additive term, we now impose an extinction per \( N(H) \) assumption to fix the multiplicative term. Cardelli et al. (1989) suggested the convention that \( A(I)/N_H = 2.6 \times 10^{-22} \) cm². To be consistent with the extinction functions presented in WD01, we define \( A(I)/N_H = 3.38 \times 10^{-22} \) cm². We denote this quantity by \( C_{\mu} \), and the normalized extinction by

\[
\frac{A_{\text{Schlafly}}(\lambda)}{N_H} = \frac{A_{\text{Schlafly}}(\lambda)}{N_H} \times C_{\mu}.
\]

Volume of the dust grains—As we let the MCMC and the optimizer explore the parameter space, we want to make sure the size distribution does not require more atoms (per H) of C and Si than are available in the universe. As such, we want to have the total mass per H atom of the dust grains as an upper bound in the parameter limits. WD01 phrases this constraint in terms of the volume per H atom, so we use this notation in this analysis.

Thus, we introduce Gaussian volume priors. For consistency, we center the priors at the values adopted by WD01 for the volume found of each type of grain in the universe, with a standard deviation of 10%. For carbonaceous grains, the total expected volume is \( V_{\text{tot, g}} \approx 2.07 \times 10^{-27} \) cm³ H⁻¹, and for silicates \( V_{\text{tot, s}} \approx 2.98 \times 10^{-27} \) cm³ H⁻¹. The mean of the Gaussian in the prior is fixed for now but later in Section 4.1.1 we will vary it.

\( b_C \) represents the overall amplitude of the bumps; to calculate the PAH volumes, one needs to also add part coming from the non-\( D(\alpha) \) part of the size distribution, integrated over the range of the PAH radii.

Since \( C \) is an overall factor, it can be calculated from a proposed combination of volume \( V \) and parameters \( \alpha, \beta, \alpha_c, \) and \( \beta_c \). As a result, we replace the \( C \) parameter with a volume parameter \( V \), and calculate the corresponding \( C \) when needed for the size distribution calculations.

Thus, the 11 parameters explored by the MCMC are \( b_C, \alpha, \beta, \alpha_c, \beta_c, \alpha_g, \beta_g, \alpha_s, \beta_s, \alpha_t, \beta_t, \) and \( V_s \). Table 2 lists the boundaries for each parameter.

**Likelihood**—We want to compare to Schlafly’s reddening vector. For each proposed set of 11 parameter the MCMC makes, the volume parameters are transformed into the size distribution parameters (converting from a set of \( b_C, \alpha, \beta, \alpha_c, \beta_c, \alpha_g, \beta_g, \alpha_s, \beta_s, \alpha_t, \beta_t, V_s \) to a set of \( b_C, \alpha, \beta, \alpha_c, \beta_c, \alpha_g, \beta_g, \alpha_s, \beta_s, \alpha_t, \beta_t, C_s, C_g, C_t \)). Using the size distribution of the grains, the resulting extinction vector \( A/N_H \) is calculated at the nine wavelengths (after \( H \) was removed when fixing the gray component) from S16 using Equation (9).

Appendix A shows the calculation for the error in extinction that gives the covariance matrix \( \Sigma^{\alpha \beta} \), Equation (A11)) for each value of \( x \), based on the errors in the reddening vectors obtained by S16.

The extinction vector \( A/N_H \) is compared to the reference extinction vector obtained with Equation (19):

\[
\frac{A_{\text{residual}}}{N_H} = \frac{A}{N_H} = \frac{A_{\text{reference}}}{N_H}.
\]

The likelihood function is

\[
\ln \mathcal{L} = -\frac{1}{2} \Delta \chi^2,
\]

with the \( \chi^2 \) given by

\[
\Delta \chi^2 = \frac{A^2_{\text{residual}}}{N_H (\Sigma^{\alpha \beta})^{-1} A_{\text{residual}}}{N_H}.
\]

To the likelihood, we add the Gaussian prior on the volume

\[
\ln \text{prior} = -\frac{1}{2} \left( \frac{V_g - V_g,\text{reference}}{0.1 \cdot V_g,\text{reference}} \right)^2 - \frac{1}{2} \left( \frac{V_s - V_s,\text{reference}}{0.1 \cdot V_s,\text{reference}} \right)^2
\]

(22)

to obtain the posterior

\[
\ln \text{posterior} = \ln \text{prior} + \ln \mathcal{L}.
\]

Here \( V_g \) represents the sum of the volumes for the PAH and carbonaceous grains, and \( V_s \) the silicate grains.
3.1. Exploring the Dust Parameters’ Posterior Distribution with an MCMC

We sample from the posterior (Equation (23)) for a target extinction curve at fixed $R_V$ (Section 2.2.1) for each of 15 values of $R_V$ linearly spaced between 2.94 and 3.67. The posterior is conditional on $R_V$ instead of letting $R_V$ float, so that the uncertainty in the target extinction curve does not depend on the parameters at each step in the Markov chain. To expedite burn-in, we initiate the MCMC at a set of dust grain size distribution parameters determined by optimization.

