TWO PROBLEMS IN INTERSTELLAR GRAIN ALIGNMENT

by

Margaret E. Jordan
A Dissertation
Submitted to the
Graduate Faculty
of
George Mason University
In Partial fulfillment of
The Requirements for the Degree
of
Doctor of Philosophy
Physics

Committee:


Joseph C. Weingartner, Dissertation Director

Maria Dworzecka, Committee Member

Shobita Satyapal, Committee Member

Timothy D. Sauer, Committee Member

Michael E. Summers, Department Chair

Richard Diecchio, Associate Dean

Vikas Chandhoke, Dean, College of Science

Date: 11/23/10

Fall Semester 2010
George Mason University
Fairfax, VA
Two Problems in Interstellar Grain Alignment

A dissertation submitted in partial fulfillment of the requirements for the degree of
Doctor of Philosophy at George Mason University

By

Margaret E. Jordan
Master of Science
George Mason University, 2009
Bachelor of Science
University of California at Irvine, 1987

Director: Joseph C. Weingartner, Professor
Department of Physics and Astronomy

Fall Semester 2010
George Mason University
Fairfax, VA
Dedication

I dedicate this dissertation to Katharine and Bernard, my Mom and Dad, who encouraged me to see what might be possible, and to believe that I might be a part of that possibility.
I would like to thank the following people who made this possible. First and foremost, I would like to thank my advisor and dissertation director, Joe Weingartner, for his support, his patience and unwavering encouragement throughout my graduate work. Joe has been not only a mentor, but has also shown by example, what it means to rigorously pursue scientific understanding. It has been a real privilege to know and work with Joe these past few years. I would also like to thank the other members of my dissertation committee, Timothy Sauer, Shobita Satyapal and Maria Dworzecka, for investing their time and effort, and providing their wisdom and guidance during this process. I have also greatly benefited from the encouragement and humor of my officemate, colleague and friend Tim Frolov. Likewise, the time has been made better by conversations with officemate and fellow former-Hawaiian Insuk Jang. I will miss both of them and look forward to hearing of their successes in the future. Last, and certainly not least, I thank my son Malcolm and my long-suffering spouse and best friend Duncan, for having faith in me and supporting my dream, and without whom I can’t imagine having completed this journey.
# Table of Contents

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>List of Tables</td>
<td>vii</td>
</tr>
<tr>
<td>List of Figures</td>
<td>viii</td>
</tr>
<tr>
<td>Abstract</td>
<td>ix</td>
</tr>
<tr>
<td>1 Introduction</td>
<td>1</td>
</tr>
<tr>
<td>1.1 Dust grains and their environment</td>
<td>2</td>
</tr>
<tr>
<td>1.2 Grain alignment and disalignment mechanisms</td>
<td>7</td>
</tr>
<tr>
<td>1.2.1 Collisional gas disalignment</td>
<td>8</td>
</tr>
<tr>
<td>1.2.2 Davis-Greenstein or paramagnetic dissipation alignment</td>
<td>11</td>
</tr>
<tr>
<td>1.2.3 Magnetic dipole due to rotating charge</td>
<td>12</td>
</tr>
<tr>
<td>1.2.4 Barnett Effect Magnetic Dipole</td>
<td>13</td>
</tr>
<tr>
<td>1.2.5 Spin-Related Internal Alignment</td>
<td>14</td>
</tr>
<tr>
<td>1.2.6 Suprathermal Rotation from Surface Conditions</td>
<td>15</td>
</tr>
<tr>
<td>1.2.7 Radiative Torque Alignment: Grain Spin-up</td>
<td>15</td>
</tr>
<tr>
<td>1.2.8 Radiative Torque Alignment: Direct Alignment</td>
<td>17</td>
</tr>
<tr>
<td>2 The Grain Alignment Effects Due to Photoemission and Photodesorption</td>
<td>19</td>
</tr>
<tr>
<td>2.1 Introduction</td>
<td>19</td>
</tr>
<tr>
<td>2.2 Point Matching Method</td>
<td>22</td>
</tr>
<tr>
<td>2.2.1 Intensity results</td>
<td>29</td>
</tr>
<tr>
<td>2.3 Efficiency factors and torques</td>
<td>32</td>
</tr>
<tr>
<td>2.3.1 Results</td>
<td>37</td>
</tr>
<tr>
<td>2.4 Photoelectric efficiency factor and torque</td>
<td>43</td>
</tr>
<tr>
<td>2.4.1 Photoelectric yield</td>
<td>45</td>
</tr>
<tr>
<td>2.4.2 Results</td>
<td>45</td>
</tr>
<tr>
<td>2.5 Photodesorption</td>
<td>48</td>
</tr>
<tr>
<td>2.6 Barton method in spheroidal coordinates</td>
<td>50</td>
</tr>
<tr>
<td>2.7 Conclusion</td>
<td>64</td>
</tr>
<tr>
<td>3 The Effect of Time-varying Electric Dipole Moments on Grain Alignment</td>
<td>67</td>
</tr>
<tr>
<td>3.1 Introduction</td>
<td>67</td>
</tr>
</tbody>
</table>
## List of Tables

<table>
<thead>
<tr>
<th>Table</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1   Solar Abundances</td>
<td>3</td>
</tr>
<tr>
<td>1.2   Interstellar Radiation Field Components</td>
<td>6</td>
</tr>
<tr>
<td>3.1   Simulation Parameters and Outputs</td>
<td>107</td>
</tr>
</tbody>
</table>
## List of Figures

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>Intensity of the internal field of an oblate grain ($\lambda = 0.1\mu m$)</td>
<td>30</td>
</tr>
<tr>
<td>2.2</td>
<td>Intensity of the external field of an oblate grain ($\lambda = 0.1\mu m$)</td>
<td>30</td>
</tr>
<tr>
<td>2.3</td>
<td>Intensity of the internal field of an oblate grain ($\lambda = 0.15\mu m$)</td>
<td>31</td>
</tr>
<tr>
<td>2.4</td>
<td>Intensity of the external field of an oblate grain ($\lambda = 0.15\mu m$)</td>
<td>31</td>
</tr>
<tr>
<td>2.5</td>
<td>$Q_{abs}$ for prolate ($\zeta = 3/2$) grains with $a_{eff} = 0.2\mu m$</td>
<td>38</td>
</tr>
<tr>
<td>2.6</td>
<td>$Q_{abs}$ for oblate ($\zeta = 2/3$) grains ($0.2\mu m$)</td>
<td>39</td>
</tr>
<tr>
<td>2.7</td>
<td>$Q_{pr}$ for prolate ($\zeta = 3/2$) grains ($0.2\mu m$)</td>
<td>40</td>
</tr>
<tr>
<td>2.8</td>
<td>$Q_{pr}$ for oblate ($\zeta = 2/3$) grains ($0.2\mu m$)</td>
<td>41</td>
</tr>
<tr>
<td>2.9</td>
<td>$\lambda Q_{\Gamma, y}$ for prolate ($\zeta = 3/2$) grains ($0.2\mu m$)</td>
<td>41</td>
</tr>
<tr>
<td>2.10</td>
<td>$\lambda Q_{\Gamma, y}$ for oblate ($\zeta = 2/3$) grains ($0.2\mu m$)</td>
<td>42</td>
</tr>
<tr>
<td>2.11</td>
<td>$\bar{Q}<em>{\Gamma, y}$ for prolate ($\zeta = 3/2$) and oblate ($\zeta = 2/3$) grains with $a</em>{eff} = 0.2\mu m$</td>
<td>42</td>
</tr>
<tr>
<td>2.12</td>
<td>The $y$-component of the torque asymmetry factor $A_{\Gamma}$</td>
<td>47</td>
</tr>
<tr>
<td>3.1</td>
<td>Parameters for trajectories of incoming charged particles</td>
<td>81</td>
</tr>
<tr>
<td>3.2</td>
<td>$\bar{J}$ vs. $\gamma$ for various values of $</td>
<td>\eta</td>
</tr>
<tr>
<td>3.3</td>
<td>$g(\cos \theta)$ vs. $\cos \theta$ for $\gamma = 0$ and various values of $\eta$</td>
<td>91</td>
</tr>
<tr>
<td>3.4</td>
<td>$g(\cos \theta)$ vs. $\cos \theta$ for $\eta = 10^2$ and various values of $\gamma$</td>
<td>91</td>
</tr>
<tr>
<td>3.5</td>
<td>$z$ component of dipole moment vs. time (perfect insulator, $a = 0.1 \mu m$)</td>
<td>110</td>
</tr>
<tr>
<td>3.6</td>
<td>$\cos \theta_{align}$ vs. time (perfect insulator, $a = 0.1 \mu m$, $\omega/\omega_T = 10^2$)</td>
<td>111</td>
</tr>
<tr>
<td>3.7</td>
<td>Disalignment time vs. suprathermality for perfectly insulating grains</td>
<td>111</td>
</tr>
<tr>
<td>3.8</td>
<td>$\tau_{dis}/\tau_{ins}$ for various models</td>
<td>112</td>
</tr>
<tr>
<td>3.9</td>
<td>$\tau_{cond}/\tau_{ins}$ for a perfectly conducting grain</td>
<td>112</td>
</tr>
</tbody>
</table>
Abstract

TWO PROBLEMS IN INTERSTELLAR GRAIN ALIGNMENT
Margaret E. Jordan, PhD
George Mason University, 2010
Dissertation Director: Joseph C. Weingartner

Starlight observed through the diffuse interstellar medium of the Galaxy is polarized and the polarization appears to track the Galactic magnetic field. This polarized starlight has been associated with non-spherical dust grains aligned with the magnetic field, and both grain aligning and disaligning mechanisms have been explored to explain the polarization. Radiative torques due to anisotropic stellar radiation incident on asymmetric grains appears to play a dominant role in alignment. Here, we investigate the importance relative to radiative torque alignment, of two possible effects on the grain’s alignment. The first is due to recoil torques as electrons and H atoms leave the grain surface and the second is due to a grains’s time-varying electric dipole moment.

A grain irradiated by starlight may experience photoelectric emission, as well as photodesorption of adsorbed surface H atoms. Each ejection event imparts an angular impulse to the grain; integrated over the grain surface, they produce non-zero net recoil torques in the grain. The effects of these torques on grain alignment is the first subject of this dissertation. To evaluate these torques we constructed models of spheroidal grains irradiated by an anisotropic radiation field, and evaluated the resulting electric field intensities immediately below and immediately above the grain surface. The variation of the internal electric field intensity with surface position provides a measure of the photoelectric emission asymmetry.
We used this asymmetry to estimate the photoelectric recoil torque on the grain. In the case of photodesorption, variation of the external electric field with surface position is used to estimate the recoil torque due to photodesorption. The maximum photoelectric torque was found to be $\sim 35\%$ the radiative torque, and the maximum photodesorption torque was $\sim 30\%$ of the photoemission torque. Because we set the conditions to maximize the torques in order to judge their relative importance, the torque contributions may be overestimated and actual torques may be on the order of $10\%$ or less of radiative torques. Given this relatively small contribution to the total torque and that additional model uncertainties contribute at comparable or greater levels, we conclude that photoelectric and photodesorption torques need not be included in radiative torque alignment models.

Charging processes, both the capture and emission of electrons from the grain, result in a net charge and an electric dipole moment that continually change for the grain. Recent analysis has shown that this changing dipole moment, in a grain drifting across the Galactic magnetic field lines, has the potential to disalign the grain. In the second half of this dissertation, the effects of the time-varying electric dipole on grain disalignment are explored. Previously, disalignment was presumed to be due principally to random collisions with interstellar gas atoms. Any successful alignment mechanism would have to align the grain on a timescale shorter than that of collisional disalignment. This is precisely what was found for radiative torque alignment. However, this new disalignment mechanism has the potential to act on a shorter timescale yet, and our investigation was designed to estimate this timescale. We considered four grain charge transport models, each subject to simulated individual charging events as a result of photoemission and capture of electrons, and tracked the effect of these events on the dipole magnitude and orientation for simulated times of up to $10^5$ years. These models covered a range of internal charge transport types, from perfect insulator to perfect conductor, and a range of rotational speeds. Our results indicate disalignment timescales that are shorter than the timescales for radiative torque alignment, even for grains rotating suprathermally. This poses a potentially significant challenge for radiative torque alignment.
Chapter 1: Introduction

Observation of the night sky has long revealed areas of darkness, showing an absence of starlight. Close examination of these dark regions has shown that stars are present but that the light has been extinguished. Further observation showed that this extinction, to varying degrees, was present throughout the Galaxy. In 1949 fractional linear polarization of starlight, on the order of a few percent, was observed widely throughout the Galaxy by Hiltner and Hall [27][26][23], and for a variety of stellar types.

The polarization was correlated with the observed extinction, with areas of greater linear polarization also showing greater extinction. The fact that the observed polarization was the same for different types of star at the same distance and in the same location pointed to a polarization mechanism that was independent of stellar processes. A model was developed to explain the linear polarization and extinction as a result of the presence of non-spherical, partially aligned dust grains in the interstellar medium, acting as a filter for observations from Earth and its orbiting observatories. These aligned grains attenuate more of the component of the electric field that coincides with the major axis of each grain, producing the observed linearly polarized starlight.

With this model of non-spherical dust grains as agents of polarization for the incident starlight, there remained the question of how the dust grains could be partially aligned to produce the observed polarization. When the polarization is observed and mapped for the entire night sky, that map shows some coherence of the polarization vectors on very large scales. This indicates that the Galactic magnetic field must somehow be relevant to the observed polarization, and in fact, the observed polarization has proven an important tool in mapping and understanding the Galactic magnetic field.

So, the model needed to explain the observed linearly polarized light must include non-spherical dust grains partially aligned with respect to the Galactic magnetic field.
examining some mechanisms for grain alignment, we first need to understand something of the nature of the dust grains and their environment.

### 1.1 Dust grains and their environment

Though there have been no sample-returns of interstellar dust grains available for examination, there is ample evidence of the existence of dust in the interstellar medium (ISM). This evidence comes in the form of wavelength-dependent extinction of starlight, excess infrared (IR) emission, polarized starlight, reflection nebulae, and the depletion of heavy elements in ISM gas. The earliest conclusive evidence of interstellar dust was the wavelength-dependent extinction of starlight from distant stars. The extinction curve (a plot of the extinction vs. wavelength) has features such as the strong ultraviolet bump ($\lambda_{\text{peak}} = 2175\,\text{Å}$) indicating the likely presence of aromatic carbon, broad featureless absorption features at 9.7 and 18$\mu$m due to bending and stretching modes of amorphous silicates, strong absorption along some lines of sight at 3.1$\mu$m indicating water ice, and more than 100 other features indicating unknown chemical constituents of interstellar dust.

In addition to the extinction spectra that point to the presence of interstellar grains, there are emission spectra that show substantial luminosity in the IR range. At the long wavelength end of the IR emission spectrum (FIR) is a component that is due to the re-radiation of starlight absorbed by dust grains. The grains absorb more effectively in the UV and visible range and radiate more effectively in the FIR. The short wavelength end of the IR emission spectrum is dominated by features caused by polycyclic aromatic hydrocarbons (PAHs), rings of $\gtrsim 10 - 50$ C atoms with H atoms bound to the outside of the rings. These broad features are indicative of the stretching and bending modes of C-C and C-H bonds, and the very broadness of the features points to a wide variety of PAH molecule types.

As discussed above, we also see large-scale polarization of starlight that correlates with the Galactic magnetic field. This polarization is caused by the excess extinction of radiation along the major axis of a non-spherical grain. Finally, we see the evidence for dust in the
Table 1.1: Solar Abundances

<table>
<thead>
<tr>
<th>Element</th>
<th>( b )</th>
<th>( c )</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>8.43</td>
<td>8.43</td>
</tr>
<tr>
<td>N</td>
<td>7.83</td>
<td>7.83</td>
</tr>
<tr>
<td>O</td>
<td>8.69</td>
<td>8.69</td>
</tr>
<tr>
<td>Ne</td>
<td>7.93</td>
<td>7.93</td>
</tr>
<tr>
<td>Na</td>
<td>6.27</td>
<td>6.24</td>
</tr>
<tr>
<td>Mg</td>
<td>7.53</td>
<td>7.60</td>
</tr>
<tr>
<td>Al</td>
<td>6.43</td>
<td>6.45</td>
</tr>
<tr>
<td>Si</td>
<td>7.51</td>
<td>7.51</td>
</tr>
<tr>
<td>S</td>
<td>7.15</td>
<td>7.12</td>
</tr>
<tr>
<td>Ar</td>
<td>6.40</td>
<td>6.40</td>
</tr>
<tr>
<td>Ca</td>
<td>6.29</td>
<td>6.34</td>
</tr>
<tr>
<td>Cr</td>
<td>5.64</td>
<td>5.64</td>
</tr>
<tr>
<td>Mn</td>
<td>5.48</td>
<td>5.43</td>
</tr>
<tr>
<td>Fe</td>
<td>7.45</td>
<td>7.50</td>
</tr>
<tr>
<td>Ni</td>
<td>6.20</td>
<td>6.22</td>
</tr>
</tbody>
</table>

\(^a\)Given as \( \log \epsilon_i \equiv \log N_i/N_H + 12 \) [3]

\(^b\)Recommended solar photospheric abundances for C, N, O, Ne and Ar; CI chondritic meteoritic values for the other elements [63]

\(^c\)Recommended solar photospheric abundances for all elements listed

scattered light of “reflection” nebulae. When a star is located in close proximity to a dust cloud, the scattered light can be intense enough to create an apparent visible glow in the dust cloud.

Interstellar grains are composed of molecular and atomic constituents drawn from the surrounding ISM gas. Therefore, elements depleted from an expected gas mix provide evidence for the composition of grains found within the gas. In order for this to be useful in determining grain composition, a baseline for gas elemental abundances, absent grains, is required. The baseline at use in current models is that of solar abundances, assuming that the solar neighborhood abundances are representative of Galactic abundances if no grains are present. The most recent recalculation of solar photospheric abundances for the volatile elements and CI chondritic meteoritic values [63] are shown in Table 1.1

Spectroscopic analysis of the diffuse clouds toward \( \xi \) Persei and \( \zeta \) Ophiuchi (see review by Savage & Sembach [62]), showed that of those elements of greatest expected abundance
(based on solar abundances), the most highly depleted were Ca, Fe, Ni, Mg, and Si. And although not highly depleted, the very high abundance levels of C and O meant that many of these atoms were missing from the gas phase. When the spectroscopic evidence of dust, as discussed above, in both absorption and emission is combined with the abundances and depletions observed in diffuse clouds, a fairly strong case is made for the presence of silicate and carbonaceous grains. There remain many uncertainties about the precise chemical compositions of dust grain populations, but it seems reasonable to adopt models consistent with silicate and graphitic compositions.

Based on the abundance/depletion evidence and emission and absorption spectra in ISM observations, one popular dust model adopts a 2 grain-type population, with silicate and graphitic grains. Size distributions for these two populations are obtained by fitting wavelength-dependent extinction from these populations to the observed extinction curve between the NIR and the UV. Mathis, Rumple & Nordsieck [51] first developed a grain size distribution based on spherical grains for these two populations. Modifications have been made to this model, as extinction observations have improved. The wavelength dependence of polarized starlight in the diffuse ISM shows a peak at $\lambda \sim 0.6\mu m$, with the most effective polarization occurring when

$$\frac{2\pi a}{\lambda} \sim 1 \quad (1.1)$$

where $a$ is the effective grain radius. This points to a large population of $\gtrsim 0.1\mu m$ grains responsible for the polarized starlight [38].

We are interested in the dust that is responsible for the observed starlight polarization. Polarization is seen for the extinction features at 9.7 and 18$\mu$m, corresponding to silicate grains, but not generally for the 2175Å feature associated with aromatic carbon. The broadening of the 9.7 and 18$\mu$m features indicate that the grains are made of amorphous rather than crystalline material. The depletion levels of non-carbon elements from the diffuse gas of the ISM provide the constituents for silicates such as olivine and pyroxine, and the most likely size for a polarizing dust grain is in the submicron range, as noted in
The dust grains are surrounded by vast regions of ISM gas. The gas of the interstellar medium is not a homogeneous mix, but rather is observed as distinct regions, each with characteristic density, temperature, and atomic and molecular composition. These distinct regions are the phases of the interstellar medium: the atomic hydrogen regions (HI) comprised of the cold neutral medium (CNM) and the warm neutral medium (WNM); the ionized hydrogen regions (HII) comprised of the warm ionized medium (WIM), photoionized nebulae and hot ionized medium (HIM) or coronal gas; and cold, dense molecular clouds. The diffuse CNM where polarized starlight is observed has a typical gas temperature of $T_{\text{gas}} \sim 100$ K.

The interstellar radiation field (ISRF) provides an energy source for the ISM. It is a composite field with contributions from stars, radiating gas and dust, and the cosmological microwave background radiation (CMB). The stellar contribution covers the range from the far ultraviolet (FUV) to the far infrared (FIR). OB-type stars provide the majority of the UV contribution, while A-type stars create most of the visible light. Late-type red giants provide infrared contributions to the composite field. Large molecule (small dust) polycyclic hydrocarbons (PAHs) and dust grains radiate in the IR range, and the CMB is the major and pervasive contributor to the microwave portion of the spectrum. Above the FUV Lyman cut-off in atomic media (HI), the intensity of the ISRF drops by orders of magnitude, as hydrogen ionization removes most of this portion of the composite field. The main contributors to this part of the spectrum come from hot gas, especially the very high-temperature coronal gas.

In 1982 and 1983 Mathis, Mezger & Panagia [52][50] provided an estimate of the average interstellar radiation field (ISRF) flux for the solar neighborhood, shown in equation 1.2 in terms of the energy density $u$ across the ISRF spectrum [17].
Table 1.2: Interstellar Radiation Field Components

<table>
<thead>
<tr>
<th>Radiation Field</th>
<th>$u_{rad}$ (ergs cm$^{-3}$)</th>
<th>$\lambda$(µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>UV [eq.(xx)]</td>
<td>$7.13 \times 10^{-14}$</td>
<td>0.1566</td>
</tr>
<tr>
<td>$W = 1 \times 10^{-14}, T = 7500$ K ($\lambda &gt; 2460$ Å)</td>
<td>$2.29 \times 10^{-13}$</td>
<td>0.7333</td>
</tr>
<tr>
<td>$W = 1.65 \times 10^{-13}, T = 4000$ K ($\lambda &gt; 2460$ Å)</td>
<td>$3.19 \times 10^{-13}$</td>
<td>1.3319</td>
</tr>
<tr>
<td>$W = 4 \times 10^{-13}, T = 3000$ K ($\lambda &gt; 2460$ Å)</td>
<td>$2.45 \times 10^{-13}$</td>
<td>1.7755</td>
</tr>
<tr>
<td>ISRF</td>
<td>$8.64 \times 10^{-13}$</td>
<td>1.2021</td>
</tr>
</tbody>
</table>

\[
\lambda u_{\text{ISRF}, \lambda} = \begin{cases} 
0 & \lambda < 912 \, \text{Å} \\
1.287 \times 10^{-9} \, (\lambda/\mu\text{m})^{4.4172} \, \text{erg cm}^{-3} & 912 \, \text{Å} - 1100 \, \text{Å} \\
6.825 \times 10^{-13} \, (\lambda/\mu\text{m}) \, \text{erg cm}^{-3} & 1100 \, \text{Å} - 1340 \, \text{Å} \\
2.373 \times 10^{-14} \, (\lambda/\mu\text{m})^{-0.6678} \, \text{erg cm}^{-3} & 1340 \, \text{Å} - 2460 \, \text{Å} \\
(4\pi\lambda/c) \sum_{i=1}^{3} W_i B_\lambda(T_i) & \lambda > 2460 \, \text{Å}
\end{cases}
\]

where $W_i$ is a dilution factor and $T_i$ a the blackbody temperature, as given in Table 1.2, and $B_\lambda$ is the Planck function. The last line of Table 1.2 gives the total energy density across the entire ISRF spectrum.

Draine & Weingartner in 1996 [17] assumed an anisotropy of the typical interstellar radiation field due to local variations in dust attenuation and the proximity of stellar sources, as well as overall concentration of starlight towards the Galactic center. In 2001, Weingartner & Draine [70] examined ISRF anisotropy, this time looking at the UV and visible range of the ISRF spectrum for the solar neighborhood, to quantify the local anisotropy. Because the major contribution in the UV and visible range is due to starlight, they summed the contributions for all cataloged stars in the specified range, finding an anisotropy of $\approx 10\%$ in the visible and UV range. The solar neighborhood ISRF with $\approx 10\%$ anisotropy is our assumed ISRF environment for grains in the diffuse ISM. The grain temperature is determined by the radiative energy balance, as the grain absorbs incident radiation from the
ISRF primarily in the FUV and re-radiates that energy in the IR. Silicate grains with radii in the submicron size range, in the diffuse ISM, have typical temperatures $T_{gr} \approx 15 \text{ K}$.

The grain environment also includes the Galactic magnetic field. The Galactic field shows large scale structure and some uniformity near the Galactic plane, but is largely characterized by chaotic non-uniformity. The source of the original magnetic field for the Galaxy is unknown, but the coupling of the field with the ISM explains at least some of the subsequent movement and observed structure in the field. This field strength in the solar region is $\approx 5 \mu \text{G}$, and increases towards the Galactic center. We adopt a field strength in the diffuse ISM of $\approx 5 \mu \text{G}$. The typical H number density of the CNM is $\approx 30 \text{ cm}^{-3}$.

The elemental composition of the interstellar gas (other than that found in the molecular clouds), is $\sim 90\%$ hydrogen, $\sim 10\%$ helium and $\lesssim 1\%$ heavier elements (as seen above in Table 1.1).

With this brief description of the aligned polarizing dust grains and their environment, we are now ready to consider grain alignment mechanisms.

### 1.2 Grain alignment and disalignment mechanisms

The first approach considered to explain grain alignment was that of direct magnetic alignment of ferromagnetic grains. Earlier spectroscopic observations of the interstellar medium led Spitzer and Tukey [66] to reason that Fe was bound up in dust grains, and might even be present at high enough levels to produce ferromagnetic grains. They proposed that a grain acted like the needle of a compass, lining up with the Galactic magnetic field lines. This approach requires a magnetic field strength greater than $10^{-4} \text{ G}$ to produce grain alignment. However, the Galactic magnetic field is only on the order of $5 \times 10^{-6} \text{ G}$, so this approach was abandoned.

In considering new alignment approaches, the rotational behavior of the non-spherical grain allows a separation of grain alignment into two components. The first is “internal” alignment of the principal axis of greatest moment of inertia $\hat{a}_1$ with the spinning grain’s
angular momentum vector, $J$, and the second is “external” alignment of $J$ with the Galactic magnetic field vector $B$. Both internal and external alignment are required to achieve overall grain alignment.

The search for other magnetic alignment mechanisms led Davis and Greenstein [9] to descriptions of both a disaligning mechanism due to gas collisions with the grain, and an external aligning mechanism based on paramagnetic dissipation coupled with an internal alignment due to the equipartition of rotational energy. First, we consider the disalignment of the grain caused by collisions with gas atoms in the surrounding ISM.

1.2.1 Collisional gas disalignment

A dust grain in the diffuse ISM will collide with gas atoms in the surrounding gas. These collisions will cause the grain to spin. In the absence of any other force, the energy of rotation about any coordinate axis will be

$$E_{\text{rot}} \simeq \frac{1}{2} k_B T_{\text{gas}} \quad (1.3)$$

where $T_{\text{gas}}$ is the temperature of the surrounding gas, approximately 100 K for the CNM, and $k_B$ is the Boltzmann constant. This is known as “thermal rotation”. The frequency of thermal rotation $\omega_T$ can be obtained from the equipartition relation between the rotational energy and the gas temperature:

$$\frac{I \omega^2}{2} = \frac{1}{2} k_B T_{\text{gas}} \quad (1.4)$$

where $I$ is the moment of inertia of the grain rotating about a single axis. Assuming a spherical grain of radius $a$,

$$\omega_T = \left( \frac{k_B T_{\text{gas}}}{I} \right)^{1/2} = \left( \frac{k_B T_{\text{gas}}}{\frac{5}{2} M_{\text{gr}} a^2} \right)^{1/2} \quad (1.5)$$
With $M_{\text{gr}} = \frac{4}{3} \pi \rho a^3$, where $\rho$ is the density of the grain

$$\omega_T = \left( \frac{15 k_B T_{\text{gas}}}{8 \pi \rho a^5} \right)^{1/2}$$  \hspace{1cm} (1.6)

$$\omega_T = 1.66 \times 10^5 \left( \frac{\rho}{3 \text{g cm}^{-3}} \right)^{-1/2} \left( \frac{T_{\text{gas}}}{100 \text{ K}} \right)^{1/2} \left( \frac{a}{0.1 \mu\text{m}} \right)^{-5/2} \text{s}^{-1}. \hspace{1cm} (1.7)$$

This is the typical rotational speed if no torques other than those due to colliding gas atoms act on the grain.

The gas collisions with the grain are random in orientation, so that the direction of angular impulse imparted to the dust grain is also random. Because of this, the grain may experience disalignment as well as rotation. Davis and Greenstein [9] determined the timescale associated with this collisional disalignment, employing an approximation for a cumulative angular momentum change that results in an angular displacement of $\mathbf{J}$ of 1 rad.

For a hydrogen gas atom of mass $m_H$ and linear speed $v_H$, the magnitude of the angular momentum imparted to a grain with radius $a$ by the atom on impact, is $\Delta J \sim a m_H v_H$. Since,

$$v_H \sim \left( \frac{k_B T}{m_H} \right)^{1/2},$$  \hspace{1cm} (1.8)

where $k_B$ is the Boltzmann constant, the change in grain angular momentum associated with each colliding hydrogen atom is

$$\Delta J \sim m_H \left( \frac{a^2 k_B T}{m_H} \right)^{1/2} = \left( \frac{m_H}{M_{\text{gr}}} \right)^{1/2} \left( a^2 k_B T M_{\text{gr}} \right)^{1/2}, \hspace{1cm} (1.9)$$

where $M_{\text{gr}}$ is the mass of the grain. The magnitude of the total angular momentum of the
grain $J$ is

$$J \sim \bar{I} \omega \sim \bar{I} \left( \frac{k_B T}{I} \right)^{1/2} \sim \left( \frac{2}{5} a^2 M_{gr} k_B T \right)^{1/2}. \quad (1.10)$$

where $\bar{I}$ is the average moment of inertia of the rotating grain. Thus,

$$\frac{\Delta J}{J} \sim \left( \frac{m_H}{M_{gr}} \right)^{1/2}. \quad (1.11)$$

This change in the angular momentum of the grain causes the angular momentum vector $\mathbf{J}$ to be angularly displaced on the order of $\left( \frac{m_H}{M_{gr}} \right)^{1/2}$ radians with each collision. When the grain has collided with $N$ gas atoms, the orientation of $\mathbf{J}$ will have changed with respect to its original position, on average, by

$$\Delta \theta \sim \sqrt{\frac{Nm_H}{M_{gr}}}. \quad (1.12)$$

When the angular displacement $\Delta \theta$ is equal to 1 rad, $Nm_H \sim M_{gr}$, meaning that the grain has collided with a number of gas atoms which is equal in mass to the grain. The average time between collisions $t_{col}$ is defined by the inverse of the collision rate $R_{col}$:

$$t_{col} = \frac{1}{R_{col}} \sim \frac{1}{n_H \pi a^2 v_H} \quad (1.13)$$

where $n_H$ is the number density of hydrogen atoms, which for the diffuse ISM is $\approx 30/\text{cm}^3$. Using the value for $v_H$ above, the average time between collisions is

$$t_{col} \sim 1.17 \times 10^3 \text{s} \quad (1.14)$$
Therefore, the disalignment timescale $\tau_{\text{col}}$ is

$$\tau_{\text{col}} \sim t_{\text{col}} \frac{M_{\text{gr}}}{n_{\text{H}}} \sim 8.8 \times 10^{12} \text{s} \sim 2.7 \times 10^5 \text{yr},$$  \hspace{1cm} (1.15)

and any effective aligning mechanism must have an alignment timescale shorter than $\tau_{\text{col}}$, if the grain is thermally rotating.

### 1.2.2 Davis-Greenstein or paramagnetic dissipation alignment

The paramagnetic dissipation alignment mechanism relies on a grain of paramagnetic material, rapidly spinning in the Galactic magnetic field $B$. Based on the levels of interstellar Fe available for grains, Davis and Greenstein reasoned [9], there was a reasonable expectation that paramagnetic grains would be present in the interstellar medium, and that these paramagnetic grains would be magnetized in the presence of the Galactic magnetic field. Grains could also be expected to be spinning due to collisions with gas atoms in the interstellar medium. For instance, a dust grain with an effective radius of $0.1 \mu m$, embedded in a gas cloud that at a temperature of $T \sim 100 \text{K}$ will spin with a rotation rate of $10^5 \text{Hz}$ due to equipartition:

$$I \omega^2 \sim kT. \hspace{1cm} (1.16)$$

The unpaired spinning electrons in the atoms of a paramagnetic grain are each magnetic dipoles with associated magnetic dipole moments $m$. These magnetic moments line up along an applied magnetic field, creating an overall magnetization vector for the grain. As the grain spins, the magnetization vector rotates (when observed in grain coordinates) and the magnetization vector lags the external magnetic field (an internal friction that tends to keep the atomic dipoles from aligning with $B$). This reduces (dissipates) both the grain rotational energy and magnetic energy. In other words, the external torque drives the grain to a minimum energy state, in which $J \parallel |B| \hat{a}_1$. In this way, paramagnetic dissipation will tend to align the grain with an external magnetic field. While the grain is experiencing this
alignment, however, the random collisions of the grain with gas atoms from the interstellar medium are simultaneously tending to disalign the grain [31][59]. The ratio of the alignment timescale for Davis-Greenstein paramagnetic dissipation $\tau_{DG}$ to the disalignment timescale due to gas atom collisions $\tau_{col}$ is a function of the grain radius $a$:

$$\frac{\tau_{DG}}{\tau_{col}} \sim 30 \left( \frac{a}{0.2 \mu m} \right).$$

(1.17)

This relationship of the alignment and disalignment timescales should produce efficient alignment of very small grains and disalignment of large grains. This is exactly the opposite of what is observed, so neither paramagnetic dissipation nor the “compass needle” model appeared to explain grain alignment.

Jones and Spitzer [31], however, observed that if small regions of more highly concentrated Fe atoms (or other strong magnetic dipole atoms) were included in the grain (“superparamagnetic” inclusions), these inclusions would increase the paramagnetic dissipation effect, speeding up the alignment discussed above. Thus, superparamagnetic inclusions had the potential to align grains on a much shorter timescale, possibly overcoming collisional gas disalignment if a grain had a sufficient number of superparamagnetic inclusions with high enough Fe atom density. There were observational constraints though, where polarization is observed even though gas/grain temperature ratios should preclude D-G alignment [1] [25] [61] [60], that seemed to require another alignment mechanism. Also, there is no direct evidence that grains contain superparamagnetic inclusions, so other alignment mechanisms were needed.

### 1.2.3 Magnetic dipole due to rotating charge

The search for other alignment mechanisms led to the consideration of the charge of a grain. Due to starlight-induced photoelectric emission, and electron and ion collisional charging, interstellar grains should be charged. A charged spinning grain will have a magnetic dipole moment $\mu$, and if $\mu$ is aligned with the grain’s angular momentum vector $J$, the presence of
an external magnetic field $\mathbf{B}$ will generate a torque that will cause the angular momentum vector to precess about $\mathbf{B}$ [49]:

$$\Gamma_\mu = \mu \times \mathbf{B}. \quad (1.18)$$

### 1.2.4 Barnett Effect Magnetic Dipole

An even larger magnetic dipole is generated by a spinning paramagnetic grain, in accordance with the Barnett effect [11]. This effect acts as some of the spinning paramagnetic grain’s rotational energy is dissipated. In the absence of external torques, as the bulk angular momentum decreases, this angular momentum is essentially transferred to the paramagnetic atoms, so that the angular momentum of the system is conserved. While the grain material is initially unmagnetized due to the random orientations of the microscopic dipole moments, the transfer of grain angular momentum to these dipoles, causes some of them to move towards alignment along the angular momentum axis of the grain $\mathbf{J}$. This results in a non-zero magnetic dipole moment in the grain. In the presence of an external magnetic field, a torque will be generated as described in Section 1.2.3, again causing the grain to precess about the external magnetic field lines.

$$\Gamma_{\mu_{\text{bar}}} = \mu_{\text{Bar}} \times \mathbf{B}. \quad (1.19)$$

The precession timescale due to the Barnett effect, $\sim 10^6\text{s}$, is much shorter than the Davis-Greenstein timescale or the gas disalignment timescale. Since the polarization vector is aligned with the grain’s principal axis of greatest moment of inertia $\mathbf{\hat{a}}_1$ (this is explained in Section 1.2.5), the precession about the magnetic field results in observed polarization that is either parallel or perpendicular to the magnetic field lines. This is due to the fact that symmetry cancels out the other components of the polarization vector for an observed ensemble of grains with angular momentum vectors already aligned at some given angle with the Galactic magnetic field.
1.2.5 Spin-Related Internal Alignment

Internal alignment of the angular momentum vector \( \mathbf{J} \) with respect to \( \hat{a}_1 \) can occur for a spinning grain due to dissipation mechanisms, as first described by Purcell [58]. If the angular momentum vector is not aligned with \( \hat{a}_1 \), friction is generated in the grain due to internal processes, and there is a net decrease in grain energy as heat is radiated away. This is a viscoelastic dissipation of grain rotational energy. In a rotating paramagnetic grain, if the angular momentum vector is not aligned with \( \hat{a}_1 \), the angular velocity vector \( \omega \) precesses in the grain coordinates and generates a “Barnett equivalent magnetic field” that opposes the direction of \( \omega \), causing a Barnett dissipation of grain rotational energy. The alignment of \( \mathbf{J} \) with \( \hat{a}_1 \) caused by this loss of energy internal to the grain can be seen in the following example. The rotational energy of an oblate spheroidal grain with angular momentum \( \mathbf{J} \), maximum moment of inertia \( I_{\text{max}} \), least moment of inertia \( I_{\perp} \), and angle \( \theta \) between \( \mathbf{J} \) and \( \hat{a}_1 \) is:

\[
E(\theta) = \frac{J^2}{I_{\text{max}}} \left[ 1 + \sin^2 \theta (h - 1) \right], \quad h = \frac{I_{\text{max}}}{I_{\perp}}. \tag{1.20}
\]

Since the angular momentum cannot be changed internally, the one thing that can be changed is the angle \( \theta \), in this case decreasing the angle, as the rotational energy of the grain is dissipated. The grain system is at its lowest energy state when \( \theta = 0 \) and, the angular momentum vector \( \mathbf{J} \) and largest principal moment of inertia \( \hat{a}_1 \) are aligned. This alignment will occur “perfectly” only in a suprathermally rotating grain (one rotating at an angular velocity much greater than that caused by random gas atom collisions), i.e. only when the rotational energy of the grain is much greater than the thermal energy of the gas \( k_B T_{\text{gas}} \) and grain \( k_B T_{\text{gr}} \). So, with suprathermal rotation, the grain is internally aligned and, if suprathermal rotation continues for a period longer than that required for external alignment with the Davis-Greenstein mechanism, both processes will result in overall grain alignment. The alignment solution now relies on finding a means to keep the paramagnetic grain rotating suprathermally.
1.2.6 Suprathermal Rotation from Surface Conditions

A solution suggested by Purcell was the existence of non-uniform surface conditions leading to unbalanced torques. He identified three possible surface-driven sources of these unbalanced torques: surface regions of uneven sticking coefficient for colliding atoms, regions of non-uniform photoelectric emission, and preferential sites on the surface of the grain for the production of H\textsubscript{2} molecules. The largest effect of these three is the production of H\textsubscript{2} from fixed sites on the grain surface, acting like small “thrusters” to spin up the grain. [58]. However, all three of these methods of producing suprathermal rotation rely on a constant surface condition over time, and the surface is changed on a timescale that is short compared to that needed to align the angular momentum vector with the magnetic field, $\tau_{DG}$. This leads to periods of slow rotation, and when $J$ approaches zero (a “crossover”), gas collision can cause disalignment of the grain [65]. Additionally, thermal fluctuations in the grain become important as the grain spins down and can also cause disalignment [40][42][41]. As $J$ approaches zero, large thermal fluctuations can actually cause the grain to flip over and, for sufficiently strong thermal fluctuations, the grain can repeatedly flip over keeping the grain from ever achieving suprathermal rotation. This repeated flipping is called “thermal trapping” and applies to small grains, when only considering paramagnetism due to electrons. When nuclear paramagnetism is also considered, the thermal trapping effect extends to large ($\sim 1\mu$m) grains, as well. Without a means to achieve suprathermal rotation, Davis-Greenstein dissipation appeared unlikely to result in the observed grain alignment, and other alignment mechanisms were needed. However, the demonstration of grain precession leading to polarization along the $\mathbf{B}$ field, and the alignment of $\mathbf{J}$ and $\hat{a}_1$ vectors when a grain is rotating suprathermally, showed that a grain alignment mechanism need not be directly magnetic and opened the door to consideration of other mechanisms.