The MCMC uses the ptemcee\textsuperscript{7} Vosunden et al. (2016) package that uses parallel tempering. This allows for a much more efficient exploration of the parameter space than something like the Metropolis–Hastings algorithm. We experimented with a number of temperatures between three and five, and found that there was no significant difference in the results, so we settled for three temperatures to reduce the computational time. Three-hundred walkers were run for each $R_V$, for 100,000 steps.

3.2. Studying the Correlation between Dust Emissivity and Absorption

Taking the final posterior distributions from all of the chains, and using the precomputed values of the temperature $T$ for each radius of the grain (Figure 6), we integrate to calculate the specific intensity, at each of the four bandpass frequencies of Planck.

The emitted radiation is modeled as an MBB shown using Equation (17), and fit to find the three parameters ($\tau_{353}$, $\beta$, $T$) corresponding to each sample from the MCMC. We generate the emission at the four wavelength bands corresponding to the Planck satellite, and then fit the four data points to the MBB law, using corresponding weighting and bandpass filters as used by the Planck team.

Next, we calculate the $R_V$ for the sample, and see if there is any correlation between $\beta$ and $R_V$, thus comparing to the results in S16 (Figure 11).

4. Results and Discussion

4.1. Correlation between Dust Extinction and Far-infrared Emissivity

We consider two hypotheses for the origin of the $R_V – \beta$ correlation:

1. the size distribution hypothesis, which attributes the variation in $R_V$ and $\beta$ to variations in grain size distribution, holding the volume (per H) of each species fixed, and\textsuperscript{8}

2. the composition hypothesis, which requires variation in the relative volumes of silicates and carbonaceous grains to vary as a function of $R_V$.

Fixing the volume priors in hypothesis I proved to be too restrictive: the MCMC does not explore the full range of the $\beta$ parameters (Figure 8). This fails to yield the observed $R_V – \beta$ correlation.

If an $R_V$-dependent prior on volumes is needed for hypothesis II, what form should it take?

4.1.1. Optimizer Results

To generate a hypothesis about what form of volume priors might give rise to the $R_V – \beta$ correlation, we begin by mapping out the volume parameter space $V_s$, $V_c$.

We use an optimizer to explore the effects of the volume priors on the resulting $\beta$. This framework is used instead of the MCMC in the beginning of the analysis in order to take advantage of the great increase in speed, which allows us to explore the parameter space of volume priors on a much finer grid. Thus, we can get an idea fast of which parameter combinations would provide useful results.

The Gaussian volume priors are defined to be centered at $V_{sil} = \alpha V_{sil} \cdot V_{0,sil}$, $V_{carb} = \alpha V_{carb} \cdot V_{0,carb}$, where $\alpha_{sil}$ and $\alpha_{carb}$ are

\textsuperscript{7} The code can be found at the Python repository at https://pypi.org/project/ptemcee/ or at the Will Vousden github repository at https://github.com/willvousden/ptemcee.

\textsuperscript{8} However, the Kramers–Kronig relation can be used to determine a lower bound on the volume of the grains for a given extinction function integrated over a finite wavelength interval (Porcelli 1969). Mishra & Li (2017) applied this relation to approximate the volumes for the silicate and carbonaceous grains. To perform this calculation, we would have to integrate over the UV part of the absorption, which is a bit uncertain (Peek & Schiminovich 2013), so it was not included in this work. Nevertheless, one should keep in mind that the bounds that we are proposing might be violating this relation slightly.
control parameters that we use to scale the total carbonaceous and silicate volumes up and down. $V_{0, \text{sil}}$ and $V_{0, \text{carb}}$ are the reference fiducial values for the volumes from WD01, as described in Section 3. We let $\alpha_{V_{\text{sil}}}$ and $\alpha_{V_{\text{carb}}}$ take values between 0.35 and 4.2, and sample the interval logarithmically at 50 values, creating a 50 by 50 grid for each $R_V$.

For each of the points in the grid, the $\chi^2$ returned by the optimizer is calculated. We smooth over the resulting image using a Gaussian filter with $\sigma = 1.5$, and calculate the contour plots over the resulting image.

For each $R_V$ panel, to compare with the expected $\beta$, we use a best fit line obtained from the $R_V$ versus $\beta$ data set from S16, given by Equation (24):

$$\beta_{\text{Schlafly}}(R_V) = 2.82 - 0.36 \cdot R_V. \quad (24)$$

Thus, for each $\beta$ obtained from the points in the grid, we calculate $\Delta \beta = \beta - \beta_{\text{Schlafly}}$. Using a Gaussian filter with $\sigma = 1.5$, we smooth over the resulting image, and calculate the contour plots. The resulting contour plots for both the $\chi^2$ and $\Delta \beta$ analysis are superimposed (Figure 9).