1.2.7 Radiative Torque Alignment: Grain Spin-up

This led to the consideration of a radiative torque alignment mechanism. It was suggested in 1970 and 1972, by Harwit and Dolginov, respectively, [24] [10] that grains could experience
a torque due to the absorption and scattering of photons. This can be seen, for example, in irregular (asymmetric) grains that absorb radiation of different circular polarization states, differently. When these irregular grains are exposed to anisotropic unpolarized radiation, torques will result. Unfortunately, due to a lack of computational capability these torques remained uncalculated for more than twenty years after the idea was originally proposed. When radiative torques were next considered in 1996 by Draine and Weingartner [17] as a means to create suprathermal rotation in the grain, a discrete (electric) dipole approximation (DDA) was developed to evaluate the torques for asymmetric arbitrarily-shaped dust grains. The DDA is based on a three-dimensional lattice of polarizable points within the boundaries of a grain. The electric dipole moments are calculated for each polarizable point within the designated grain boundaries, taking into account both the incident radiation and the interaction of the electric dipoles with one another. The incident radiation is modeled as anisotropic, consistent with a finding of 10% anisotropy in the local interstellar medium [17]. A few asymmetric grain shapes were evaluated using the DDA and the torques were found to be large for grain radii greater than \( \sim 0.1 \mu m \) but small for grain radii less than \( \sim 0.05 \mu m \). Since these torques are based on the overall grain geometry rather than on surface conditions as with the \( \text{H}_2 \) “thrusters”, the torques can be expected to be stable over long periods of time compared to the gas collision disalignment timescale. This makes “crossovers” (when the grain flips over) unlikely but not impossible. However, because the radiative torque alignment mechanism relies on an anisotropic radiation source and the grain is asymmetric, the torque is not fixed in grain coordinates. When the grain does flip over, the torques do not exactly reverse and the grain’s time-averaged torque does not go to zero. Thus, the grain avoids thermal “trapping”. The ability of radiative torques to suprathermally spin up a grain makes the grain insensitive to disalignment by gas collisions, and gives time for Davis-Greenstein dissipation to align the grain.
1.2.8 Radiative Torque Alignment: Direct Alignment

In addition to being able to spin up a grain to suprathermal rotation rates, Draine and Weingartner found that radiative torques could directly align dust grains with the Galactic magnetic field [18]. This direct alignment process is based on the ability of the radiative torques to change the direction of the grain’s rotation with respect to the direction of radiation anisotropy and the magnetic field $\mathbf{B}$. The radiative torque components that are perpendicular to the principal axis of greatest moment of inertia $\hat{a}_1$, act directly to align the grain, for larger grains: $a \gtrsim 0.1\mu\text{m}$. The direct alignment with respect to $\mathbf{B}$ is dependent on short periods for both grain rotation and grain precession, relative to the timescale for any other rotational and re-orienting process affecting the grain, and is also highly dependent on the anisotropy of the interstellar radiation. Draine and Weingartner included the effects of H$_2$ production torques (per the discussion just above), and found that alignment times due to radiative torques were always less than those of Davis-Greenstein dissipation alignment, when the H$_2$ production site density was $> 1/10^6$ Å$^2$. For their assumed characteristic H$_2$ site density of $1/10^2$ Å$^2$, the alignment time is $\sim 5 \times 10^5$ yr. These anisotropy-generated radiative torques appear to be the principal mechanism responsible for interstellar grain alignment.

The work discussed in the remainder of this dissertation, investigates effects of two other sources of torque for asymmetric grains in an anisotropic radiation field. The first of these torques examined in Chapter 2 is that due to photoelectric emission and photodesorption of surface atoms. Incident radiation resulting in the emission of electrons or desorption of H atoms from the grain surface creates a recoil in the grain. The work discussed in Chapter 2 investigates whether this recoil would produce torques that significantly affect grain alignment in asymmetric grains. Photoelectric emission and electron capture can also change the electric charge and the electric dipole moment of the grain.

Recent work by Weingartner [68] described a torque that would be generated by an interaction of the electric dipole moment of a grain drifting across Galactic magnetic field
lines. This torque changes with the changing electric dipole as the grain acquires and loses charge randomly across the grain surface. The timescale and the magnitude of these changes and their effect on grain alignment are the subject of the work discussed in Chapter 3. This dissertation concludes with an afterword in Chapter 4, which discusses the broader context of this work.
Chapter 2: The Grain Alignment Effect of Torques Due to Photoemission and Photodesorption

2.1 Introduction

In this chapter, we estimate the importance of recoil torques generated by photoelectric emission and photodesorption of atoms from a grain surface, relative to the radiative torques that are thought to play a critical role in aligning grains with the Galactic magnetic field.

In 2003 Weingartner and Draine [72] found that recoil forces due to photoelectric emission and photodesorption could be significant - comparable to or greater than radiation pressure in some cases. This finding suggests that recoil torques due to the same phenomena might also be significant relative to radiative torques. Draine and Weingartner used the “discrete dipole approximation” to evaluate radiative torques [17] [18] for three irregular grain shapes using the DDSCAT [14] computer code. In this approximation, the grain body is represented as an array of polarizable points, and torques (due to the incident electric field and dipole field of each other point) are calculated for each point. This approach, however, is not practical for the calculation of recoil torques. With photoemission, most of the electrons originate in the outer $\approx 10\,\AA$ of a grain. We use the fact that the photoemission rate is proportional to the internal electric field intensity just below the surface, and calculate the field intensity. To do that using the discrete dipole approximation for a 0.2$\mu$m grain, with a 10$\AA$ resolution, would require an array too large to be computationally feasible. We adopt a more computationally manageable approach. We employ two alternative methods to find the position-dependent internal and external field intensities. Then, using an approach developed by Kerker and Wang [37] the internal field intensity just below the surface is used to obtain the photoemission rate and, similarly, the external field intensity
just above the surface provides a photodesorption rate, as a function of positon on the grain surface. With these rates, the recoil torques can be calculated.

The following simplified scenario provides a heuristic description of the origin of the photoelectric and photodesorption torques. A photon arriving at a neutral dielectric grain is absorbed. In the case of photoemission, the absorbed photon sometimes has enough energy to free an electron from the valence band, propel that electron through the grain and out the surface with enough energy to overcome any surface energy barrier. The escaping electron carries angular momentum away from the grain; integration over all electrons emitted over a period of time results in "recoil" in the grain. The rate of electron emission can vary across the grain surface as the material work function varies, and we consider both uniform and non-uniform surface conditions for photoemission. In the case of photodesorption, the same angular momentum change argument applies, with the photon energy going to break the bond of a H atom attached to the grain surface. This binding energy is associated with either a chemisorption site, where the atom is chemically bound to the surface, or a physisorption site, a "shallow" potential well in the surface lattice structure of the grain material with a potential barrier much smaller than that of a chemical bond. The angular momentum change imparted by the desorbing atom, again when integrated for all desorbing atoms for a period of time, generates a recoil in the grain.

We adopt a spheroidally shaped grain (either prolate or oblate) with an effective radius (i.e. the radius for a sphere of the same volume), \( a_{\text{eff}} = 0.2 \mu \text{m} \). The grain material is amorphous silicate, with dielectric characteristics as described by Draine [13]. The grain material is homogeneous, including at the surface, except when noted otherwise, and the grain is charge neutral. The \( z \) axis is the axis of symmetry for the spheroidal grain. The anisotropic starlight incident on the grain is modeled as an unpolarized monochromatic harmonic plane wave, where the angle of incidence \( \theta_0 \) is measured relative to the \( z \) axis. The wavelength of the incident radiation is on the order of the grain effective radius, and the scattering of starlight is elastic so that the wavelength of the radiation is the same for incident and scattered waves. The medium external to the grain is vacuum.
As stated above, in order to determine the photoelectric and photodesorption torques, the internal and external field intensities are needed near the grain surface. Two independent means were used to solve for these intensities. The first method, the Point Matching Method (PMM), uses expansions in spherical vector wavefunctions to describe the internal and scattered fields, using surface boundary conditions at discrete points to solve for the expansion coefficients (Morrison and Cross [55] and Al-Rizzo and Tranquilla [2]). The asymmetry of these intensities provide surface-position-dependent rates of photoemission [37] and photodesorption that are responsible for the recoil torques. We also use the spherical expansion coefficients to calculate radiative torques and forces and their respective efficiency factors, in order to validate the PMM code against the same torques and forces evaluated with the DDSCAT code (at the same time providing another validation of DDSCAT). In the second method, developed by Barton [32] the internal and scattered fields are expressed as expansions in spheroidal vector wavefunctions. The spheroidal expansion coefficients are found, again employing boundary conditions at the surface, but this time integrating the surface boundary conditions rather than matching at specific points. The intensities found with this second method are used to verify the PMM results. This verification is important because the computer codes used for each method are long and complex, with ample opportunity for error. With a high level of agreement for intensity values from two very different approaches, we can have confidence in our calculated torque results.

In the following sections, we first describe the PMM method and resulting intensities. Following this, the expressions for radiative efficiency factors are discussed and the calculated results using PMM-derived intensities are shown. In the next section, the calculation of photoelectric and photodesorption efficiency factors and torques, again using PMM-derived intensities, are described and calculated results shown. A section describing the Barton method for finding internal and scattered intensities follows. The final section presents conclusions.
2.2 Point Matching Method

Solutions of the vector Helmholtz equation

$$\nabla^2 V + k^2 V = 0 \quad (2.1)$$

are found for the spherical coordinate system, by first solving the scalar wave equation in spherical coordinates

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial^2 \psi}{\partial \phi^2} + k^2 \psi = 0 \quad (2.2)$$

where $$\psi(r, \theta, \phi)$$ is a fully separable solution in spherical coordinates, and $$k$$ is the wave number. The scalar solution is then used to construct the vector solution

$$M_{nm}(r, \theta, \phi) = \nabla \times r \psi \quad (2.3)$$

$$N_{nm}(r, \theta, \phi) = \frac{1}{k} \nabla \times M_{nm}(r, \theta, \phi) \quad (2.4)$$

where $$M_{nm}(r, \theta, \phi)$$ and $$N_{nm}(r, \theta, \phi)$$ are the vector spherical wavefunctions, with components

$$M_r(r, \theta, \phi) = 0 \quad (2.5)$$

$$M_\theta(r, \theta, \phi) = \frac{im}{\sin \theta} Z(kr) P(\cos \theta) e^{im\phi} \quad (2.6)$$

$$M_\phi(r, \theta, \phi) = \sin \theta Z(kr) P'(\cos \theta) e^{im\phi} \quad (2.7)$$

$$N_r(r, \theta, \phi) = \frac{n(n+1)}{kr} Z(kr) P(\cos \theta) e^{im\phi} \quad (2.8)$$

$$N_\theta(r, \theta, \phi) = -\sin \theta \left[ Z'(kr) + \frac{Z(kr)}{kr} \right] P'(\cos \theta) e^{im\phi} \quad (2.9)$$
\[
N_\phi(r, \theta, \phi) = \frac{im}{\sin \theta} \left[ Z'(kr) + \frac{Z(kr)}{kr} \right] P(\cos \theta) e^{im\phi} \tag{2.10}
\]

where \( P(\cos \theta) = P_n^{[m]}(\cos \theta), \ P'(\cos \theta) = dP_n^{[m]}(\cos \theta)/d(\cos \theta), \) \( k \) is the wave number \((k = k_0 \equiv 2\pi/\lambda \) outside the grain and \( k = n_{\text{ref}}k_0 \) inside the grain, where \( n_{\text{ref}} \) is the grain index of refraction and \( \lambda \) is the wavelength of the incident radiation), \( Z(kr) = j_n(kr) \) (spherical Bessel function of the first kind) inside the grain and \( Z(kr) = h_n^{(1)}(k_0r) \) (spherical Hankel function of the first kind) outside the grain, and \( Z'(kr) = dZ(kr)/d(kr) \). We adopt Jackson’s [30] convention for associated Legendre polynomials \( P_{nm}(\cos \theta) \).

The scattered electric (\( E^s \)) and magnetic (\( H^s \)) fields are given by

\[
E^{(s)} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \left[ a_{nm}(1) N_{nm}^{(s)} + a_{nm}(2) M_{nm}^{(s)} \right] \tag{2.11}
\]

\[
H^{(s)} = -i \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \left[ a_{nm}(1) M_{nm}^{(s)} + a_{nm}(2) N_{nm}^{(s)} \right] \tag{2.12}
\]

and the internal fields are given by

\[
E^{(t)} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \left[ a_{nm}(3) N_{nm}^{(t)} + a_{nm}(4) M_{nm}^{(t)} \right] \tag{2.13}
\]

\[
H^{(t)} = -i n_{\text{ref}} \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \left[ a_{nm}(3) M_{nm}^{(t)} + a_{nm}(4) N_{nm}^{(t)} \right] \tag{2.14}
\]

where superscripts \((s)\) and \((t)\) refer to evaluation in the grain exterior and interior, respectively.

We will take the \( z \)-axis as the symmetry axis of the spheroidal grain and assume that the incident radiation field wave vector \( k_0 \) lies in the \( x-z \) plane with \( k_0 = k_0(\cos \theta_0 \hat{z} - \sin \theta_0 \hat{x}) \). We also adopt unit amplitude for the incident electric field \( E^i \). When \( E^i \) lies in the \( x-z \) plane.
plane (TM mode),

\[
\mathbf{E}^{(i)}_{\text{TM}} = i \hat{r} (\cos \theta_0 \sin \theta \cos \phi + \sin \theta_0 \cos \theta) \\
+ \hat{\theta} (\cos \theta_0 \cos \theta \cos \phi - \sin \theta_0 \sin \theta) - \hat{\phi} \cos \theta_0 \sin \phi \exp (i k_0 \cdot \mathbf{r}) , \tag{2.15}
\]

\[
\mathbf{H}^{(i)}_{\text{TM}} = i \hat{r} \sin \theta \sin \phi + \hat{\theta} \cos \theta \sin \phi + \hat{\phi} \cos \phi \exp (i k_0 \cdot \mathbf{r}) \tag{2.16}
\]

with

\[
k_0 \cdot \mathbf{r} = k_0 r (\cos \theta_0 \cos \theta - \sin \theta_0 \sin \theta \cos \phi) . \tag{2.17}
\]

For the orthogonal polarization state (TE mode),

\[
\mathbf{E}^{(i)}_{\text{TE}} = - \mathbf{H}^{(i)}_{\text{TM}} ; \quad \mathbf{H}^{(i)}_{\text{TE}} = - \mathbf{E}^{(i)}_{\text{TM}} . \tag{2.18}
\]

At the surface, the tangential components of \( \mathbf{E} \) and \( \mathbf{H} \) and the normal components of \( \mathbf{D} \equiv \epsilon \mathbf{E} \) (\( \epsilon \) is the dielectric function) and \( \mathbf{H} \) are continuous.

For the grain surface, the radius \( r \) as a function of polar angle \( \theta \) is given by

\[
r(\theta) = a \left[ \cos^2 \theta + \zeta^2 \sin^2 \theta \right]^{-1/2} . \tag{2.19}
\]

For prolate grains, \( a \) is the semimajor axis length and \( \zeta > 1 \) is the ratio of the semimajor axis length to the semiminor axis length. For oblate grains, \( a \) is the semiminor axis length and \( \zeta < 1 \) is the ratio of the semiminor axis length to semimajor axis length. Given the radius \( a_{\text{eff}} \) of a sphere of equal volume, \( a = a_{\text{eff}} \zeta^{2/3} \).

In this case, the boundary conditions on the tangential field components become

\[
E^{(i)}_{\phi} + E^{(s)}_{\phi} = E^{(t)}_{\phi} \tag{2.20}
\]

\[
H^{(i)}_{\phi} + H^{(s)}_{\phi} = H^{(t)}_{\phi} \tag{2.21}
\]
\[(1 - \zeta^2) \sin \theta \cos \theta (E_r^{(i)} + E_r^{(s)} - E_r^{(t)}) + (\cos^2 \theta + \zeta^2 \sin^2 \theta) (E_\theta^{(i)} + E_\theta^{(s)} - E_\theta^{(t)}) = 0 \quad (2.22)\]

\[(1 - \zeta^2) \sin \theta \cos \theta (H_r^{(i)} + H_r^{(s)} - H_r^{(t)}) + (\cos^2 \theta + \zeta^2 \sin^2 \theta) (H_\theta^{(i)} + H_\theta^{(s)} - H_\theta^{(t)}) = 0 \quad . \quad (2.23)\]

The boundary conditions on the normal field components are

\[(\cos^2 \theta + \zeta^2 \sin^2 \theta) (D_r^{(i)} + D_r^{(s)} - D_r^{(t)}) + (\zeta^2 - 1) \sin \theta \cos \theta (D_\theta^{(i)} + D_\theta^{(s)} - D_\theta^{(t)}) = 0 \quad (2.24)\]

\[(\cos^2 \theta + \zeta^2 \sin^2 \theta) (H_r^{(i)} + H_r^{(s)} - H_r^{(t)}) + (\zeta^2 - 1) \sin \theta \cos \theta (H_\theta^{(i)} + H_\theta^{(s)} - H_\theta^{(t)}) = 0 \quad . \quad (2.25)\]

The incident radiation field can be expressed as follows [2]:

\[E_r^{(i), \text{TM}} = \exp(ik_0 r \cos \theta_0 \cos \theta) \sum_{m=-\infty}^{\infty} i^m [J_m(u) \sin \theta_0 \cos \theta - iJ'_m(u) \cos \theta_0 \sin \theta] \exp(im\phi) \quad (2.26)\]

\[E_\theta^{(i), \text{TM}} = -\exp(ik_0 r \cos \theta_0 \cos \theta) \sum_{m=-\infty}^{\infty} i^m [J_m(u) \sin \theta_0 \sin \theta + iJ'_m(u) \cos \theta_0 \cos \theta] \exp(im\phi) \quad (2.27)\]

\[E_\phi^{(i), \text{TM}} = \exp(ik_0 r \cos \theta_0 \cos \theta) \cos \theta_0 \sum_{m=-\infty}^{\infty} i^m mu^{-1} J_m(u) \exp(im\phi) \quad (2.28)\]

\[H_r^{(i), \text{TM}} = -\sin \theta \exp(ik_0 r \cos \theta_0 \cos \theta) \sum_{m=-\infty}^{\infty} i^m mu^{-1} J_m(u) \exp(im\phi) \quad (2.29)\]

\[H_\theta^{(i), \text{TM}} = -\cos \theta \exp(ik_0 r \cos \theta_0 \cos \theta) \sum_{m=-\infty}^{\infty} i^m mu^{-1} J_m(u) \exp(im\phi) \quad (2.30)\]

\[H_\phi^{(i), \text{TM}} = -\exp(ik_0 r \cos \theta_0 \cos \theta) \sum_{m=-\infty}^{\infty} i^{m+1} J'_m(u) \exp(im\phi) \quad (2.31)\]

with \( u = -k_0 r \sin \theta_0 \sin \theta \), \( J_m(u) \) the Bessel function, and \( J'_m(u) = dJ_m(u)/du \).
To find the expansion coefficients \( a_{nm} \), the field expressions in Eqns. (2.11) through (2.14) and (2.26) through (2.31) are substituted into the boundary conditions in Eqns. (2.20) through (2.23). In the resulting equations, each term contains a factor \( \exp(im\phi) \) and no other \( \phi \)-dependence. Multiplying by \( \exp(-im'\phi) \) and integrating over \( \phi \), we find the following equations, which must be satisfied for each value of \( m, \theta, \) and \( i = 1 \) through 4:

\[
\sum_{n=|m|}^{\infty} \sum_{j=1}^{4} C_{nm}(i,j) \cdot a_{nm}(j) = D_{m}(i) \quad (2.32)
\]

with

\[
C_{nm}(1, 1) = (1 - \zeta^2) \sin \theta \cos \theta N_{nm,r}^{(s)}(\phi = 0) + (\cos^2 \theta + \zeta^2 \sin^2 \theta) N_{nm,\theta}^{(s)}(\phi = 0) \quad (2.33)
\]

\[
C_{nm}(1, 2) = (\cos^2 \theta + \zeta^2 \sin^2 \theta) M_{nm,\theta}^{(s)}(\phi = 0) \quad (2.34)
\]

\[
C_{nm}(1, 3) = -(1 - \zeta^2) \sin \theta \cos \theta N_{nm,r}^{(t)}(\phi = 0) - (\cos^2 \theta + \zeta^2 \sin^2 \theta) N_{nm,\theta}^{(t)}(\phi = 0) \quad (2.35)
\]

\[
C_{nm}(1, 4) = -(\cos^2 \theta + \zeta^2 \sin^2 \theta) M_{nm,\theta}^{(t)}(\phi = 0) \quad (2.36)
\]

\[
C_{nm}(2, 1) = N_{nm,\phi}^{(s)}(\phi = 0) \quad (2.37)
\]

\[
C_{nm}(2, 2) = M_{nm,\phi}^{(s)}(\phi = 0) \quad (2.38)
\]

\[
C_{nm}(2, 3) = -N_{nm,\phi}^{(t)}(\phi = 0) \quad (2.39)
\]

\[
C_{nm}(2, 4) = -M_{nm,\phi}^{(t)}(\phi = 0) \quad (2.40)
\]

\[
C_{nm}(3, 1) = C_{nm}(1, 2) \quad (2.41)
\]

\[
C_{nm}(3, 2) = C_{nm}(1, 1) \quad (2.42)
\]
\( C_{nm}(3, 3) = n_{\text{ref}} C_{nm}(1, 4) \) (2.43)
\( C_{nm}(3, 4) = n_{\text{ref}} C_{nm}(1, 3) \) (2.44)
\( C_{nm}(4, 1) = C_{nm}(2, 2) \) (2.45)
\( C_{nm}(4, 2) = C_{nm}(2, 1) \) (2.46)
\( C_{nm}(4, 3) = n_{\text{ref}} C_{nm}(2, 4) \) (2.47)
\( C_{nm}(4, 4) = n_{\text{ref}} C_{nm}(2, 3) \) (2.48)

and

\[
D_m(1) = i^m [J_m(u) \sin \theta_0 \sin \theta]^2 + i J'_m(u) \cos \theta_0 \cos \theta \exp(ik_0 r \cos \theta_0 \cos \theta) \tag{2.49}
\]
\[
D_m(2) = -i^m m u^{-1} \cos \theta_0 J_m(u) \exp(ik_0 r \cos \theta_0 \cos \theta) \tag{2.50}
\]
\[
D_m(3) = i^{m+1} m u^{-1} J_m(u) \cos \theta \exp(ik_0 r \cos \theta_0 \cos \theta) \tag{2.51}
\]
\[
D_m(4) = -i^m J'_m(u) \exp(ik_0 r \cos \theta_0 \cos \theta) \tag{2.52}
\]

In practice, we impose an upper cutoff for \(|m|, m_{\text{max}}\), and for \(n, n_{\text{max}}\). For each \(m\), we find the expansion coefficients \(a_{nm}\) by performing a least-squares minimization of

\[
\left\| \sum_{\theta,i} \left\{ \sum_{n=|m|}^{n_{\text{max}}} \sum_j [C_{nm}(i, j; \theta) \cdot a_{nm}(j) - D_m(i; \theta)] \right\} \right\|^2 \tag{2.53}
\]

where,

\[
\left\| \sum_{\theta,i} f(\theta, i) \right\|^2 \equiv \sum_{\theta,i} f^2(\theta, i). \tag{2.54}
\]

We generally take \(2n_{\text{max}}\) to \(3n_{\text{max}}\) values of \(\theta\), evenly spaced in \(\cos \theta\). Minimizing Eqn.
2.53 according to the numerical approach described by Press et al. [57] results in a matrix equation

\[(C^T \cdot C) \cdot a = C^T \cdot D\] (2.55)

where \(C^T\) is the transpose of \(C\). The design matrix for the least-squares problem is a \(4n_\theta\) by \(4(n_{\text{max}} - |m| + 1)\) matrix, made up from \(C_{nm}(i, j; \theta)\), and does not depend on \(\theta_0\). Because the least-squares solution is prone to roundoff error [57], we first apply QR-decomposition to the design matrix. This results in

\[C = Q \cdot R,\] (2.56)

where \(R\) is an upper triangular matrix and \(Q\) is orthogonal (\(Q \cdot Q^T = 1\)). Using this form of \(C\), the \(a_{nm}\) coefficients can be solved for in the matrix equation

\[R \cdot a = Q^T \cdot D.\] (2.57)

The computational time required to then complete the solution is small compared with the time to accomplish the factorization. Thus, several additional values of \(\theta_0\) can be treated without substantially increasing the computational time. The matrix equations often exhibit serious ill-conditioning. We work around this problem by implementing the solution using Mathematica, which supports arbitrary-precision arithmetic.

Note that, when \(m\) changes sign, \(C'(1, 2), C'(1, 4), C'(2, 1), C'(2, 3), C'(3, 1), C'(3, 3), C'(4, 2), C'(4, 4), D(2),\) and \(D(3)\) change sign, while the other components retain their sign. Thus, for the TM mode,

\[a_{n, -m}(1) = a_{n, m}(1) ; \quad a_{n, -m}(2) = -a_{n, m}(2) ; \quad a_{n, -m}(3) = a_{n, m}(3) ; \quad a_{n, -m}(4) = -a_{n, m}(4)\] (2.58)
and for the TE mode,

\[ a_{n,-m}(1) = -a_{n,m}(1) ; \quad a_{n,-m}(2) = a_{n,m}(2) ; \quad a_{n,-m}(3) = -a_{n,m}(3) ; \quad a_{n,-m}(4) = a_{n,m}(4) \]

(2.59)

As a result, it is not necessary to separately compute the expansion coefficients for \( m < 0 \). When \( m = 0 \), \( a_{n,m}(2) \) and \( a_{n,m}(4) \) equal zero for the TM mode and \( a_{n,m}(1) \) and \( a_{n,m}(3) \) equal zero for the TE mode.

When \( \theta_0 = 0 \), all of the azimuthal modes vanish, except for those with \( m = \pm 1 \). In this case, the above expressions for the incident field components (Eqns. 2.26–2.31) contain the ill-defined terms \( J'_m(u) \) and \( J_m(u)/u \) with \( u = 0 \). Equations (2.49) through (2.52) must be replaced with

\[ D_1(1) = D_1(3) = -\frac{1}{2} \cos \theta \exp(ik_0r \cos \theta) \]

(2.60)

\[ D_1(2) = D_1(4) = -\frac{i}{2} \exp(ik_0r \cos \theta) . \]

(2.61)

To verify the solution, we check that the boundary conditions, Eqns. (2.20) through (2.25) are indeed satisfied. This is particularly powerful for conditions (2.24) and (2.25), since these are not used in the solution. In addition, we check that the field intensity exhibits the following symmetry: \( |E|^2(2\pi - \phi) = |E|^2(\phi) \), and that the intensity is independent of \( \phi \) when \( \theta_0 = 0 \).

### 2.2.1 Intensity results

Figures 2.1 - 2.4 are examples of the internal and external intensity \( |E|^2 \) results obtained at the surface of a spheroidal grain using the PMM approach described above. (The external intensity is a sum of the incident and scattered field intensities.) These examples show \( |E|^2 \) for an oblate grain with \( \zeta = 2/3 \) and \( a_{\text{eff}} = 0.2\mu m \), at two different wavelengths of incident radiation (\( \lambda = 0.1\mu m \), and \( \lambda = 0.15\mu m \)).
Figure 2.1: The intensity $I = |E|^2$ of the internal field (averaged over the TE and TM modes and normalized to the incident intensity $I_0$) at the grain surface, for an oblate ($\zeta = 2/3$) silicate grain with $a_{\text{eff}} = 0.2\mu m$, incident wavelength $\lambda = 0.1\mu m$, and angle between the incident radiation and grain symmetry axis $\theta_0 = \cos^{-1} 0.6$.

Figure 2.2: Same as Figure 2.1 except that the external field intensity at the grain surface is plotted.
Figure 2.3: Same as Figure 2.1 except that $\lambda = 0.15\mu m$

Figure 2.4: Same as Figure 2.2 except that $\lambda = 0.15\mu m$
2.3 Efficiency factors and torques

Here we describe electromagnetic efficiency factors, which are computed in order to validate the PMM code.

The scattering efficiency factor is defined [6] as:

\[ Q_{\text{sca}} = \frac{C^{(s)}}{\pi a_{\text{eff}}^2}. \]  

The scattering cross section \( C^{(s)} \) is defined as the ratio of scattered power \( P_{\text{sca}} \) to the incident flux \( F_{\text{inc}} \). Thus, \( Q_{\text{sca}} \) is defined by:

\[ P_{\text{sca}} = F_{\text{inc}} Q_{\text{sca}} \pi a_{\text{eff}}^2 \]  

The power scattered by a spheroid [55],

\[ P_{\text{sca}} = \frac{1}{2} \Re \int_0^{2\pi} \int_0^{\pi} \left[ E^s_{\theta} (H^s_{\phi})^* - E^s_{\phi} (H^s_{\theta})^* \right] r^2 \sin \theta d\theta d\phi \]  

(where \(^*\) indicates the complex conjugate, and \((r, \theta, \phi)\) are spherical coordinates), when integrated over a sphere located at infinity, gives

\[ P_{\text{sca}} = \frac{2\pi}{\omega \mu_0 k_0} \sum_{m,n}^{m>0} \frac{n(n+1)(n+|m|)!}{(2n+1)(n-|m|)!} \left( |a_{m,n}|^2 + |b_{m,n}|^2 \right) \]  

and the ratio of \( P_{\text{sca}} \) to the incident flux \( F_{\text{inc}} \) gives the scattering efficiency factor:

\[ Q_{\text{sca}} = \frac{4\pi}{\kappa_0^2 E^{(i)} E^{(i)*} \pi a_{\text{eff}}^2} \sum_{m,n}^{m>0} \frac{n(n+1)(n+|m|)!}{(2n+1)(n-|m|)!} \left( |a_{m,n}|^2 + |b_{m,n}|^2 \right) \]
where the magnitude of the incident intensity is set to 1 and $\epsilon_m = 1$ when $m = 0$ and $\epsilon_m = 2$ when $m > 0$.

The extinction efficiency factor is the sum of the scattering and absorption efficiency factors, and is defined in the same way:

$$P_{\text{ext}} = F_{\text{inc}}Q_{\text{ext}}\pi a^2$$  \hspace{1cm} (2.67)

$$P_{\text{ext}} = P_{\text{sca}} + P_{\text{abs}}$$  \hspace{1cm} (2.68)

Using the optical theorem, the extinction efficiency factors for the TE and TM modes are found \[2\]:

$$Q_{\text{ext}} = \frac{4}{(k_0 a_{\text{eff}})^2} \text{Im} \left\{ \sum_{m,n} \epsilon_m (-1)^n (-1)^m \left[ a_{m,n}(1) \sin \theta_0 P'(\cos \theta_0) - \frac{ma_{m,n}(2)P(\cos \theta_0)}{\sin \theta_0} \right] \right\} \text{ (TM)}$$  \hspace{1cm} (2.69)

$$Q_{\text{ext}} = \frac{4}{(k_0 a_{\text{eff}})^2} \text{Im} \left\{ \sum_{m,n} \epsilon_m (-1)^n (-1)^m \left[ a_{m,n}(2) \sin \theta_0 P'(\cos \theta_0) - \frac{ma_{m,n}(1)P(\cos \theta_0)}{\sin \theta_0} \right] \right\} \text{ (TE)}$$  \hspace{1cm} (2.70)

The radiation pressure efficiency factor $Q_{\text{pr}}$ is defined by

$$F_{\text{rad}} = \pi a_{\text{eff}}^2 u_{\text{rad}} Q_{\text{pr}}$$  \hspace{1cm} (2.71)

where $F_{\text{rad}}$ is force due to absorption and scattering and $u_{\text{rad}}$ is the the incident field energy density. In a similar way, the efficiency factor $Q_{\Gamma}$ for the radiative torque $\Gamma_{\text{rad}}$ is defined by \[17\]

$$\Gamma_{\text{rad}} = \pi a_{\text{eff}}^2 u_{\text{rad}} \frac{\lambda}{2\pi} Q_{\Gamma}.$$  \hspace{1cm} (2.72)

In order to solve Eqns. (2.71) and (2.72) for their respective efficiency factors, the force and torque due to both the incident and scattered fields must be known. Expressions for
both force and torque, expanded in vector spherical harmonics, were derived by Farsund and Felderhof [21]. They provide Cartesian components for the extinction and scattered contributions to force and torque, with the incident field terms derived as a difference of those of the extinction and scattered fields. The Cartesian components of the extinction contribution to force and torque are (in the following, $\epsilon_\sigma = \epsilon_0$ when $\sigma = e$ and $\epsilon_\sigma = \mu_0$ when $\sigma = h$):

\begin{align}
\bar{F}_x^{(\text{ext})} &= \bar{F}_{eex}^{(\text{ext})} + \bar{F}_{ehx}^{(\text{ext})} + \bar{F}_{hhx}^{(\text{ext})} \\
\bar{F}_y^{(\text{ext})} &= \bar{F}_{eey}^{(\text{ext})} + \bar{F}_{ehy}^{(\text{ext})} + \bar{F}_{hhy}^{(\text{ext})} \\
\bar{F}_z^{(\text{ext})} &= \bar{F}_{eez}^{(\text{ext})} + \bar{F}_{ehz}^{(\text{ext})} + \bar{F}_{hhz}^{(\text{ext})}
\end{align}

where

\begin{align}
\bar{F}_{\sigma xx}^{(\text{ext})} + i\bar{F}_{\sigma xy}^{(\text{ext})} &= i \frac{\epsilon_\sigma}{16\pi} \sum_{m,n} \frac{n(n+2)}{\sqrt{(2n+1)(2n+3)}} \\
&\times \left[ \sqrt{(n + m + 1)(n + m + 2)} \left( c_{\sigma,m+1,n+1}^{is} c_{\sigma,m,n}^{s} + c_{\sigma,m+1,n+1}^{ss} c_{\sigma,m,n}^{i} \right) \\
&+ \sqrt{(n - m + 1)(n - m + 2)} \left( c_{\sigma,m,n}^{is} c_{\sigma,m+1,n+1}^{s} + c_{\sigma,m,n}^{ss} c_{\sigma,m+1,n+1}^{i} \right) \right] \\
\bar{F}_{\sigma zz}^{(\text{ext})} &= \frac{\epsilon_\sigma}{8\pi} \Im \sum_{m,n} \frac{n(n+2)}{\sqrt{(n + m + 1)(n - m + 1)}} \\
&\times \left( c_{\sigma,m,n}^{is} c_{\sigma,m+1,n+1}^{s} + c_{\sigma,m,n}^{ss} c_{\sigma,m+1,n+1}^{i} \right),
\end{align}
with cross terms for the components:

\[ F_{e_{chx}}^{(ext)} + iF_{e_{chy}}^{(ext)} = \frac{\sqrt{\varepsilon_0 \mu_0}}{16\pi} \sum_{m,n} \sqrt{(n-m)(n+m+1)} \]

\[ \times \left[ c_{h,m+1,n}^{s*} c_{e,m,n}^d + c_{h,m+1,n}^{s*} c_{e,m,n}^e - c_{e,m+1,n}^{s*} c_{h,m,n}^d - c_{e,m+1,n}^{s*} c_{h,m,n}^e \right] \]

\[ F_{e_{ehz}}^{(ext)} = \frac{\sqrt{\varepsilon_0 \mu_0}}{8\pi} \text{Im} \sum_{m,n} m \left( c_{e,m,n}^{s*} c_{h,m,n}^d + c_{e,m,n}^{s*} c_{h,m,n}^e \right) \]  

The Cartesian components of the torque are:

\[ \tilde{N}_x^{(ext)} = \tilde{N}_{eex}^{(ext)} + \tilde{N}_{hhx}^{(ext)} \]  

\[ \tilde{N}_y^{(ext)} = \tilde{N}_{eey}^{(ext)} + \tilde{N}_{hhy}^{(ext)} \]  

\[ \tilde{N}_z^{(ext)} = \tilde{N}_{eez}^{(ext)} + \tilde{N}_{hhz}^{(ext)} \]  

where,

\[ \tilde{N}_{\sigma\sigma}^{(ext)} + i\tilde{N}_{\sigma\sigma}^{(ext)} = \frac{i \varepsilon_\sigma}{16\pi k_0} \sum_{m,n} n(n+1) \sqrt{(n-m)(n+m+1)} \]

\[ \times \left( c_{\sigma,m+1,n}^{s*} c_{\sigma,m,n}^d + c_{\sigma,m+1,n}^{s*} c_{\sigma,m,n}^e \right) \]  

\[ \tilde{N}_{\sigma\sigma}^{(ext)} = \frac{\varepsilon_\sigma}{8\pi k_0} \text{Re} \sum_{m,n} n(n+1) m c_{\sigma,m,n}^{d*} c_{\sigma,m,n}^e. \]  

The Cartesian components of the scattered field force \( F_{e_{\sigma\sigma}}^{(sca)}, F_{e_{e\sigma}}^{(sca)} \) and torque \( \tilde{N}_{\sigma\sigma}^{(sca)} \) are obtained by changing the superscript \( i \) to \( s \) in Eqns. 2.76 through 2.84 above, and multiplying the equations by -1. In order to use the expansion coefficients derived using the PMM code, those coefficients need to be converted to the form for the \( c_{\sigma,m,n} \) coefficients of
Farsund and Felderhof. In the PMM approach, the incident wave was expanded in terms of the vector spherical harmonics $M_{m,n}$ and $N_{m,n}$

$$E^{(i)} = \sum_{m,n} [p_{mn}N_{m,n} + q_{mn}M_{m,n}]$$  \hspace{1cm} (2.85)

where, for the TM mode

$$p_{m,n} = -d_{m,n} \sin \theta_0 P'(\cos \theta_0) \hspace{1cm} q_{m,n} = d_{m,n}m \frac{P'(\cos \theta_0)}{\sin \theta_0}$$  \hspace{1cm} (2.86)

and for the TE mode

$$p_{m,n} = -im d_{m,n}m \frac{P(\cos \theta_0)}{\sin \theta_0} \hspace{1cm} q_{m,n} = im d_{m,n} \sin \theta_0 P'(\cos \theta_0).$$  \hspace{1cm} (2.87)

The factor $d_{m,n}$ is

$$d_{m,n} = i^{n+1}(-1)^m \frac{(2n+1)(n-m)!}{n(n+1)(n+m)!}.$$  \hspace{1cm} (2.88)

We convert these coefficients to those needed in the force and torque equations above using, for the TM mode,

$$c_{h,m,n}^{(i)} = -id_{m,n} P'(\cos \theta_0)$$  \hspace{1cm} (2.89)

$$c_{e,m,n}^{(i)} = -d_{m,n} \sin \theta_0 P'(\cos \theta_0)$$  \hspace{1cm} (2.90)

$$c_{h,m,n}^{(s)} = \frac{\omega_{m|n|,n}(2)}{k_0} \left[ \frac{4\pi(n + |m|)!}{(2n+1)(n-|m|)!} \right]^{1/2}$$  \hspace{1cm} (2.91)

$$c_{e,m,n}^{(s)} = \frac{\beta_{m|n|,n}(1)}{k_0} \left[ \frac{4\pi(n + |m|)!}{(2n+1)(n-|m|)!} \right]^{1/2}$$  \hspace{1cm} (2.92)
where \( \alpha_m = (-1)^{|m|}(-1) \) for \( m < 0 (m \geq 0) \) and \( \beta = (-1)^{|m|}(1) \) for \( m < 0 (m \geq 0) \). The conversion for the TE mode is

\[
c^{(i)}_{h,m,n} (TE) = -c^{(i)}_{e,m,n} (TM); \quad c^{(i)}_{e,m,n} (TE) = c^{(i)}_{h,m,n} (TM)
\]

\[
c^{(s)}_{h,m,n} (TE) = c^{(s)}_{h,m,n} (TM); \quad c^{(s)}_{e,m,n} (TE) = c^{(s)}_{e,m,n} (TM)
\]

except when \( m < 0 \), in which case \( c^{(s)}_{h,m,n}(TE) \) and \( c^{(s)}_{e,m,n}(TE) \) are multiplied by \(-1\).