For each grid, we find the point of minimum $\chi^2$ that has $\Delta \beta = 0$. We read the corresponding $\alpha_{V_{\text{sil}}}$ and $\alpha_{V_{\text{carb}}}$ values, and plot them against $R_V$ (Figure 10). The points show a log-linear dependence. Performing linear fits of $\ln \alpha_{V_{\text{sil}}}$ versus $R_V$ and $\ln \alpha_{V_{\text{carb}}}$ versus $R_V$, the functions shown in Equations (25) and (26) are obtained:

$$\ln \alpha_{V_{\text{sil}}}(R_V) = -1.42 \cdot R_V + 5.32, \quad (25)$$

$$\ln \alpha_{V_{\text{carb}}}(R_V) = 1.66 \cdot R_V - 5.85. \quad (26)$$

This relation of the volume priors on $R_V$ also depends on extinction per $N(H)$, assumed to be $A_1/N_H = 3.38 \times 10^{-22} \text{cm}^2$ (beginning of Section 3). The $R_V$–$\beta$ relation itself does not depend on this assumption, because neither $R_V$ nor $\beta$ depend on the column density per se. However an increase in the assumed $A_1/N_H$ would require an increase in the volume (per H) of each species, by the same factor. In other words, a different $A_1/N_H$ convention would simply slide the contours in Figure 9 up and to the right. If a different $A_1/N_H$ is chosen, such as $A_1/N_H = 2.6 \times 10^{-22} \text{cm}^2$ (Zhu et al. 2017), the volume
Table 3
Optimized Parameter Values of the Dust Grain Size Distributions for Each \( \chi/R_\nu \) for Hypothesis II

| \( \chi \) | \( R_\nu \) | \( 10^3 \) bC | \( \alpha_\nu \) | \( \beta_\nu \) | \( a_{\nu,1} (\mu m) \) | \( a_{\nu,2} (\mu m) \) | \( 10^3 \nu \) (cm\(^3\) H\(^{-1}\)) | \( \alpha_c \) | \( \beta_c \) | \( a_{c,1} (\mu m) \) | \( a_{c,2} (\mu m) \) | \( 10^3 \nu_c \) (cm\(^3\) H\(^{-1}\)) |
|-----|-----|-----|-----|-----|-----|-----|----------------|-----|-----|-----|-----|----------------|
| -0.040 | 2.94 | 3.00 | -0.66 | 0.07 | 0.00035 | 0.68 | 0.813 | -1.83 | -5.41 | 0.16 | 0.19 | 8.355 |
| -0.034 | 2.99 | 3.00 | -0.72 | 0.12 | 0.06709 | 0.73 | 0.871 | -1.60 | -23.45 | 0.13 | 0.21 | 8.385 |
| -0.029 | 3.04 | 3.00 | -0.83 | -0.00 | 0.00035 | 1.02 | 0.975 | -1.59 | -20.81 | 0.22 | 0.11 | 7.460 |
| -0.023 | 3.09 | 3.00 | -1.47 | -0.00 | 0.00282 | 1.27 | 1.047 | -1.56 | -19.47 | 0.17 | 0.16 | 7.364 |
| -0.017 | 3.14 | 3.00 | -1.05 | -0.17 | 0.00883 | 1.34 | 1.111 | -1.94 | -2.78 | 0.21 | 0.14 | 7.187 |
| -0.011 | 3.20 | 3.00 | -1.49 | -0.00 | 0.00035 | 1.72 | 1.204 | -1.65 | -5.28 | 0.16 | 0.18 | 6.662 |
| -0.006 | 3.25 | 4.70 | -1.30 | -0.01 | 0.00119 | 1.41 | 1.315 | -1.76 | -8.79 | 0.35 | 0.00 | 6.496 |
| 0.000 | 3.30 | 4.66 | -1.30 | -0.08 | 0.00036 | 1.54 | 1.466 | -1.78 | -2.72 | 0.26 | 0.09 | 5.683 |
| 0.006 | 3.35 | 4.11 | -2.50 | 0.00 | 0.00141 | 1.53 | 1.526 | -1.23 | -6.84 | 0.14 | 0.20 | 5.176 |
| 0.011 | 3.40 | 5.40 | -1.93 | -0.01 | 0.00241 | 2.58 | 1.672 | -1.05 | -30.00 | 0.16 | 0.17 | 4.944 |
| 0.017 | 3.46 | 5.81 | -2.56 | 0.00 | 0.00035 | 1.78 | 1.868 | -0.80 | -20.84 | 0.18 | 0.14 | 4.176 |
| 0.023 | 3.51 | 5.94 | -2.01 | -0.00 | 0.00065 | 4.83 | 1.991 | -0.52 | -19.04 | 0.09 | 0.22 | 4.126 |
| 0.029 | 3.56 | 6.09 | -1.67 | -0.53 | 0.00041 | 2.48 | 2.110 | -0.61 | -4.43 | 0.15 | 0.17 | 3.684 |
| 0.034 | 3.61 | 6.07 | -2.85 | 0.02 | 0.00348 | 1.85 | 2.303 | -0.87 | -10.25 | 0.33 | 0.02 | 3.654 |
| 0.040 | 3.66 | 6.41 | -1.78 | -0.25 | 0.00047 | 3.68 | 2.406 | -0.50 | -3.92 | 0.19 | 0.14 | 3.325 |

The fits described in Section 4.1.1 represent a hypothesis for how carbonaceous and silicates volumes might change as a function of \( R_\nu \), and now we must validate that hypothesis using an MCMC analysis.