Using these conversions, values are calculated for the force and torque on the grain due to radiation pressure, and, given a known incident flux, the efficiency factors \( Q_{pr} \) and \( Q_{\Gamma} \) are found using Eqns. (2.71) and (2.72).

### 2.3.1 Results

In Figures 2.5-2.11, the radiation efficiency factors found in the PMM code are presented for a silicate grain with \( a_{\text{eff}} = 0.2 \mu m \). The silicate grain has the dielectric function \( \epsilon = \epsilon_1 + i\epsilon_2 \) (index of refraction: \( n_{\text{ref}} = \sqrt{\epsilon_1 + \epsilon_2} \) given by Draine [13]) for astronomical silicates. For each of the three efficiency factor types there are two figures, one for a prolate grain of \( \zeta = 3/2 \) and one for an oblate grain with \( \zeta = 2/3 \). Each graph contains the results for six different incident angles for the incoming radiation, from \( \cos \theta_0 = 1 \) where the incident radiation is approaching the grain “head-on” (aligned with the body axis-of-symmetry, \( \hat{z} \)), to \( \cos \theta_0 = 0 \). In all of the calculations represented by the results below, the TE and TM modes of incident radiation are averaged together to approximate the assumed unpolarized incident starlight.

In order to check these efficiency factors, the same factors were generated using the widely distributed discrete dipole approximation code, DDSCAT (version 6.1, Draine & Flatau 2004). The values were found to be the same within the uncertainty associated with convergence of the solution. The PMM code converged in each case, although, in some cases, the truncation factor for the summation over \( n, n_{\max} \) had to be as large as 80 in
order to achieve convergence within 1%. For some wavelengths, we were unable to converge to within 10% with DDSCAT, due to limitations on the size of the dipole arrays when using the GNU Fortran compiler. The agreement between these two sources on the values for the efficiency factors, validated both the PMM and the DDSCAT code.

In Figures 2.5 and 2.6, $Q_{\text{abs}}$ is calculated as $Q_{\text{ext}} - Q_{\text{sca}}$ using Eqns. (2.66), (2.69), and (2.70).

![Graph](image)

Figure 2.5: $Q_{\text{abs}}$ for prolate ($\zeta = 3/2$) grains with $a_{\text{eff}} = 0.2\mu m$

Figures 2.7 and 2.8 show the scalar radiation pressure efficiency factor for prolate and oblate grains, respectively. The scalar radiation pressure efficiency factor $Q_{\text{pr}} = Q_{\text{pr}} \cdot \hat{k}_0$ describes the component of the force that is directed along $\hat{k}_0$, and given by [6]:

$$Q_{\text{pr}} = Q_{\text{ext}} - Q_{\text{sca}} < \cos \theta >$$  \hspace{1cm} (2.95)

$$Q_{\text{pr}} = Q_{\text{abs}} + (1 - < \cos \theta >) Q_{\text{sca}}$$  \hspace{1cm} (2.96)

where $< \cos \theta >$ is the mean scattering angle.
Figures 2.9 and 2.10 show the calculated results for the radiation-induced torque efficiency factor, again for both the prolate and oblate grain geometries. These results again use the converted expansion coefficients, this time substituted into Farsund’s and Felderhof’s expressions for the torque, Eqns. (2.83) and (2.84).

For a given incident radiation field, the spectrally averaged force and torque efficiency factors are given by:

$$\bar{Q}_{pr} = \frac{1}{u_{\text{rad}}} \int Q_{pr} u_{\nu} d\nu$$  \hspace{1cm} (2.97)

$$\bar{Q}_\Gamma = \frac{1}{\lambda_{\text{rad}}} \int Q_\Gamma \lambda u_{\nu} d\nu$$  \hspace{1cm} (2.98)

In Figure 2.11 the spectrally-averaged torque efficiency factor $\bar{Q}_{\Gamma,y}$ is displayed, where the spectral averaging is over the interstellar radiation field (ISRF). This averaging was done using the estimation of the solar neighborhood average ISRF spectrum made by Mathis, Mezger and Panagia [52],[50], as shown in Eqn.(1.2.)
Both the wavelength-dependent and spectrally averaged efficiency factors are comparable in magnitude to those for an irregular grain studied by Draine and Weingartner [17]. For a spherical silicate grain with $a_{\text{eff}} = 0.2\mu$m exposed to the ISRF, $\bar{Q}_{pr} = 0.82$. For prolate spheroids with $\zeta = 3/2$, $\bar{Q}_{pr}$ ranges from 0.73 to 0.85, while for oblate spheroids with $\zeta = 2/3$, $\bar{Q}_{pr}$ ranges from 0.78 to 0.89, with larger values corresponding to larger cross-sectional areas. The transverse component of $Q_{pr}$ takes values as high as $\approx 0.1$. 

Figure 2.7: $Q_{pr}$ for prolate ($\zeta = 3/2$) grains (0.2µm)
Figure 2.8: $Q_{pr}$ for oblate ($\zeta = 2/3$) grains (0.2\,\mu m)

Figure 2.9: $\lambda Q_{\Gamma, y}$ for prolate ($\zeta = 3/2$) grains (0.2\,\mu m)
Figure 2.10: $\lambda Q_{\Gamma, y}$ for oblate ($\zeta = 2/3$) grains (0.2$\mu$m)

Figure 2.11: The torque efficiency factor averaged over the MMP radiation field $\bar{Q}_{\Gamma, y}$ for prolate ($\zeta = 3/2$) and oblate ($\zeta = 2/3$) grains with $a_{\text{eff}} = 0.2\mu$m
2.4 Photoelectric efficiency factor and torque

To find the photoelectric torque, we extended an approach developed by Kerker and Wang [37] to find the photoelectric force. For an irradiated grain, the probability that an electron will be emitted from a given surface site is directly proportional to the intensity of the electric field immediately under the surface at that site. (The superscript $t$ indicates the internal field.) Any variation of this field intensity across the grain’s surface will result in a corresponding variation in the probability of photoemission from the surface. Kerker and Wang use this intensity variation to define an asymmetry factor for photoemission, in this case determining the average fraction of momentum photoelectrons carry in the incident wave direction:

$$A = \frac{\int_S |E(t)|^2 (\hat{n} \cdot \hat{e}) dS}{\int_S |E(t)|^2 dS}$$  \hspace{1cm} (2.99)

where $\hat{e}$ is in the direction of the incident wave and $\hat{n}$ is the unit surface normal vector and $dS$ is the surface area element. We adopted this asymmetry factor approach, modified to examine the photoelectric torque, as well as the force. The photoelectric force on a grain, as given by Weingartner and Draine [70] is a sum of the force due to the photoemission of valence electrons and the emission of any “attached” electrons ($Z > 0$). Since we adopt $Z = 0$, the photoelectric force includes only those forces due to photoemitted valence electrons. We also assume that all electrons are emitted along the normal surface vector $\hat{n}$, and that the electrons emerge from the grain with energy $E_e = h\nu - W$, where $h\nu$ is the incident photon energy and $W$ is the work function of the grain material. An actual grain is expected to have a slight positive charge [71]. Our assumption of a neutral grain increases the expected rate of photoelectric emission and the average energy per emitted electron, that would occur for a positively charged grain. These simplifications serve to overestimate the torque and force, which is appropriate given that we are initially attempting to determine the importance of photoelectric torque and force relative to radiative torque and force. The following expression is used to calculate the force the grain experiences due
to photoemission:

\[ F_{pe} = \pi a_{\text{eff}}^2 u_{\text{rad}} Q_{\text{pr,pe}} \] (2.100)

where the photoelectric force efficiency factor \( Q_{\text{pr,pe}} \) includes the force asymmetry factor \( A_{\text{pr}} \),

\[ Q_{\text{pr,pe}} = \frac{c Q_{\text{abs}}}{h \nu} Y p_e A_{\text{pr}} \] (2.101)

\[ A_{\text{pr}} = \frac{\int |E_{\text{surf}}|^2 \hat{n} dS}{\int |E_{\text{int}}|^2 dS}. \] (2.102)

where \( p_e \) is the photoelectron momentum and \( Y \) is the photoelectric yield (the probability that an electron will be emitted after a photon is absorbed). The photoelectric torque similarly includes an efficiency factor \( Q_{\Gamma,\text{pe}} \) and a photoemission torque asymmetry factor \( A_{\Gamma} \):

\[ \Gamma_{\text{pe}} = \pi a_{\text{eff}}^2 u_{\text{rad}} \frac{\lambda}{2\pi} Q_{\Gamma,\text{pe}} \] (2.103)

\[ Q_{\Gamma,\text{pe}} = \frac{c Q_{\text{abs}}}{h \nu} Y p_e \frac{2\pi a_{\text{eff}}}{\lambda} A_{\Gamma} \] (2.104)

\[ A_{\Gamma} = \frac{\int |E_{\text{surf}}|^2 r \times \hat{r} dS}{a_{\text{eff}} \int |E_{\text{int}}|^2 dS}. \] (2.105)

Expressions for the unit surface normal \( \hat{n} \) and the surface area element \( dS \) needed for the above calculations in spherical coordinates are:

\[ n = \frac{\partial r}{\partial \theta} \times \frac{\partial r}{\partial \phi} ; \quad \hat{n} = \frac{n}{|n|} \] (2.106)

\[ dS_{\theta \phi} = |n| d\theta d\phi \] (2.107)

\[ \hat{n} = [1 + (\zeta^4 - 1) \sin \theta^2]^{-1/2} [\zeta^2 \sin \theta (\hat{x} \cos \phi + \hat{y} \sin \phi) + \hat{z} \cos \theta] \] (2.108)
\[ dS_{\theta \phi} = r^2 \sin \theta \left[ 1 + \left( \frac{r}{a} \right)^4 \left( 1 - \frac{\zeta^2}{2} \right)^2 \sin^2 \theta \cos^2 \theta \right]^{1/2} d\theta d\phi. \]  
\hspace{1cm} (2.109)

### 2.4.1 Photoelectric yield

The photoelectric yield \( Y \) above is estimated based on the model developed by Weingartner and Draine [70]. For the grain size we consider, the threshold energy for photoemission is approximately equal to the work function for the bulk silicate material, estimated by [70] as \( W = 8 \text{eV} \). Using these assumptions, the photoelectric yield is:

\[
Y(h\nu, Z, a) \approx \frac{0.5(h\nu - W)}{5h\nu - 4W}.  
\hspace{1cm} (2.110)
\]

These estimates, based on bulk silicate, are expected to vary little with grain size for the sizes under consideration. However, there is little experimental data of photoemission yields for submicron grains. Some recent photoemission experiments using submicron-size grains [53] actually found much larger yields than those found for bulk material; however, even bulk silicate is not experimentally well characterized in terms of the work function and yield. Until such laboratory characterization of bulk and submicron grain-size silicate is done, the assumptions made above for the photoelectric yield provide only rough estimates of the photoelectric torque.

### 2.4.2 Results

Figure 2.12 shows the results of the calculation of the \( y \)-component of the photoelectric torque asymmetry factor, for six different angles of incidence \((\cos \theta_0)\) for starlight irradiating the grain. (Recall that, the grain is positioned in the coordinate system with its axis of symmetry aligned with the \( z \)-axis and the origin of the coordinate system at the center of mass of the grain. The incident field propagation vector is \( k_0(\hat{z} \cos \theta_0 - \hat{x} \sin \theta_0) \). Due to symmetry, the \( x \)- and \( z \)-components of the torque vanish, leaving only the \( y \)-component. These results are shown for a prolate \((\zeta = 3/2)\) and an oblate \((\zeta = 2/3)\) spheroidal grain,
and for two incident radiation wavelengths, $\lambda = 0.1\mu m, 0.15\mu m$. Based on these results, a maximum approximate value for $|A|_{\Gamma,y} \approx 0.05$ (independent of the wavelength) was adopted for calculation of the photoelectric recoil torque $\Gamma_{pe}$. In addition, we used $Q_{abs} \approx 1$, a reasonable approximation given that the incident (photoemission-inducing) photon energy will be $> 8$ eV ($\lambda < .15\mu m$) per the values displayed in Figures 2.5 and 2.6. We used the definition for the spectrally averaged radiative torque efficiency factor Eqn. (2.98), this time to calculate the photoelectric recoil torque efficiency factor, finding that $\bar{Q}_{\Gamma,pe,y} \approx 3.8$. Given a relevant ISRF energy range of 8 - 13.6 eV, the energy density $u = 3.86 \times 10^{-14}$ erg s$^{-1}$ and $\bar{\lambda} = 0.124\mu m$, for the calculation of $\bar{Q}_{\Gamma,pe,y}$. Figure 2.11 shows that the spectrally-averaged torque efficiency factor for the ISRF has values as high as $|\bar{Q}_{\Gamma,y}| \approx 0.05$. Using these values to calculate each torque, we compare them at the incident angle ($\cos \theta_0$) at which they peak, and find: $\Gamma_{pe} \approx 0.35\Gamma_{rad}$.

Non-uniform surface conditions, even for symmetrical grain shapes, could result in torques that are not confined to $\hat{y}$, as first suggested by Purcell [58]. A non-uniform distribution of photoelectric yield (e.g. due to a variation of the work function) could result in a photoelectric torque with components in both the $\hat{y}$ and $\hat{x}$ directions. (There can be no component of torque in the $\hat{z}$ direction for a spheroid, as $r \times \hat{n}$ has no $z$ component.) To model this condition, the photoelectric torque asymmetry factor $A_{\Gamma}$ is modified so that the yield $Y$ appears in both integrals. We positioned a large spot on the grain surface where the yield was enhanced by 10%. When the spot is on the illuminated side of the grain, $A_{\Gamma,y}$ changes by as much as $\approx 20\%$ and $|A_{\Gamma,x}|$ (and $|A_{\Gamma,y}|$ for $\cos \theta_0 = 0, 1$) reaches values as high as $\approx 0.005$. These relatively small enhancements in the photoelectric torque asymmetry factor result in little change in the photoelectric torque, relative the the radiative torque. Therefore, the radiative torques are likely to dominate the photoelectric torques.

The forward-direction force asymmetry factor ($A_{pr} \equiv A_{pr} \cdot \hat{k}_0$) has a range of values for the different angles of incidence $\approx 0.4$ to 0.6. The asymmetry factor for the transverse
direction has values from 0 to \( \approx 0.15 \). Using \( A_{pr} \approx 0.5 \) and \( Q_{abs} \approx 1 \), the ISRF spectrally-averaged efficiency factor \( \bar{Q}_{pr,pe} \approx 3.7 \), yielding a photoelectric force magnitude \( F_{pe} \approx 0.2F_{abs} \).

Figure 2.12: The \( y \)-component of the torque asymmetry factor \( A_{\Gamma} \).
2.5 Photodesorption

A dust grain in the neutral diffuse ISM will collide with the hydrogen atoms of the gas, as well as with the free electrons. Some of these atoms are expected to bind to the surface of the grain, “migrate” over the surface (via quantum mechanical tunneling or thermally activated hopping), be ejected from the surface due to photodesorption, or bind with other atoms on the surface to form H$_2$ molecules. The surface binding energy of these adsorbed atoms (adatoms), and other surface characteristics of this process are not well known at this time, so there is a great deal of uncertainty in modelling the torques that could result from the photodesorption of these atoms from the grain surface. In order to make an estimate of the relative importance of the photodesorption torque, we adopt the approach taken by Weingartner and Draine [70] on examining the photodesorption force, and consider the maximum contribution to torque possible for this process. As the photodesorption torque ($\Gamma_{pd}$) magnitude is proportional to the coverage of the surface by adatoms, assuming that surface conditions are uniform, the maximum torque generation occurs when the surface is fully covered with adatoms.

A model for estimating the torque due to photodesorption of H atoms from the grain surface would begin with a grain surface fully populated with adatom binding sites. The surface area of each binding site is $l^2$ and we adopt an estimate for the value of $l^2 \approx 10 \, \text{Å}^2$. The maximum number of surface binding sites is combined with the desorption rate per adatom ($R_{pd}^0$) to give the maximum desorption rate for the entire grain surface ($S$):

$$R_{pd} \leq \frac{R_{pd}^0 S}{l^2}. \quad (2.111)$$

Following [70], we estimate $R_{pd}^0 \approx 2 \times 10^{-10} \, \text{s}^{-1}$ for silicate grains and assume that the kinetic energy of the photoejected adatom is comparable to that of a photoemitted electron, $\sim 1\text{eV}$. As with our model for photoemission of electrons, we assume that the the photodesorption rate will be proportional to the intensity of the field at a given position on the surface, this
time the external field (scattered + incident) just above the surface. The torque generated by adatom photodesorption will be based on the asymmetry of the external field intensity over the grain surface.

The torque asymmetry factor due to adatom photodesorption is defined in the same way as that for photoemitted electrons, except that the field intensities are for the external field

\[ A_{\Gamma, pd} = -\frac{\int |\mathbf{E}_{\text{surf}}^\text{ext}|^2 \mathbf{r} \times \mathbf{n} dS}{\alpha_{\text{eff}} \int |\mathbf{E}_{\text{ext}}|^{2} dS}. \]  

(2.112)

The magnitude of the maximum photodesorption torque \( \Gamma_{pd} \) can be estimated as a ratio with the photoemission torque \( \Gamma_{pe} \), using the definition of \( A_{\Gamma, pd} \) from above

\[ \frac{|\Gamma_{pd}|}{|\Gamma_{pe}|} \approx \frac{R_{pd}^0 S h \nu}{\pi \alpha_{\text{eff}}^2 c u_{\text{rad}} Q_{\text{abs}} Y_l r^2} \left( \frac{m_H}{m_e} \right)^{1/2} \frac{|A_{\Gamma, pd}|}{|A_{\Gamma, pe}|} \]  

(2.113)

with the ratio of H momentum to \( e^- \) momentum

\[ \frac{p_H}{p_e} = \left( \frac{m_H}{m_e} \right)^{1/2} \]  

(2.114)

due to the equivalence of the kinetic energy of the ejected adatom and the photoemitted electron. The surface area \( S \) is estimated to be \( \approx 4\pi \alpha_{\text{eff}}^2 \) for \( \zeta = 3/2, 2/3 \) for the prolate and oblate grain models considered here. The asymmetry factors \( A_{\Gamma, pd} \) and \( A_{\Gamma, pe} \) are very similar for \( \lambda = 0.15\mu m \), while \( A_{\Gamma, pd} \) is as much as three times smaller than \( A_{\Gamma, pe} \) for \( \lambda = 0.1\mu m \). Therefore, we estimate the value of \( \Gamma_{pd} \) relative to \( \Gamma_{pe} \) for \( \lambda = 0.15\mu m \), using \( A_{\Gamma, pd} \approx A_{\Gamma, pe}, Q_{\text{abs}} \approx 1, \) and the photoelectric yield \( Y \approx 0.07, \) and find \( \Gamma_{pd} \approx 0.3\Gamma_{pe} \).

The force asymmetry factor due to photodesorption \( A_{pd} \) was as little as half the magnitude of \( A_{pe} \), the photoelectric force asymmetry factor, but generally was comparable in magnitude to \( A_{pe} \). Thus, for the prolate and oblate grain models here (\( \zeta = 3/2, 2/3 \)) the
force due to photodesorption $F_{pd}$ was comparable to the photoelectric force $F_{pe}$, as was found by Weingartner and Draine [70] for spheres.

### 2.6 Barton method in spheroidal coordinates

**Overview of spheroidal coordinates and wavefunctions**

Spheroids are generated by rotating an ellipse about either its major axis or its minor axis. Rotation about the minor axis creates an oblate spheroid and rotation about the major axis results in a prolate spheroid. The oblate and prolate coordinate systems are the result of the rotation of the elliptic coordinate system, similarly, about the two axes. A standard reference to the geometry of an ellipse is the semi-focal length $f$, half the distance between the two ellipse foci.

The transformation between spheroidal and Cartesian coordinates is:

\[
x = f \left[ (1 - \eta^2) \left( \xi^2 \pm 1 \right) \right]^{\frac{1}{2}} \cos \phi
\]  
\[
y = f \left[ (1 - \eta^2) \left( \xi^2 \pm 1 \right) \right]^{\frac{1}{2}} \sin \phi
\]  
\[
z = f \eta \xi
\]

with the upper sign ($\pm$) for the oblate coordinates and the lower sign for the prolate coordinates. The ranges of the oblate coordinates are:

\[-1 \leq \eta \leq 1, \quad 0 \leq \xi < \infty, \quad 0 \leq \phi \leq 2\pi, \quad (2.118)\]

and the prolate coordinate ranges are:

\[-1 \leq \eta \leq 1, \quad 1 \leq \xi < \infty, \quad 0 \leq \phi \leq 2\pi. \quad (2.119)\]
The Cartesian basis vectors in terms of the spheroidal coordinates are:

\[ \hat{e}_x = -\eta \left( \frac{\xi^2 \pm 1}{\xi^2 \pm \eta^2} \right)^{\frac{1}{2}} \cos \phi \ \hat{e}_\eta + \xi \left( \frac{1 - \eta^2}{\xi^2 \pm \eta^2} \right)^{\frac{1}{2}} \cos \phi \ \hat{e}_\zeta - \sin \phi \ \hat{e}_\phi \] (2.120)

\[ \hat{e}_y = -\eta \left( \frac{\xi^2 \pm 1}{\xi^2 \pm \eta^2} \right)^{\frac{1}{2}} \sin \phi \ \hat{e}_\eta + \xi \left( \frac{1 - \eta^2}{\xi^2 \pm \eta^2} \right)^{\frac{1}{2}} \sin \phi \ \hat{e}_\zeta + \cos \phi \ \hat{e}_\phi \] (2.121)

\[ \hat{e}_z = \xi \left( \frac{1 - \eta^2}{\xi^2 \pm \eta^2} \right)^{\frac{1}{2}} \hat{e}_\eta + \eta \left( \frac{\xi^2 \pm 1}{\xi^2 \pm \eta^2} \right)^{\frac{1}{2}} \hat{e}_\zeta, \] (2.122)

with the upper sign for the oblate spheroidal coordinates and the lower sign for the prolate spheroidal coordinates.

The scale factors for the spheroidal coordinate systems are:

\[ h_\eta = f \left( \frac{\xi^2 \pm \eta^2}{1 - \eta^2} \right)^{\frac{1}{2}} \] (2.123)

\[ h_\xi = f \left( \frac{\xi^2 \pm \eta^2}{\xi^2 \pm 1} \right)^{\frac{1}{2}} \] (2.124)

\[ h_\phi = f \left[ (1 - \eta^2) \left( \frac{\xi^2 \pm 1}{\xi^2 \pm \eta^2} \right) \right]^{\frac{1}{2}} \] (2.125)

and the position vector \( \mathbf{r} \) in spheroidal coordinates is:

\[ \mathbf{r} = \mp f \eta \left( \frac{1 - \eta^2}{\xi^2 \pm \eta^2} \right)^{\frac{1}{2}} \hat{e}_\eta + f \xi \left( \frac{\xi^2 \pm 1}{\xi^2 \pm \eta^2} \right)^{\frac{1}{2}} \hat{e}_\zeta. \] (2.126)

Both the surface of a spheroid, designated by \( \xi_0 \) and the semi-focal length \( f \) are related to
the semi-major \((a_{\text{semi}})\) and semi-minor \((b_{\text{semi}})\) axes of the ellipse:

\[
\xi_0 = \frac{\zeta}{(\zeta^2 - 1)^{1/2}} \tag{2.127}
\]

\[
f = a_{\text{semi}} \left(1 - \zeta^2\right)^{1/2} \tag{2.128}
\]

where \(\zeta = a_{\text{semi}}/b_{\text{semi}}\).

The spheroidal scalar Helmholtz equation

The first step in expressing electromagnetic fields in spheroidal coordinates is to write the Helmholtz equation in spheroidal coordinates and solve for the scalar wave function \(\psi\). Using the transformations and scale factors defined above, the Laplacian is rewritten in spheroidal coordinates. This equation, with the prolate coordinate system represented by the lower sign and the oblate by the upper, is:

\[
\frac{4}{d^2 (\xi^2 \pm \eta^2)} \left[ \frac{\partial}{\partial \xi} \left( (\xi^2 \pm 1) \frac{\partial}{\partial \xi} \right) + \frac{\partial}{\partial \eta} \left( (1 - \eta^2) \frac{\partial}{\partial \eta} \right) + \frac{\partial}{\partial \phi} \left( \frac{\xi^2 \pm \eta^2}{(\xi^2 \pm 1) (1 - \eta^2)} \frac{\partial}{\partial \phi} \right) \right] \psi + k^2 \psi = 0 \tag{2.129}
\]

The equations for the Laplacian in both the oblate and prolate coordinates are fully separable, and the details of that separation (for the prolate system) are presented in Appendix A. Applying the separation of variables approach results in Lame product solutions to Eqn. (2.129)

\[
\psi_{m,n} = S_{m,n}(c, \eta) R_{m,n}(c, \xi)e^{im\phi} \tag{2.130}
\]

and,

\[
\psi_{m,n} = S_{m,n}(-ic, \eta) R_{m,n}(-ic, \xi)e^{im\phi} \tag{2.131}
\]
that are, respectively, a solution to the two differential equations for the prolate coordinate system,

\[
\frac{d}{d\xi} \left[ (\xi^2 + 1) \frac{d}{d\xi} \right] - \left[ \lambda_{m,n} - c^2 \xi^2 + \frac{m^2}{(\xi^2 \pm 1)} \right] R^{(i)}_{[m,n]}(c,\xi) = 0 \tag{2.132}
\]

\[
\frac{d}{d\eta} \left[ (1 - \eta^2) \frac{d}{d\eta} S_{m,n}(c,\eta) \right] + R^{(i)}_{[m,n]}(c,\xi) \left[ \lambda_{m,n} - c^2 \eta^2 - \frac{m^2}{(1 - \eta^2)} \right] S_{m,n}(c,\eta) = 0 \tag{2.133}
\]

and a solution to the two differential equations for the oblate coordinate system,

\[
\frac{d}{d\xi} \left[ (\xi^2 + 1) \frac{d}{d\xi} R^{(i)}_{[m,n]}(-ic,ix) \right] - \left[ \lambda_{m,n} - c^2 \xi^2 - \frac{m^2}{(\xi^2 + 1)} \right] R^{(i)}_{[m,n]}(-ic,ix) = 0 \tag{2.134}
\]

\[
\frac{d}{d\eta} \left[ (1 - \eta^2) \frac{d}{d\eta} S_{m,n}(-ic,\eta) \right] + \left[ \lambda_{m,n} + c^2 \eta^2 - \frac{m^2}{(1 - \eta^2)} \right] S_{m,n}(-ic,\eta) = 0 \tag{2.135}
\]

The characteristic value \( c \) above is the product of the wave number \( k \) of the medium through which the electromagnetic wave is traveling, and the spheroid’s semi-focal distance \( f \), \( c = kf \).

**The spheroidal angular and radial functions**

The solutions to the spheroidal scalar Helmholtz differential equation include the spheroidal angular \( S_{m,n}(c,\eta) \) and radial \( R^{(i)}_{[m,n]}(c,\xi) \) functions, as described in Flammer’s [22] foundational work of 1957 on spheroidal wavefunctions. Here we summarize the functions and their properties.

When \( c \) is equal to zero in the differential equation derived for the spheroidal angular function in the prolate coordinates Eqn. (2.133),

\[
\frac{d}{d\eta} \left[ (1 - \eta^2) \frac{dS}{d\eta} \right] + \left[ \lambda_{m,n} - c^2 \eta^2 - \frac{m^2}{(1 - \eta^2)} \right] S_{m,n}(c,\eta) = 0, \tag{2.136}
\]
the solution is satisfied by the associated Legendre functions, \( P_n^m(\eta) \). For the solution to be finite at \( \pm 1 \), these must be associated Legendre functions of the first kind, where \( m \) and \( n \) again correspond, respectively, to the integral order and degree of the functions. When \( c \) is not equal to zero, the spheroidal angular function can be described by the infinite sum,

\[
S_{m,n} = \sum_{r=0,1}^{\infty} d_r^m c P_{m+r}(\eta)
\]  

(2.137)

for the prolate system, and

\[
S_{m,n}(-ic,\eta) = \sum_{r=0,1}^{\infty} d_r^m (-ic) P_{m+r}(\eta)
\]  

(2.138)

for the oblate system. The prime (') over the summation symbol indicates that only even values \( r \) are summed when \( m - n \) is even, and only odd values of \( r \) are summed when \( m - n \) is odd.

The spheroidal radial functions are infinite sums involving the spherical Bessel, Neumann and Hankel functions \( (z^i; i = 1, 2, 3, 4) \), shown here for the prolate coordinate system

\[
R_{|m|,n}(c, \xi) = \sum_{r=0,1}^{\infty} \frac{1}{d_r^{m,n}(c)(2|m|+r)!} \left( \frac{\xi^2 \pm 1}{\xi^2} \right)^{|m|/2}
\]

\[
\times \sum_{r=0,1}^{\infty} i^{r+|m|-n} d_r^{m,n}(c) (2|m|+r)! \xi^{i} c_{|m|+r}(c \xi)
\]  

(2.139)

The spheroidal expansion coefficients \( d_r^{m,n}(c) \) above, and the separation constants \( \lambda_{m,n} \) in the differential equations above were solved for using an eigenvalue/eigenvector solution approach developed by Eide, Stamnes, Stamnes and Schulz [19]. This approach was implemented in Fortran making use of a LAPACK library routine for complex coefficients. The
details of this solution approach are in Appendix B.

**The vector spheroidal wavefunctions**

Next we expand the electromagnetic field in vector spheroidal wavefunctions. The vector spheroidal wavefunctions must have the characteristics of the electromagnetic field vectors. Any real electromagnetic field \((\mathbf{E}, \mathbf{H})\) propagating through a linear, homogeneous and isotropic medium in the absence of free charge must be a solution of the vector wave equation:

\[
\nabla^2 \mathbf{E} = k^2 \mathbf{E} = 0, \quad \nabla^2 \mathbf{H} = k^2 \mathbf{H} = 0.
\]

(2.140)

The constant \(k\), above, is equal to \(\omega^2 \epsilon \mu\), where \(\epsilon\) and \(\mu\) are the dielectric and the permeability constants of the medium through which the wave is propagating, with \(k_0\) for fields in the vacuum external to the grain, and \(k_l\) for the internal field. The electric and magnetic fields \((\mathbf{E}, \mathbf{H})\) are related and interdependent

\[
\nabla \times \mathbf{E} = n\omega \mu \mathbf{H}, \quad \nabla \times \mathbf{H} = -n\omega \epsilon \mathbf{E},
\]

(2.141)

as well as being divergenceless

\[
\nabla \cdot \mathbf{E} = 0, \quad \nabla \cdot \mathbf{H} = 0
\]

(2.142)

so that any expansion in vector spheroidal wavefunctions must have these characteristics. The vector spheroidal wavefunctions are based on a divergenceless vector representation of the spheroidal scalar Helmholtz equation solution, \(\psi\), with an interdependence as defined by that between \(\mathbf{E}\) and \(\mathbf{H}\):

\[
\mathbf{M}_{m,n} = \nabla \times (r\psi_{m,n})
\]

(2.143)

\[
\mathbf{N}_{m,n} = \frac{1}{k} \nabla \times \mathbf{M}_{m,n}
\]

(2.144)
where, the pilot vector used in Eqn. (2.143) is the position vector Eqn. (2.126) in spheroidal coordinates, and \( k \) is the wave number of the medium through which the wave is propagating. The following vector wavefunction components result, where a harmonic time dependence \( e^{-i\omega t} \) is assumed but suppressed throughout the section. (\( \tilde{c} = c \) and \( \tilde{\xi} = \xi \) for prolate coordinates, while \( \tilde{c} = -ic \) and \( \tilde{\xi} = i\xi \) for oblate coordinates):

\[
M_{m,n;\eta} = \frac{-im\xi}{[(\xi^2 \pm \eta^2)(1 - \eta^2)]^{1/2}} R^{(i)}_{|m|,n}(\tilde{c},\tilde{\xi}) S_{m,n}(\tilde{c},\eta) e^{im\phi}
\]  

(2.146)

\[
M_{m,n;\xi} = \frac{m\eta}{[(\xi^2 \pm \eta^2)(\xi^2 \pm 1)]^{1/2}} R^{(i)}_{|m|,n}(\tilde{c},\tilde{\xi}) S_{m,n}(\tilde{c},\eta) e^{im\phi}
\]  

(2.147)

\[
M_{m,n;\phi} = \frac{[(\xi^2 \pm 1)(1 - \eta^2)]^{1/2}}{\tilde{c}(\xi^2 \pm \eta^2)^{1/2}} \left[ \xi R^{(i)}_{|m|,n}(\tilde{c},\tilde{\xi}) S'_{m,n}(\tilde{c},\eta) - \eta R^{(i)}_{|m|,n}(\tilde{c},\tilde{\xi}) S_{m,n}(\tilde{c},\eta) \right] e^{im\phi}
\]  

(2.148)

\[
N_{m,n;\eta} = \frac{(1 - \eta^2)^{1/2}}{\tilde{c}(\xi^2 \pm \eta^2)^{1/2}} \left[ S'_{m,n}(\tilde{c},\eta) \frac{\partial}{\partial \xi} \left( \frac{\xi (\xi^2 \pm 1)}{(\xi^2 \pm \eta^2)} R^{(i)}_{|m|,n}(\tilde{c},\tilde{\xi}) \right) \right.
\]

\[
\pm \eta S_{m,n}(\tilde{c},\eta) \frac{\partial}{\partial \xi} \left( \frac{(\xi^2 \pm 1)}{(\xi^2 \pm \eta^2)} R^{(i)}_{|m|,n}(\tilde{c},\tilde{\xi}) \right)
\]

\[
\pm \frac{m^2\eta}{(1 - \eta^2)(\xi^2 \pm 1)} S_{m,n}(\tilde{c},\eta) R^{(i)}_{|m|,n}(\tilde{c},\tilde{\xi}) e^{im\phi}
\]  

(2.149)
\[ N_{m,n;\xi} = - \frac{(\xi^2 \pm 1)^{1/2}}{\tilde{c}(\xi^2 \pm \eta^2)^{1/2}} \left[ \pm \frac{\partial}{\partial \eta} \left( \frac{\eta (1 - \eta^2)}{(\xi^2 \pm \eta^2)} S_{m,n}(\tilde{c}, \eta) \right) R_{|m|,n}^{(i)}(\tilde{c}, \tilde{\xi}) \right. \\
\left. \xi \frac{\partial}{\partial \eta} \left( \frac{(1 - \eta^2)}{(\xi^2 \pm \eta^2)} S_{m,n}'(\tilde{c}, \eta) \right) R_{|m|,n}^{(i)}(\tilde{c}, \tilde{\xi}) \right. \\
\left. - \frac{m^2 \xi}{(1 - \eta^2) (\xi^2 \pm 1)} S_{m,n}(\tilde{c}, \eta) R_{|m|,n}^{(i)}(\tilde{c}, \tilde{\xi}) \right] e^{im\phi} \] (2.150)

\[ N_{m,n;\phi} = -im \frac{(1 - \eta^2)^{1/2}}{\tilde{c}(\xi^2 \pm \eta^2)^{1/2}} \left[ \pm \frac{1}{(\xi^2 \pm 1)} \frac{d}{d\eta} (\eta S_{m,n}(\tilde{c}, \eta)) R_{|m|,n}^{(i)}(\tilde{c}, \tilde{\xi}) \right. \\
\left. - \frac{1}{(1 - \eta^2)} S_{m,n}(\tilde{c}, \eta) \frac{d}{d\xi} \left( \xi R_{|m|,n}^{(i)}(\tilde{c}, \tilde{\xi}) \right) \right] e^{im\phi}. \] (2.151)

**Obtaining the internal and scattered field intensities**

The internal and scattered fields can be expressed as expansions in vector spheroidal wavefunctions, guaranteeing that Maxwell’s equations are satisfied. The medium-specific parameters of \( \psi \) are set based on whether the field is interior or exterior to the grain. The characteristic value \( \tilde{c} = k_f \) is replaced below with \( c_t (c_s) \) when describing the internal field (scattered or incident field); and \( R^{(i)} \) is a radial spheroidal function of the first kind for the internal field \( R_{|m|,n}^{(1)}(\tilde{c}_t, \tilde{\xi}) \), and of the third kind for the external scattered field \( R_{|m|,n}^{(3)}(\tilde{c}_s, \tilde{\xi}) \).