The resulting values for each parameter can be seen in Table 3. Using the functions found in Equations (25) and (26), we now set up volume priors correspondingly, and turn to performing an MCMC analysis as described in the Section 3.1. The optimizer is run with the new volume priors. The resulting values for each parameter (Table 3) are used as initializing points for the MCMC. We run 15 MCMCs for 15 \( R_\nu \) values linearly spaced between 2.936 and 3.664 (\( \chi \) varies between \(-0.04 \) and \( 0.04 \)). For each of the MCMC runs, we calculated the dust emissivity and the \( R_\nu \) for each sample from the posterior, using the procedure described in Section 3.2. The results can be seen in Figure 11. The spectral index \( \beta \) is spread between 1.4 and 1.8. The variation in spectral index value is significant, which indicates that having different size distributions of dust grains in different directions of the sky can motivate the need to model these different lines of sight with different spectral index values. The values of \( R_\nu \) and \( \beta \) obtained are in the same range as the ones obtained by S16. Most importantly, our values reproduce the trend of the \( R_\nu - \beta \) anticorrelation. The log posterior of all the end positions of the chains in the runs is contained within a modest range (Figure 12). The systematic uncertainty in the Planck \( \beta \) measurements is thought to be of order 0.05.
Volume and composition—As expected for hypothesis II, we find that a composition with higher ratio of carbonaceous to silicate grains leads to higher \( R_V \) and lower \( \beta \). (Figure 13)

While the functions (25) and (26) seem very precise, they do not represent unique solutions. We are making a plausibility argument, not a final determination of model parameters for a
firmed established model. One might be able to find other solutions that explain the $R_V - \beta$ correlation. But it is suggestive that $R_V$-dependent volume priors give this behavior, and fixed priors do not.

Size of grain distribution—One of the intuitive expectations of the analysis was that larger grains would lead to higher $R_V$. In order to test this hypothesis, we plot the cumulative density function of the volume of the grains versus radii. Figure 14 shows what percentage of the volume of the grains is made up of radii smaller than each possible radius value. For example, for the case of silicates, 80% of low $R_V$ volume is in grains with radius smaller than 0.1 $\mu$m, but 20% of high $R_V$ volume. For both silicates and carbonaceous grains, as $R_V$ increases, at least 50% of the volume is in grains of larger and larger size.

The size distributions coming from the posterior resulting from the MCMC are calculated (Figure 15). They reproduce acceptable size distributions as proposed by WD01 (Figure 2).

There is a broad range of parameters that can produce each $R_V$, but the distributions are largely distinct from each other as $R_V$ changes (Figure 16). Each parameter has a different impact on the $R_V - \beta$ anticorrelation (Figure 17). Further work may be warranted to isolate the effect of each parameter on $R_V$ independently of the others.

Ultraviolet extinction—The model is constrained to match the S16 extinction curve in 10 bands, but is not sufficient to constrain the 2175 Å feature. We compare extinction functions derived from the MCMC with reference functions from WD01 (calculated for the fourth row of Table 1 of WD01) and find good agreement across a wide wavelength range (Figure 18). In particular the 2175 Å feature varies between the Milky Way, Small Magellanic Galaxy, and Large Magellanic Galaxy Fitzpatrick & Massa (2007), with the feature being prominent in the Milky way and less prominent outside of it. The 2175 Å bump is often associated with PAHs (Joblin et al. 1992; Li & Draine 2001; Mishra & Li 2015) and in the WD01 model its amplitude is explicitly controlled by the $b_C$ parameter. Since in our study we were aiming to replicate the conditions in the Milky Way, we restricted $b_C$ to values greater than $3 \times 10^{-5}$ to make sure we have a minimum amount of PAH involved.

The maximum value of $b_C$ is set between (5.0, 6.5) as $R_V$ goes from low to high since the total volume of the carbonaceous grains increases with $R_V$ as well. The formula used is $\max b_C = 6 \times \frac{1}{(1 + 0.28 \times \tanh(\alpha_Rv - 1))}$.

4.2. Effect of the Interstellar Radiation Field

The effect of the ISRF on our analysis is very significant. As described in Section 2.3, we assume the ISRF is isotropic and homogeneous, an assumption which is obviously not reflected at the large scales of the universe where variations in proximity, types, and density of stars (and other objects), as well as the cloud thickness, influence the local ISRF dust grains are exposed to. To try to get a glimpse of what the effects of changing the ISRF look like, we modified the ISRF multiplication factor $\chi_{ISRF}$ over a log-spaced array with values between 0.5 and 2 (Figures 19 and 20). However, the effect is not that drastic, as a factor of 4 in $\chi_{ISRF}$ leads to a change of up to 0.1 in $\beta$ at low $R_V$ and 0.15 at high $R_V$.

In addition, the effect of the variation of the ISRF on the MBB temperature fit is explored, averaged for each of the 15 MCMC posterior points (Figure 20). For each $R_V$ value, a linear relationship is obtained between $\ln \tau_{MBB}$ and $\ln \chi_{ISRF}$. The slope of this linear function decreases as $R_V$ increases. One could expect the slope to be close to $1/(4 + \beta)$, and due to the $R_V-\beta$ anticorrelation relation discussed in this paper, the average value of $\beta$ decreases as $R_V$ increases. This would result in the slope increasing at higher $R_V$. However, the discrepancy is explained by the fact that we are doing an MBB fit over a collection of grains with variable dust composition. For each grain individually (Figures 3 and 7), the relationship $1/(4 + \theta)$ is recovered when calculating the equilibrium temperatures at different $\chi_{ISRF}$ Values. However, the value of the optical power law index $\theta$ varies with the type and size of grain (Figure 3). At high $R_V$, our runs have a higher ratio of carbonaceous to silicate than at low $R_V$. Since carbonaceous grains have higher $\theta$ than
silicate grains, it results in a lower slope obtained when integrating over the contributions from all the particles in the distributions to obtain the MBB fit.