The radial function \( R_{|m|,n}^{(1)}(\tilde{c}_t, \tilde{\xi}) \) is selected for the internal field because the function has a finite value at the grain center (origin). The scattered radial function \( R_{|m|,n}^{(3)}(\tilde{c}_s, \tilde{\xi}) \) is formed as a combination \( R^{(3)} = R^{(1)} + sR^{(2)} \), with this combination providing for finite values at infinity. \( R^{(3)} \) diverges at the origin, but this is not a problem for the scattered field which is defined as starting at the grain surface. The internal electromagnetic field can be expressed as an expansion in the two vector wavefunctions \( M \) and \( N \), (noting that \( t \) indicates the
internal field, and \( s \) indicates the scattered field):

\[
E^{(t)} = \sum_{m,n} \left[ c_{m,n} N_{m,n}^{(t)} + d_{m,n} M_{m,n}^{(t)} \right] 
\]

\[
H^{(t)} = -i n_{\text{int}} \sum_{m,n} \left[ c_{m,n} M_{m,n}^{(t)} + d_{m,n} N_{m,n}^{(t)} \right], 
\]

where \( c_{m,n} \) and \( d_{m,n} \) are the expansion coefficients of the internal field. In a similar manner, the scattered field is expanded:

\[
E^{(s)} = \sum_{m,n} \left[ a_{m,n} N_{m,n}^{(s)} + b_{m,n} M_{m,n}^{(s)} \right] 
\]

\[
H^{(s)} = -i \sum_{m,n} \left[ a_{m,n} M_{m,n}^{(s)} + b_{m,n} N_{m,n}^{(s)} \right], 
\]

where \( a_{m,n} \) and \( b_{m,n} \) are the expansion coefficients of the scattered field.

If the incident field, \( E^{(i)}, H^{(i)} \), is known, with the approach developed by Barton [32] it is now possible to derive a set of linear equations in order to determine the unknown expansion coefficients for the internal and scattered fields. First, the boundary conditions for the tangential (tg) fields are applied at the particle surface:

\[
E_{\text{tg}}^{(i)} + E_{\text{tg}}^{(s)} = E_{\text{tg}}^{(t)} 
\]

\[
H_{\text{tg}}^{(i)} + H_{\text{tg}}^{(s)} = H_{\text{tg}}^{(t)} 
\]

At the surface defined as \( \xi = \xi_0 \), the tangential field boundary conditions result in the following equations,

\[
E_{\eta}^{(i)} + E_{\eta}^{(s)} = E_{\eta}^{(t)} 
\]
\[ E^{(i)} + E^{(s)} = E^{(t)} \]  \hspace{1cm} (2.159)

\[ H^{(i)} + H^{(s)} = H^{(t)} \]  \hspace{1cm} (2.160)

\[ H^{(i)} + H^{(s)} = H^{(t)} \]  \hspace{1cm} (2.161)

The incident electromagnetic field for this model is that of a plane linearly polarized wave propagating through the vacuum surrounding the grain. The angle between the wave propagation vector \( \mathbf{k}_0 \) and the spheroidal grain symmetry axis \( \mathbf{z} \) is \( \theta_0 \), the angle of incidence. With this orientation, in the TE mode \( \mathbf{E} \) lies entirely along the \( \mathbf{y} \) axis and in the TM mode \( \mathbf{E} \) lies within the x-z plane. With a coordinate system centered on the grain center of mass, the propagation direction selected is one which is positive in both the x and z directions. The propagation vector for the incident wave is:

\[ \mathbf{k}_0 = k_0 (\hat{x} \sin \theta_0 + \hat{z} \cos \theta_0) . \]  \hspace{1cm} (2.162)

(Note that the direction of the propagation vector \( \mathbf{k} \) is different from that of the one used in the PMM approach presented earlier. The incident polar angle \( \theta_0 \) is the same; however, the azimuthal angle \( \phi \) is shifted by \( \pi \) so that the intensities plotted over the surface of the grain are mirror-images of one another. The prescription was adopted here to allow comparison with published values of the spheroidal coefficients, \( S_{m,n} \) and \( R_{m|n|,m}^{(i)} \), to verify the code.)

In the TE mode, the electric and magnetic vectors of the incident wave are,

\[ \mathbf{E}^{i}_{TE} = \hat{y} E_0 e^{i \mathbf{k} \cdot \mathbf{r}} \]  \hspace{1cm} (2.163)

\[ \mathbf{B}^{i}_{TE} = (\hat{z} \sin \theta_0 - \hat{x} \cos \theta_0) E_0 e^{i \mathbf{k} \cdot \mathbf{r}} \]  \hspace{1cm} (2.164)

with the TM mode electromagnetic vectors being,

\[ \mathbf{E}^{i}_{TM} = -\mathbf{B}^{i}_{TE} \]  \hspace{1cm} (2.165)
\[ \mathbf{B}^{(i)}_{TM} = \mathbf{E}^{(i)}_{TE} \] (2.166)

where \( E_0 \) is the amplitude of the incident wave, which is set to 1. The incident field components in spheroidal coordinates are (for the TE mode):

\[ E^{(i)}_{TE, \eta} = -\eta \frac{(\xi^2 + 1)^{1/2}}{(\xi^2 - \eta^2)^{1/2}} \sin \phi e^{ikr} \] (2.167)

\[ E^{(i)}_{TE, \phi} = \cos \phi e^{ikr} \] (2.168)

\[ B^{(i)}_{TE, \eta} = \left( \frac{1 - \eta^2}{2} \sin \theta_0 + \eta \frac{(\xi^2 + 1)^{1/2}}{(\xi^2 - \eta^2)^{1/2}} \cos \phi \cos \theta_0 \right) e^{ikr} \] (2.169)

\[ B^{(i)}_{TE, \phi} = \sin \phi \cos \theta_0 e^{ikr} \] (2.170)

where,

\[ k \cdot r = c_s \left[ \left( \xi^2 + 1 \right) \left( 1 - \eta^2 \right)^{1/2} \cos \phi \sin \theta_0 + \xi \eta \cos \theta_0 \right]. \] (2.171)

With the components of the incident wave defined, the expanded wavefunction expressions for the internal and the scattered fields are substituted into Eqns. (2.158), (2.159), (2.160), and (2.161), generating four sets of equations, for each mode. (The term \( n_{int} \) below is the index of refraction of the grain material, \( n_{int} = (\epsilon_{int})^{1/2} \) based on the wavelength of the incident field.)

TE:

\[ E^{(i)}_{TE, \eta} = \sum_{m, n} \left[ c_{m,n} N^{(i)}_{\eta} + d_{m,n} M^{(i)}_{\eta} - a_{m,n} N^{(s)}_{\eta} - b_{m,n} M^{(s)}_{\eta} \right] \] (2.172)

\[ E^{(i)}_{TE, \phi} = \sum_{m, n} \left[ c_{m,n} N^{(i)}_{\phi} + d_{m,n} M^{(i)}_{\phi} - a_{m,n} N^{(s)}_{\phi} - b_{m,n} M^{(s)}_{\phi} \right] \] (2.173)

\[ H^{(i)}_{TE, \eta} = \sum_{m, n} \left[ -n_{int} \left( c_{m,n} M^{(i)}_{\eta} + d_{m,n} N^{(i)}_{\eta} \right) + \left( a_{m,n} M^{(s)}_{\eta} + b_{m,n} N^{(s)}_{\eta} \right) \right] \] (2.174)
\[ H^{(i)}_{TE, \phi} = \sum_{m,n} \left[ -n_{int} \left( c_{m,n} M^{(t)}_{\phi} + d_{m,n} N^{(t)}_{\phi} \right) + \left( a_{m,n} M^{(s)}_{\phi} + b_{m,n} N^{(s)}_{\phi} \right) \right] \] (2.175)

TM:

\[ E^{(i)}_{TM, \eta} = \sum_{m,n} \left[ n_{int} \left( c_{m,n} M^{(t)}_{\eta} + d_{m,n} N^{(t)}_{\eta} \right) - \left( a_{m,n} M^{(s)}_{\eta} + b_{m,n} N^{(s)}_{\eta} \right) \right] \] (2.176)

\[ E^{(i)}_{TM, \phi} = \sum_{m,n} \left[ n_{int} \left( c_{m,n} M^{(t)}_{\phi} + d_{m,n} N^{(t)}_{\phi} \right) - \left( a_{m,n} M^{(s)}_{\phi} + b_{m,n} N^{(s)}_{\phi} \right) \right] \] (2.177)

\[ H^{(i)}_{TM, \eta} = \sum_{m,n} \left[ c_{m,n} N^{(t)}_{\eta} + d_{m,n} M^{(t)}_{\eta} - a_{m,n} N^{(s)}_{\eta} - b_{m,n} M^{(s)}_{\eta} \right] \] (2.178)

\[ H^{(i)}_{TM, \phi} = \sum_{m,n} \left[ c_{m,n} N^{(t)}_{\phi} + d_{m,n} M^{(t)}_{\phi} - a_{m,n} N^{(s)}_{\phi} - b_{m,n} M^{(s)}_{\phi} \right] \] (2.179)

At this point, the method developed by Barton [34],[33],[32] extends the Point Matching Method (PMM) (discussed above) to what Barton calls the “boundary matching method”. Instead of matching boundary conditions at a set of discrete points on a defined surface as in the PMM, Barton multiplies Eqns. 2.172 through 2.179 by \( S_{m',n'} e^{-im'\phi} \) and integrates over \( \eta = (-1,1) \), \( \phi = (0,2\pi) \). This results in a set of linear equations that can be solved for the unknown field expansion coefficients \( a_{m,n}, b_{m,n}, c_{m,n}, d_{m,n} \). (This approach was originally developed for spherical surfaces, using spherical coordinates [34]; then extended to slightly non-spherical surfaces, again using spherical coordinates [33]; and finally applied to spheroidal surfaces using spheroidal coordinates [32].)

When the incident field is integrated for each of the four above equations (for a given mode) 2.172 through 2.179, four surface integrals are obtained for \( E^{(i)}_{\eta}, E^{(i)}_{\phi}, H^{(i)}_{\eta}, H^{(i)}_{\phi} \):

\[ A^{\eta}_{m,n'} = \int_{0}^{2\pi} \int_{-1}^{1} E^{(i)}_{\eta} S_{m,n'}(c_{s}, \eta) e^{-im\phi} d\eta d\phi \] (2.180)
Similarly, integrating the vector wavefunctions of the expanded scattered and internal fields in Eqns. (2.172), (2.173), (2.174), and (2.175) above, results in the following line integrals (integration of $\phi$ over the surface is completed, and integration with respect to $\eta$ is performed over only half the range and doubled, due to the symmetry of the spheroidal angular function $S_{m,n}$):

\[
A_{m,n'}^\phi = \int_0^{2\pi} \int_{-1}^1 E_{m,n'}(c_s, \eta)e^{-im\phi}d\eta d\phi
\]

(2.181)

\[
B_{m,n'}^\eta = \int_0^{2\pi} \int_{-1}^1 H_{m,n'}(c_s, \eta)e^{-im\phi}d\eta d\phi
\]

(2.182)

\[
B_{m,n'}^\phi = \int_0^{2\pi} \int_{-1}^1 H_{m,n'}(c_s, \eta)e^{-im\phi}d\eta d\phi.
\]

(2.183)

\[
I_{m,n,n'}^1 = 4\pi \int_0^1 N_{m,n; \eta}^{(s)} S_{m,n'}(c_s, \eta)d\eta
\]

(2.184)

\[
I_{m,n,n'}^2 = 4\pi \int_0^1 M_{m,n; \eta}^{(s)} S_{m,n'}(c_s, \eta)d\eta
\]

(2.185)

\[
I_{m,n,n'}^3 = 4\pi \int_0^1 N_{m,n; \eta}^{(t)} S_{m,n'}(c_s, \eta)d\eta
\]

(2.186)

\[
I_{m,n,n'}^4 = 4\pi \int_0^1 M_{m,n; \eta}^{(t)} S_{m,n'}(c_s, \eta)d\eta
\]

(2.187)

\[
I_{m,n,n'}^5 = 4\pi \int_0^1 N_{m,n; \phi}^{(s)} S_{m,n'}(c_s, \eta)d\eta
\]

(2.188)

\[
I_{m,n,n'}^6 = 4\pi \int_0^1 M_{m,n; \phi}^{(s)} S_{m,n'}(c_s, \eta)d\eta
\]

(2.189)

\[
I_{m,n,n'}^7 = 4\pi \int_0^1 N_{m,n; \phi}^{(t)} S_{m,n'}(c_s, \eta)d\eta
\]

(2.190)
\[ I_{m,n,n'}^8 = 4\pi \int_0^1 M_{m,n;\phi}^{(i)} S_{m,n'}(c_s, \eta) d\eta. \]  

(2.191)

(The integration of the line and surface integrals above required some significant integral “deconstruction”. Series were used to represent some functions, odd and even integral forms were used to reduce the integration load in other cases. The details of this methodology are included in Appendix C, for the adventurous reader.)

When both the surface and line integrals are included in the boundary condition matching equations, a set of \(4(L - |m| + 1)\) simultaneous linear equations results for each value of \(m \neq 0\). The variable \(L\) is a truncation number selected based on the level of precision required for convergence. Each equation has \(4(L - |m| + 1)\) terms, \((L - |m| + 1)\) terms for each integral.

\[
\sum_{n=|m|}^{L} (-I_{m,n,n'}^{1} a_{m,n} - I_{m,n,n'}^{2} b_{m,n} + I_{m,n,n'}^{3} c_{m,n} + I_{m,n,n'}^{4} d_{m,n}) = \frac{A_{m,n'}}{2\pi} \quad (2.192)
\]

\[
\sum_{n=|m|}^{L} (-I_{m,n,n'}^{5} a_{m,n} - I_{m,n,n'}^{6} b_{m,n} + I_{m,n,n'}^{7} c_{m,n} + I_{m,n,n'}^{8} d_{m,n}) = \frac{A_{m,n'}}{2\pi} \quad (2.193)
\]

\[
\sum_{n=|m|}^{L} (-I_{m,n,n'}^{2} a_{m,n} - I_{m,n,n'}^{1} b_{m,n} + n_{int} I_{m,n,n'}^{4} c_{m,n} + n_{int} I_{m,n,n'}^{3} d_{m,n}) = \frac{\imath B_{m,n'}}{2\pi \sqrt{\varepsilon_{\text{ext}}}} \quad (2.194)
\]

\[
\sum_{n=|m|}^{L} (-I_{m,n,n'}^{6} a_{m,n} - I_{m,n,n'}^{5} b_{m,n} + n_{int} I_{m,n,n'}^{8} c_{m,n} + n_{int} I_{m,n,n'}^{7} d_{m,n}) = \frac{\imath B_{m,n'}}{2\pi \sqrt{\varepsilon_{\text{ext}}}} \quad (2.195)
\]

When \(m = 0\), the spheroidal wavefunction components \(M_{m,n;\eta}\) and \(N_{m,n;\phi}\) equal 0, resulting in a smaller set of equations to be solved.

\[
\sum_{n=0}^{L} (-I_{0,n,n'}^{1} a_{0,n} + I_{0,n,n'}^{3} c_{0,n}) = \frac{A_{0,n'}}{2\pi} \quad (2.196)
\]
\[
\sum_{n=0}^{L} (-I_{0,n,n'}^6 b_{0,n} + I_{0,n,n'}^8 d_{0,n}) = \frac{A_{0,n'}^6}{2\pi} 
\]

(2.197)

\[
\sum_{n=0}^{L} (-I_{0,n,n'}^4 b_{0,n} + n_{int} I_{0,n,n'}^3 d_{0,n}) = \frac{iB_{0,n'}^3}{2\pi \sqrt{\varepsilon_{\text{ext}}}} 
\]

(2.198)

\[
\sum_{n=0}^{L} (-I_{0,n,n'}^6 a_{0,n} + n_{int} I_{0,n,n'}^8 c_{0,n}) = \frac{P_{0,n'}^6}{2\pi \sqrt{\varepsilon_{\text{ext}}}} . 
\]

(2.199)

When these sets of linear equations are solved for the internal and scattered expansion coefficients \((c_{m,n} \text{ and } d_{m,n}, \text{ and } a_{m,n} \text{ and } b_{m,n})\), the internal electric field at a discrete set of points on the grain surface can be calculated using Eqn. (2.152). Once the electric field is found for both the TE and TM modes, the intensity of each mode is calculated (the complex components of each field are multiplied by their conjugates and and then summed for the mode). The average of the intensities of the two modes is used \(I = (E_{\text{TE}}^2 + E_{\text{TM}}^2)\), since the incident field is assumed to be unpolarized (with only the radiation scattered and emitted by the grain, being polarized).

When the intensity results obtained using Barton’s Method were compared to those obtained using the Point Matching Method, the two were found to be in excellent agreement. This confirmation of the intensity results, based on two completely independent methods, validated the complex code developed to implement each method and added confidence to our subsequent recoil torque evaluations.

### 2.7 Conclusion

With this work, we have investigated the importance of recoil torques due to photoelectric emission and photodesorption, relative to the radiative torques, in grain alignment. We have found that these recoil torques, given our assumptions about photoelectric yield and grain surface conditions, are approximately an order of magnitude smaller than the aligning radiative torques, with the photoelectric torque \(\Gamma_{\text{pe}} \approx 0.35 \Gamma_{\text{rad}}\), and the photodesorption
torque $\Gamma_{\text{pd}} \approx 0.1 \Gamma_{\text{rad}}$. These values are for models that tend to maximize the recoil torques. So, if the values we adopted for physical parameters are realistic, then the actual recoil torques will likely be even smaller than these. At this time, we recommend against inclusion of recoil torques in grain alignment models. The vastly greater effort required to include these recoil torques in an alignment model does not seem justified, given the expected small impact on grain alignment.

However, the photoelectric yield of submicron astronomical silicate grains is not well characterized. If laboratory work done by Abbas et al. [53] showing substantially higher photoelectric yields for submicron grains proves to be accurate, then the photoelectric recoil torque may need to be included in dust grain alignment models. A higher yield would increase the torque. But the higher levels of photoemission would also result in a larger positive charge for the grain, which would have a moderating effect on the increased yield. Yet, the possibility that the photoelectric torque would be of the same order of magnitude as the radiative torque cannot be ruled out. Further laboratory characterization of the yield is needed to definitely ascertain the role of photoelectric torques.

There is also the possibility that less symmetric grains than the spheroids studied here would yield higher recoil torques, although the radiative torque values used are comparable to those found for a highly asymmetric grain model by Draine and Weingartner [17]. It may not be computationally feasible to use either the Point Matching Method or Barton’s method to determine torques for highly asymmetric grain shapes. However, the fact that the near-surface fields found here for spheroids are very smooth, may mean that there is sufficient resolution for the discrete dipole approximation to be used to accurately evaluate recoil torques for highly asymmetric grains.

In modeling the surface environment associated with photodesorption, we assumed a relatively large binding energy ($>1\text{eV}$). With a smaller binding energy, the desorption rate would be higher and the angular impulse per photodesorption would be greater as less of the incident energy is required to overcome the binding energy. Physical characteristics of the grain’s surface may be significantly different than those of the bulk material, and
amorphous silicates are not yet well characterized for photodesorption (or other electronic characteristics, as described in the next chapter). In addition to characterizing the photoelectric yield, further laboratory work is needed to fully understand the grain surface environment and determine with certainty the photodesorption torque.
Chapter 3: The Effect of Time-varying Electric Dipole Moments on Grain Alignment

3.1 Introduction

In searching for efficient grain alignment processes, each new alignment mechanism has been evaluated in terms of its alignment timescale. A successful alignment mechanism must have a shorter timescale than that of any disaligning mechanism. Until recently, thermal gas collision was the only grain disalignment mechanism considered. As discussed in Chapter 1, the gas collisional disalignment timescale $\tau_{\text{coll}}$ is shorter than that associated with Davis-Greenstein alignment (unless the grains contain superparamagnetic inclusions [31]), but appears to be longer than that due to radiative torque alignment mechanisms $\tau_{\text{rad}}[17]$. Thus, radiative torque alignment mechanisms appear to provide the means to align dust grains with the Galactic magnetic field, even in the presence of disalignment torques due to gas atom collisions with the grain.