Emission-based interstellar dust maps such as that in Schlegel et al. (1998) have been a very valuable tool for

4.3. Effect on $A(\lambda)/\tau_{353}$

Figure 16. Binned histograms of each of the 11 parameters of the size distributions, shown for three different $R_V$ MCMC runs. The distributions for each of the 11 parameters change substantially as $R_V$ changes, and are largely distinct from each other.
They make the assumption that the ratio of near-infrared extinction to the emission optical depth does not vary with $R_V$. Using the results for our 15 MCMC runs, we calculate the ratio of $A(\lambda)/\tau_{353}$ to see how it varies with $R_V$ (Figures 21 and 22).

We find that there can be a lot of variation in $A(\lambda)/\tau_{353}$. For the K band (Figure 21), the best fit power law for hypothesis II predicting extinction across the sky.
\[ \ln(A(\lambda)/3.38 \times 10^{-22} cm^2 N_H) = 4.00 \ln R_V + 4.36. \]  
(27)

For \( E(B - V)/\tau_{353} \) (Figure 22) the power law index is smaller, given by
\[ \ln(E(B - V)/\tau_{353}) = 1.72 \ln R_V + 7.91, \]  
(28)

and there is a tendency for it to be 20% lower at 2.9 and 20% higher at 3.7, compared to \( R_V = 3.3 \).

Figure 18. The left panel shows the extinction functions obtained from the MCMC for three values of \( R_V \) (2.993, 3.300, 3.664) for wavelengths ranging from far infrared to X-rays. Looking over the entire wavelength range, we can see that the extinction functions resulting from the MCMC are in agreement with the reference function from WD01. The right panel is a zoomed-in view on the UV feature at 2175 Å; the feature varies between the Milky Way, Small Magellanic Galaxy, and Large Magellanic Galaxy (Fitzpatrick & Massa (2007)), with the feature being prominent in the Milky Way and less prominent outside of it. The 2175 Å bump is often associated with PAHs (Joblin et al. 1992; Li & Draine 2001; Mishra & Li 2015) and in the WD01 model its amplitude is explicitly controlled by the \( b_C \) parameter. Since in our study we were aiming to replicate the conditions in the Milky Way, we restricted the \( b_C \) parameter to make sure we have a minimum of PAHs involved.

Figure 19. The emissivity of the collection of dust particles for each run is calculated using a modified ISRF multiplication factor \( \chi_{ISRF}. \) \( \chi_{ISRF} \) takes 10 log spaced values between 0.5 and 2. This results in the \( R_V - \beta \) correlation being shifted left and right relatively uniformly across \( R_V, \) with a change of up to 0.1 in \( \beta \) at low \( R_V \) and 0.15 at high \( R_V. \) For each \( \chi_{ISRF} \) value, the lines on the plot were generated from the 15 average \( R_V \) and \( \beta \) value from the MCMC posteriors.

Figure 20. The logarithm of the average \( T_{MBB}, \) for each of the 10 values of \( \chi_{ISRF}, \) for each of the 15 MCMC runs. This results in a linear relationship between \( \ln T_{MBB} \) and \( \ln \chi_{ISRF}. \) The legend shows the slope of the linear fit for each \( R_V \) value. The slope decreases with \( R_V, \) a result due to the variable dust composition, as explained in Section 4.2.

We took the \( E(B - V) \) of the stars studied by S16, and the corresponding \( \tau_{353} \) data from Planck Collaboration et al. (2016a), and obtained the average value of \( \mu_{E(B - V)/\tau_{353}} = 10,501. \) Figure 22 shows that both hypothesis are above this value. Hypothesis II is closer and thus preferred, but this indicates that the overall dust model could be improved.

This is a potentially impactful result that can motivate future research into the effect of \( R_V \) variation on emission-based interstellar dust map calibrations. The fact that sign of the trend changes depending on whether we assume \( R_V \) variation is caused only by size variation, or by size and composition variation, suggests that additional research will be required.
before we can confidently derive extinction from emission-based dust maps as \( R_V \) varies.

4.4. Correlation between Spectral Index and Temperature

Researchers have been looking at the \( T - \beta \) correlation and there is not quite a consensus on whether it is real (Dupac et al. 2003; Désert et al. 2008) or a subtle statistical artifact (Shetty et al. 2009; Kelly et al. 2012). To address this question we consider the MBB fit to models at varying \( R_V \) but with fixed radiation field \( (\chi_{\text{ISRF}} = 1) \). It is important to mention that we do not have noise in our model, thus, we cannot comment on studies that presented results on that. In addition, the optical properties of the dust grains can change with the temperature of the grains, and this can lead to a change in the spectral index. However, we do not account for this effect in our models, so we cannot probe this.

The intensity emission of the collection of dust particles is fit using an MBB function, as described in Section 2.4.2, for each point in the posterior resulting from the MCMC. When plotting the resulting distribution of the spectral index (\( \beta \)) as a function of the collective MBB temperature (\( T \)) we observe an anticorrelation (Figure 23).

One explanation for this interesting result is that \( T \) does not affect the long wavelength end very much, so if we boost those points (e.g., with more cold dust) to get the \( R_V \) correct, the fit must lower \( \beta \), but then that lower \( \beta \) means a higher \( T \) to get the peak in roughly the right place. As a result, there is a natural inverse correlation between \( T \) and \( \beta \) built into the problem.

At high \( R_V \) one has larger grains, and larger grains tend to have lower equilibrium temperatures (Figure 6). However, our runs also have different dust composition. Carbonaceous grains have higher temperature than the silicates, and the ratio of carbonaceous grains to silicate increases as \( R_V \) increases. This explains why in our results, higher \( R_V \) means higher temperature for the MBB fit over the collection of dust grains.

5. Conclusion

We started from the size distribution of the grains of dust, and we varied the parameters for it using an MCMC while adding the constraints from the reddening vector obtained by S16. We used the MCMC results to generate the dust emission spectrum for each sample from size distribution space. We suspected that the \( R_V - \beta \) correlation would arise naturally from the size distribution alone, but in the case of fixed total volume priors for each dust species, variation of \( R_V \)
does not produce an appreciable correlation. This is an interesting outcome, and to follow up in the search for a full explanation we force the $R_V - \beta$ and see what parameters give it. We find again that larger grains are correlated with high $R_V$, but in addition we find an explicit function of carbonaceous and silicates volume priors as functions of $R_V$ that gives the $R_V - \beta$ correlation and satisfy the constraints WD01 used. The properties of the optical absorption coefficients for carbonaceous and silicates offer an explanation for the results of the analysis; carbonaceous grains have optical properties that lower the $\beta$ for a collection of dust grains, while silicates raise it (Figure 3).

Widely used dust maps like those in Schlegel et al. (1998) and Planck Collaboration et al. (2016b) assume the ratio of $E(B-V)/\tau_{353}$ is constant. In Section 4.3, we find a dependence of $E(B-V)/\tau_{353}$ and $\Lambda(\lambda)/\tau_{353}$ on $R_V$. This dependence is a testable consequence of our understanding of the $R_V - \beta$ relation in the context of the WD01 models. Other optical models and size distribution parameterizations are possible, but if this dependence on $R_V$ persists in future models, it would have serious consequences for the recalibration of emission-based interstellar dust maps as a function of $R_V$.

Moreover, this result might provide some guidance on how to improve these dust models in the future. $E(B-V)/\tau_{353}$ can become an additional constraint used during modeling. Reproducing the correct function of $E(B-V)/\tau_{353}$ versus $R_V$ based on real data could be a good target for the next studies.

Modeling the size distribution and composition of dust is an area of active research. The parameterizations of the size distributions and the optical parameters of the grains can be revisited. An alternative model for the size distribution and optical parameters has been proposed by Zubko et al. (2004), which can be explored in a future work. In the future, we might have to explore grains that are a combination of both carbon and silicate. The model we are using here, though it reproduces many empirical facts about dust, is necessarily a simplification of nature. Future work may involve other materials, complex grain geometries, composites, and coatings, etc. Our work is intended as a plausibility argument, not a final determination of parameters for a truly complete model. One might be able to
find other solutions that explain the $R_V - \beta$ correlation. The robust effect we observe is that a composition with higher ratio of carbonaceous to silicate grains leads to more $R_V$ and lower $\beta$. It is an open question whether this tendency is a generic property of all dust models or if it is a specific feature of the precise dust models we are using.

The fact that larger $R_V$ corresponds to smaller silicate volume can be difficult to understand. Denser regions that have larger $R_V$ are expected to have depleted Si, Mg, and Fe from the gas phase. However, in the dense clouds it may not be possible to know how much hydrogen there is. Since we perform our calculations per $N_H$, this could play a significant role. Also, if the carbon is coming out of the gas faster than the silicate is, there might be more carbon per $N_H$ in the dust cloud. Carbonaceous grains could also be misidentified with grains coated with carbons. The exchange of carbon between the solid and gaseous phases of the ISM is not fully understood, but upcoming missions such as SPHEREx (Doré et al. 2014) will shed light on this issue.

This work depends critically on the S16 reddening vectors. Their pre-Gaia (Gaia Collaboration et al. 2016) analysis of the reddening law was performed in absence of information regarding distances to the stars whose extinction they were modeling. As a result, the absolute extinction cannot be determined, only the relative difference of extinction between bands, after the gray component had been removed from the analysis. This can be improved in future work when the gray component to the extinction can be fixed using Gaia measurements. In addition, this analysis is performed at fixed $A(I)/N(H)$, so we still have a free parameter left. If future data constrains $A(I)/N(H)$ as a function of $R_V - \beta$, we can modify the volume relations and get the similar results again with different functions, as $A(I)/N(H)$ scale linearly with the $b_c$, $C_3$, $C_5$ parameters combined.

The results of this study provide a possible explanation of the observed $R_V - \beta$ correlation in the context of the WD01, Laor & Draine (1993), Draine & Lee (1984), Li & Draine (2001) family of models. Although this explanation may not be unique, it increases our confidence that the $R_V - \beta$ correlation can be used to our advantage. For example, the relation can be use as a cross check for CMB experiments: one can start from a sensitive map of the sky in $R_V$, like one created from the data sets from LSST (LSST Science Collaboration et al. 2009), and determine the corresponding $\beta$. Conversely, one can make predictions of $R_V$ given precise measurements in $\beta$. The $R_V - \beta$ correlation provides valuable information about the size distribution and composition of interstellar dust grains, and may lead us toward a more complete model of the interstellar medium.

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9 http://mkweb.bcgsc.ca/biovis2012/color-blindness-palette.png
10 https://mariechatfield.com/simple-pdf-viewer/
Software: pteemce (Vousden et al. 2016), emcee (Foreman-Mackey et al. 2013), NumPy (van der Walt et al. 2011), Matplotlib (Hunter 2007), pandas McKinney (2010), scikit-learn (Pedregosa et al. 2012), IPython (Perez & Granger 2007), Python (Millman & Aivazis 2011; Oliphant 2007).

Appendix A
Error in Extinction

We calculate the errors in the extinction function to be used as a reference in the MCMC (Equation (19)). Denote with \( e_0 \) and \( e_1 \) the error vectors in \( R_0 \) and \( \frac{dR}{dx} \), respectively. The values for these error vectors are given in Table 2 of S16.

First, we calculate the error propagation in the extinction formula, given by \( A(\lambda) = R_0(\lambda) + x \frac{dR}{dx} \).

Let us assume we have a function \( y \) expressed as a linear combination of the variables \( x_i \):

\[
y(x) = \sum_i a_i x_i.
\]

(A1)

Let \( \Sigma^x \) be the covariance matrix for the parameters \( x_i \), such that

\[
\Sigma^x_i = E[(x_i - \mu_x)(x_k - \mu_x)].
\]

The mean (first moment) of \( y \) is then given by Equation (A2):

\[
E[y] = \mu_y = E\left[ \sum_i a_i x_i \right] = \sum_i a_i E[x_i] = \sum_i a_i \mu_x i,
\]

and the variance (second moment) by Equation (A3):

\[
\sigma^2_y = E[(y - \mu_y)^2] = E\left[ \left( \sum_i a_i x_i - \sum_i a_i \mu_x i \right)^2 \right] = E\left( \sum_i a_i (x_i - \mu_x i)^2 \right) = \sum_i \sum_k a_i a_k E[(x_k - \mu_x k)(x_i - \mu_x i)].
\]

(A2)

(A3)

Let \( \Sigma^A \) be the covariance matrix of \( A(\lambda) \). For our case, the coefficient vector is \( (1, x) \), and the variable vector \( x = \left( R_0(\lambda), \frac{dR(\lambda)}{dx} \right) \). S16 make the assumption that there is no covariance between the errors in the vectors \( R_0 \) and \( \frac{dR}{dx} \). As a result, only the diagonal terms of the covariance matrix are nonzero. Then the error \( \sigma_A(\lambda) \) is given by Equation (A4):

\[
\sigma^2_A(\lambda) = \sigma^2_0(\lambda) + x^2 \sigma^2_1(\lambda).
\]

(A4)

S16 also assume there is no covariance between the errors at different wavelength. As a result, the covariance matrix \( \Sigma^A \) is given by Equation (A5):

\[
\Sigma^A_{ij} = \delta_{ij} \sigma^2_A(\lambda).
\]

(A5)

Second, we calculate the error introduced by fixing the gray component \( A(\lambda) \rightarrow A(\lambda) + C \) such that \( A'(H)/A'(K) = 1.55 = r \) (Indebetouw et al. 2005):

\[
A'(\lambda) = A(\lambda) + C
\]

\[
C = \frac{1}{r^{-1}} A(H) - \frac{r}{r^{-1}} A(K)
\]

A'(\lambda) = A(\lambda) + \frac{1}{r^{-1}} A(H) - \frac{r}{r^{-1}} A(K)

(A6)

We calculate the error in \( A'(\lambda) \). Since the errors in the different bands from the reddening vector were not correlated, neither are the errors of \( A(\lambda) \). The \( r \) parameter comes from a measurement given with 10% precision. We keep \( r \) fixed in this analysis. The effect of having \( r \) values with ±10% difference can be easily explored by fixing \( r \) to different values and rerunning the analysis.

The covariance matrix of \( A'(\lambda) \) is given by Equation (A7):

\[
\Sigma^{A'}_{ij} = E[(A'(k) - \mu_{A'(k)})(A'(l) - \mu_{A'(l)})] = \Sigma^A_{ij} + \frac{1}{r^{-1}} (\Sigma^A_{kh} + \Sigma^A_{hk}) + \frac{1}{(r^{-1})^2} \Sigma^A_{kk}.
\]

(A7)

Due to fixing the gray component, the covariance matrix of \( A'(\lambda) \) is not diagonal, but it is still symmetrical.

The indexes of the matrix run over the 10 filters, in the order g,r,i,z,y,J,H,K,W1,W2. Labeling with \( b = \frac{\sigma^2_{A(H)} + \sigma^2_{A(K)}}{(r^{-1})^2} \),

\[
c = \frac{\sigma^2_{A(H1)} + \sigma^2_{A(W1)}}{(r^{-1})^2},
\]

\[
d = \frac{\sigma^2_{A(H2)} + \sigma^2_{A(W2)}}{(r^{-1})^2}.
\]

(A8)
Due to fixing of the gray component by requiring \( A(H)/A(K) = r \), the rows (and columns) of \( H \) and \( K \) in the covariance matrix are now related by the constant \( r \), making the covariance matrix singular. As such, we remove the row and column corresponding to the \( H \) band, and redefine the matrix in Equation (A9):

\[
\Sigma_A' = \frac{1}{\mu_{A'(l)}^2} C_{\mu_{A'}}^2 \begin{bmatrix}
\sigma_{A(l)^2} + b & b & b & b & b & b & b & b & b & d & b & b \\
 b & \sigma_{A(l)^2} + b & b & b & b & b & b & b & d & b & b & b \\
 b & b & \sigma_{A(l)^2} + b & b & b & b & b & d & d & b & b & b \\
 b & b & b & \sigma_{A(l)^2} + b & b & b & d & b & d & b & b & b \\
 b & b & b & b & \sigma_{A(l)^2} + b & d & d & b & d & b & b & b \\
 d & d & d & d & d & d & \sigma_{A(l)^2} + \sigma_{A(K)^2} & (r-1)^2 & d & d & \sigma_{A(l)^2} + \sigma_{A(K)^2} & d & d & b & b \\
 b & b & b & b & b & b & d & d & \sigma_{A(l)^2} + \sigma_{A(K)^2} & d & b & b & b & b & b & b & b \\
 b & b & b & b & b & b & d & d & \sigma_{A(l)^2} + \sigma_{A(K)^2} & d & b & b & b & b & b & b & b \\
 b & b & b & b & b & b & d & d & \sigma_{A(l)^2} + \sigma_{A(K)^2} & d & b & b & b & b & b & b & b \\
 b & b & b & b & b & b & d & d & \sigma_{A(l)^2} + \sigma_{A(K)^2} & d & b & b & b & b & b & b & b \\
 b & b & b & b & b & b & d & d & \sigma_{A(l)^2} + \sigma_{A(K)^2} & d & b & b & b & b & b & b & b \\
 b & b & b & b & b & b & d & d & \sigma_{A(l)^2} + \sigma_{A(K)^2} & d & b & b & b & b & b & b & b \\
 b & b & b & b & b & b & d & d & \sigma_{A(l)^2} + \sigma_{A(K)^2} & d & b & b & b & b & b & b & b \\
 b & b & b & b & b & b & d & d & \sigma_{A(l)^2} + \sigma_{A(K)^2} & d & b & b & b & b & b & b & b \\
\end{bmatrix}
\]

\( (A9) \)

The third step is to normalize at the third bandpass value of 7572 Å = 0.7572 μm, corresponding to the I filter. This is done in order to fix the extinction per hydrogen column density \((N_H)\) to the chosen prior convention value at the I band. As a result, we want to divide by the average of \( A'(l) \), \( \mu_{A'(l)} \), and multiply by our chosen prior convention value of \( C_{\mu_{A}} \):

\[
A''(\lambda) = \frac{A'(\lambda)}{\mu_{A'(l)}} C_{\mu_{A}}
\quad (A10)
\]

Since we treat the average of \( A'(l) \) as a fixed quantity without errors, the covariance matrix for the elements of the vector \( A'' \) (\( \lambda \)) is given by Equation (A11):

\[
\Sigma_{kl}'' = \frac{\Sigma_{kl}'}{\mu_{A'(l)}^2} C_{\mu_{A}}^2.
\quad (A11)
\]

---

### Appendix B

**Extending the Dust Optical Properties**

The optical properties of the dust grains were extended beyond the wavelengths given by Laor & Draine (1993), Draine & Lee (1984), and Li & Draine (2001), to values between 10^3 and 10^4 μm. The extension was done by modeling \( Q_{\text{radi}}(\lambda) = \tau (\lambda/\lambda_0)^{-\theta} \), with \( \lambda_0 = 1 \) mm and fitting for the \( \theta \) and \( \tau \) parameters for each radii, using the last 20 bins. Then, the optical parameters were calculated for the new range. The calculation was performed separately for the scattering and absorption coefficients (Figures 24–27).

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**Figure 24.** Extending the graphite optical properties for absorption and scattering between 10^3 and 10^4 μm. The gray-dotted line indicates the boundary of the extension.
Figure 25. Extending the silicate optical properties for absorption and scattering between $10^3$ and $10^4$ μm. The gray-dotted line indicates the boundary of the extension.

Figure 26. Extending the neutral PAH optical properties for absorption and scattering between $10^3$ and $10^4$ μm. The gray-dotted line indicates the boundary of the extension.
Figure 27. Extending the ionized PAH optical properties for absorption and scattering between 10³ and 10⁴ μm. The gray-dotted line indicates the boundary of the extension.

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