However, in 2006 Weingartner [68] proposed a new mechanism with the potential to disalign grains with respect to $B$. This new mechanism affects the alignment of the grain’s rotational axis $\omega$ with $B$ via torques produced by the interaction between the grain’s changing electric dipole moment and the Galactic magnetic field lines across which the grain is drifting. The timescale $\tau_{\text{dis}}$ of the new disalignment mechanism will determine whether this mechanism poses a challenge to grain alignment via radiative torques. A brief and simplified description of the problem follows.

The grain of interest in this work is most probably a highly amorphous [46] [35] [36] [48] submicron silicate grain. We assume a spherical grain shape for this work and consider two grain sizes, with radii 0.1$\mu$m and 0.2$\mu$m. The grain is expected to have a high level of impurity based on observations of the ISM that indicate depleted elements in the gas
surrounding the dust grains [62] [3]. The grain can be expected to have a lattice structure that has many randomly positioned irregularities that result in shallow potentials throughout the grain material, because of its highly amorphous and impure state [5]. The silicate is expected to be a dielectric with negligible intrinsic conductivity. As the grain is exposed to charging events associated with electron collision and photoemission (discussed in the previous Chapter), the distribution of these charges may result in an electric dipole moment for the grain, as well as a net charge. The dipole comes about as the charges get trapped in the randomly positioned shallow potentials in the grain structure. They are able to move in the grain to encounter these traps, and to sometimes recombine. The traps have an energy distribution, so that some are deeper than others, and therefore tend to be occupied most often. As these deep traps fill and empty as a result of charging events, the electric dipole moment varies in time. As the grain drifts across the Galactic magnetic field lines, this time-varying dipole interacts with the field to produce torques that change the grain’s orientation to that magnetic field [68]. This is the disaligning scenario that we consider in this work. Each of the elements introduced here are described in detail in what follows.

In the next Section 3.2, the physical basis of the disaligning effects of the changing electric dipole is discussed, and a means is presented for estimating the grain disalignment timescale based on the rate of dipole changes. In Section 3.3, charging processes and rates due to collisonal electron capture and photoemission will be described. The effects of the electric dipole moment on electron capture trajectories is also included in this Section. Following this, in Section 3.4, we describe four simplified models of charge transport and distribution within the grain. We put specific emphasis on describing the physical and charge-related characteristics of the grain that pertain to the electric dipole moment. Section 3.5 describes the simulations run for each model, with simulations of up to $10^5$ years of charging events and for a range of grain rotation rates. The results of these simulations are reported and presented graphically in Section 3.6. The Chapter finishes with Section 3.7 describing the conclusions resulting from this work. Appendix D describes a model used to investigate the movement of charges through the grain volume, providing a basis for some
of the simplifying assumptions that made simulated runtimes of $10^5$ yr computationally possible.

### 3.2 Disalignment due to time-varying electric dipole moments

A grain in the diffuse ISM is expected to be spinning and, in the general case, is expected to be spinning suprathermally as a result of collisional and other torques, as described in Sections 1.2.1 and 1.2.6. If the grain is charged and spinning, it will acquire a magnetic dipole moment $\mathbf{\mu}$ parallel to the rotational velocity $\mathbf{\omega}$. If the spinning grain is comprised of paramagnetic material, whether charged or not, it will tend to become magnetized either parallel or anti-parallel to $\mathbf{\omega}$ per the Barnett effect described in Chapter 1 [11], potentially acquiring a much stronger magnetic moment $\mathbf{\mu}_{\text{Bar}}$ than that due to spinning charge. For a grain of volume $V$ and magnetic susceptibility $\chi_0$, the Barnett magnetic moment $\mathbf{\mu}_{\text{Bar}} = \chi_0 \omega V / \gamma_g$, where $\gamma_g$ is the gyromagnetic ratio (the ratio of the magnetic moment to the angular momentum of the microscopic dipoles).

The grain material is expected to be an amorphous mix of olivine-type silicate (MgFeSiO$_4$) with a high level of impurity, so the distribution and density of the ions, nuclei and defects responsible for paramagnetism, and susceptibility, in the grain is somewhat uncertain. The susceptibility $\chi_0$ adopted ([12] [68]) is given by Curie’s law [54]

$$\chi_0 = \frac{n \gamma_g^2 \hbar^2 J (J + 1)}{3 k_B T_{gr}}$$  \hspace{1cm} \text{(3.1)}

where $n$ is the approximated number density of Fe ions ($\text{Fe}^{3+}; S_{5/2}$) responsible for the magnetization of the grain material (the gram molar weight of olivine is used, here)

$$n_{\text{Fe}} \sim 3 \text{ g cm}^{-3} \frac{1 \text{ mol}}{153.31 \text{ g}} \times 6.0221 \times 10^{23} \text{ mol}^{-1} \sim 1 \times 10^{22}$$  \hspace{1cm} \text{(3.2)}
and \( J = 5/2 \), with the electron gyromagnetic ratio \( \gamma_g = -1.76 \times 10^7 \text{s}^{-1} \text{G}^{-1} \), leading to

\[
\chi_0 \sim 5 \times 10^{-3} \left( \frac{T_{\text{gr}}}{15 \text{K}} \right)^{-1}. \tag{3.3}
\]

Based on this estimate for the magnetic susceptibility, the Barnett magnetic moment can be approximated for a silicate grain:

\[
|\mu_{\text{Bar}}|_{\text{sil}} \approx 1.2 \times 10^{-19} \left( \frac{T_{\text{gr}}}{15 \text{K}} \right)^{-1} \left( \frac{a}{0.1 \mu\text{m}} \right)^3 \left( \frac{\omega}{10^5 \text{s}^{-1}} \right) \text{statC cm}. \tag{3.4}
\]

In the presence of an external magnetic field \( \mathbf{B} \), the grain experiences a torque, \( \mathbf{\Gamma}_\mu = \mu_{\text{Bar}} \times \mathbf{B} \). When \( \mu_{\text{Bar}} \) is parallel or anti-parallel to the angular momentum vector \( \mathbf{J} \), the torque produced causes \( \mathbf{J} \) to precess about \( \mathbf{B} \) with a constant angle \( \theta_{\text{align}} \) (the angle between \( \mathbf{B} \) and \( \mathbf{J} \)). The equation of motion associated with this torque

\[
\frac{d\mathbf{J}}{dt} = \mu_{\text{Bar}} \times \mathbf{B} = \mathbf{J} \times \frac{\chi_0 V}{\gamma_g I} \mathbf{B} \tag{3.5}
\]

takes the form of the Larmor equation, where the rate of precession \( \Omega_0 \), also constant, is

\[
|\Omega_0| = \frac{\chi_0 V B}{\gamma_g I} = \frac{|\mu_{\text{Bar}}| B}{J} \tag{3.6}
\]

and, using the values derived above for \( \mu_{\text{Bar}} \) and \( \omega_T \), the precession rate \( \Omega_0 \) is:

\[
|\Omega_0| \approx 314 \left( \frac{|\mu|}{10^{-19} \text{statC cm}} \right) \left( \frac{\rho}{3 \text{g cm}^{-3}} \right)^{-1} \left( \frac{B}{5 \mu\text{G}} \right) \left( \frac{a}{0.1 \mu\text{m}} \right)^5 \left( \frac{\omega}{10^5 \text{s}^{-1}} \right)^{-1} \text{yr}^{-1}. \tag{3.7}
\]

This precession rate is not dependent on the rotational speed \( \omega \), as both \( \mu \) and \( J \propto \omega \). It
is also clear that $\Omega_0$ is very rapid in comparison to the timescale for collisional disalignment $\tau_{\text{coll}} \approx 10^5\text{yr}$. Because of the short timescale of precession with respect to collisional disalignment, at any given time an ensemble of identical grains would show a uniform distribution of precessional phase. This averaging over precessional phase, given internal grain alignment of $\mathbf{a}_1$ with $\mathbf{J}$, will result in starlight polarization that is either parallel or perpendicular to $\mathbf{B}$.

In addition to a magnetic dipole moment, the grain may also have an electric dipole moment $\mathbf{p}$. In a grain made of dielectric material with limited or no conductivity, individual excess charges may be randomly and non-uniformly distributed in the grain body, leading to an electric dipole moment. As the grain drifts with velocity $\mathbf{v}$ across the Galactic magnetic field lines, in the reference frame in which the grain is stationary there is an electric field

$$\mathbf{E} \approx \frac{\mathbf{v}}{c} \times \mathbf{B} \tag{3.8}$$

and the interaction of $\mathbf{p}$ with $\mathbf{E}$ produces a torque $\Gamma_p$

$$\Gamma_p = \mathbf{p} \times \left( \frac{\mathbf{v}}{c} \times \mathbf{B} \right). \tag{3.9}$$

In the case where the electric dipole lies entirely along the grain angular momentum vector, $\mathbf{p} = p \mathbf{J}$, the grain will no longer precess around $\mathbf{B}$ (the result of the torque due to the magnetic moment of the grain), but will now precess around an axis tilted at an angle $\delta$ relative to $\mathbf{B}$. This can be seen when the two torques are added:

$$\Gamma = \Gamma_\mu + \Gamma_p = (\mu \times \mathbf{B}) + \mathbf{p} \times \left( \frac{\mathbf{v}}{c} \times \mathbf{B} \right). \tag{3.10}$$

When $\mu = \mu \hat{\mathbf{J}}$, $\mathbf{p} = p \hat{\mathbf{J}}$, $\mathbf{B}$ lies along the z-axis $\hat{\mathbf{z}}$, and the grain drift velocity is written as
a sum of its components parallel and perpendicular to \( \mathbf{B} \), \( \mathbf{v} = v_\parallel \hat{z} + v_\perp \hat{y} \)

\[
\mathbf{\Gamma} = \left( \mu \mathbf{J} \times \hat{z} \right) + \left( p \mathbf{J} \times \frac{v_\perp B}{c} \hat{x} \right)
\]

(3.11)

\[
\mathbf{\Gamma} = \mu \mathbf{J} B \times \left( \hat{z} + \frac{p v_\perp}{\mu c} \hat{x} \right).
\]

(3.12)

The angle \( \delta \) between \( \hat{z} \) and the new axis of precession is

\[
\delta = \arctan |\Upsilon|; \quad \Upsilon \equiv \frac{p v_\perp}{\mu c},
\]

(3.13)

and the rate of precession is increased, as shown in the Larmor-type equation of motion for the combined torques

\[
\frac{d\mathbf{J}}{dt} = \mathbf{J} \times \Omega_0 B \left( \hat{z} + \Upsilon \hat{x} \right)
\]

(3.14)

where the new precession rate is

\[
\Omega = \Omega_0 \left( 1 + \Upsilon^2 \right)^{1/2}.
\]

(3.15)

In order to discuss the motion of the grain when \( \mathbf{p} \) and \( \mathbf{\mu} \) do not lie along \( \mathbf{J} \), we adopt the approach taken by Weingartner and Draine \[68\] \[72\]. Using this approach, the torques associated with \( \mathbf{p} \) and \( \mathbf{\mu} \) are averaged over the grain’s rotation, as this motion has a timescale that is orders of magnitude shorter than any other process affecting the grain. For the grain, which is an asymmetric rigid body, three moments of inertia, \( I_1 \geq I_2 \geq I_3 \), correspond to three principal axes \( \hat{a}_1 \), \( \hat{a}_2 \), and \( \hat{a}_3 \). A dimensionless quantity \( q \) is used to express the rotational energy of the body,

\[
q \equiv \frac{2 I_1 E}{J^2}.
\]

(3.16)
Defined thus, \( 1 \leq q \leq I_1/I_3 \). Using the averages over grain rotation for the torques due to the magnetic moment \( (\Gamma_\mu) \) and the electric dipole moment \( (\Gamma_p) \), the torques are redefined

\[
\bar{\Gamma}_\mu = \bar{\mu} \times \mathbf{B} = \left( \frac{\mu}{\bar{\omega}} \right) \frac{q\mathbf{J}}{I_1} \times \mathbf{B}
\]

\[ (3.17) \]

\[
\bar{\Gamma}_p = \bar{p} \times \left( \frac{\mathbf{v} \times \mathbf{B}}{c} \right)
\]

\[ (3.18) \]

where the rotation-averaged angular velocity \( \bar{\omega} \) and electric dipole moment are used [72]

\[
\bar{\omega}(q) = \frac{q\mathbf{J}}{I_1}
\]

\[ (3.19) \]

\[
\bar{p}(q, \pm) = \pm (\mathbf{p} \cdot \hat{a}_i) f_i(q) \hat{J}.
\]

\[ (3.20) \]

The ± refers to the one of two “flip” states the grain can assume. This flip state is with respect to one principal axis \( \hat{a}_i \), where the axis is selected based on the value of \( q \). When \( q < I_1/I_2 \) the axis is \( \hat{a}_1 \); when \( q > I_1/I_2 \) the axis is \( \hat{a}_3 \). A positive flip state is defined as one where the component of angular velocity around the selected axis \( \omega_i \) is always positive as the grain rotates. A negative flip state occurs when \( \omega_i \) remains negative throughout the rotation. The factor \( f_i \) is defined in [68] as

\[
f_i(q) = \left( \frac{|I_1 - I_3q|}{I_1 - I_3} \right)^{1/2} \frac{\pi}{2F(\pi/2, k^2)},
\]

\[ (3.21) \]

The function \( F \) is an elliptic integral of the first kind

\[
F(\pi/2, k^2) \equiv \int_0^{\pi/2} d\theta \left( 1 - k^2 \sin^2 \theta \right)^{-1/2}
\]

\[ (3.22) \]
with

\[ k^2 \equiv \frac{(I_2 - I_3) (q - 1)}{(I_1 - I_2) (1 - I_3q/I_1)} \quad (3.23) \]

when \( q < I_1/I_2 \). The definition for \( k^2 \) in Eqn. (3.23) is inverted for \( q > I_1/I_2 \). Weingartner [68] identified two sources of rapid change for the grain precession axis angle and the rate of rotation through change to \( \Upsilon \): 1) changes to the grain rotational state when the grain flips or \( q \) changes; and 2) changes to the grain electric dipole moment \( \mathbf{p} \). The first source of rapid change was investigated in [68] with the conclusion that grain disalignment can result from changes in \( \Upsilon \) due to flipping, and the timescale for flipping could be much shorter than that due to thermal collisions. Weingartner also took a preliminary look at disalignment time-scale \( \tau_{\text{dis}} \) due to a changing electric dipole, and it is this second source of rapid change, that due to electric dipole variation, that is the subject of this research.

When the grain rotates suprathermally, the grain angular momentum is not significantly changed by torques produced by random thermal gas atom collisions [39] [45] [40] [42] [41] [69] [29]. Also, rapid dissipation of rotational energy due to viscoelastic or Barnett effects (as discussed in Chapter 1) will bring \( \mathbf{J} \) into alignment with \( \hat{\mathbf{a}}_1 \). This case results in \( q = 1, k^2 = 0, F(\pi/2, k^2) = \pi/2, \) and \( f_1(q) = 1 \). Thus, for a suprathermally rotating grain, where \( \mu \) and \( \mathbf{p} \) do not lie along \( \mathbf{J} \), and the Barnett effect is primarily responsible for \( \mu \),

\[ \mu_J = \left( \frac{\mu_{\text{Bar}}}{\omega} \right) \frac{qJ}{I_1} = \left( \frac{\chi_0 V}{\gamma g} \right) \frac{J}{I_1} \quad (3.24) \]

\[ p_J = \pm (\mathbf{p} \cdot \hat{\mathbf{a}}_1) f_i(q). \quad (3.25) \]

Both \( \mu_J \) and \( p_J \) depend on the grain’s rotational state through \( q \) [Eqn. (3.16)]. The sign in Eqn. (3.25) is + (-) when \( \mathbf{J} \cdot \hat{\mathbf{a}}_i > 0 \) (< 0). These expressions for \( \mu_J \) and \( p_J \) are used in the following research, and while justified for the suprathermally rotating grain case, are less rigorous for the thermally rotating grain case.

A grain in the diffuse ISM is subject to changes in the electric dipole moment \( \mathbf{p} \) that
are rapid as compared to the mechanisms of alignment. These changes come as a result of discrete charging events, photoemission and collisional electron charging. Due to the dielectric nature of the grain, the capture and emission of electrons can result in non-uniform distribution of charge in the grain and a subsequent non-zero electric dipole moment. The magnitude and direction of this dipole moment can change with each charging event. The timing between these charging events also varies, as each charging process occurs at its own average rate, but the timing intervals of each process are stochastic distributions about the average interval for that rate. The time interval between any two charging events, then, is drawn from a combination of these two distributions. When the dipole changes, the phase of precession can be at any value between 0 and $2\pi$. The change in $\mathbf{p}$ results in a change in $\Upsilon$, that will shift the precession axis, as well as change the rate of precession. A subsequent change to the dipole will again interrupt the (already-reset) precession at a new and most probably different point in precession phase, again shifting the precession axis and the rate. After some number of these shifts, the grain can become significantly disaligned if the resulting alignment angle $\theta_{\text{align}}$ between the precession axis and $\mathbf{B}$ is large and the time required to accumulate the disalignment is short compared to the timescale for alignment by radiative torques.

Weingartner [68] found formulas for approximating the time-scale $\tau_{\text{dis}}$ for the simple scenario where $\Upsilon$ has a constant magnitude but stochastically reverses sign. When $\tau_{\text{flip}}$ is short compared to the precession time-scale $|\Omega_0|^{-1}$,

$$\tau_{\text{dis}} \sim \Upsilon^{-2} |\Omega_0|^{-2} \tau_{\text{flip}}^{-1}; \quad \text{if} \quad \tau_{\text{flip}} \ll |\Omega_0|^{-1} (1 + \Upsilon^2)^{-1/2}$$

(3.26)

and, when $\tau_{\text{flip}}$ is long compared to $|\Omega_0|^{-1}$

$$\tau_{\text{dis}} \sim (1 + \Upsilon^{-2}) \tau_{\text{flip}}; \quad \text{if} \quad \tau_{\text{flip}} \gg |\Omega_0|^{-1} (1 + \Upsilon^2)^{-1/2}.$$  

(3.27)
3.3 Charging Processes

Two charging processes, photoemission due to exposure to the interstellar radiation field in the far ultraviolet (FUV) range, and the capture of gas-phase electrons (resulting in part from the ionization of carbon in the ISM), are expected to provide a continual source of charging events for dust grains in the CNM. (UV penetration of the diffuse neutral medium is the source for a rate of photoemission from the grain that is far greater than that due to ion collision, so that ion collisional charging is a negligible contributor to grain charge and is ignored here.) The simultaneous operation of the two charging processes results in the establishment of an equilibrium average charge state for the grain, $Z_0$. The actual charge varies stochastically about $Z_0$. For a silicate grain of effective radius $= 0.1 \, \mu m$ in the CNM, the expected potential $U \approx 0.3 \, V$ [71]. This potential will result in an average of approximately 20 positive charges, or “holes”, per grain

$$N_{\text{charges}} = \frac{Ua}{e}. \quad (3.28)$$

3.3.1 Collisional Charging

The collisional charging rate $J_c$, for a grain at rest with respect to the surrounding gas, is dependent upon the CNM gas temperature ($T_{\text{gas}}$), the effective radius ($a$) of the grain, the number density of charged particles ($n$), the mass of the particle ($m$), the sticking coefficient ($s_e$) and the “reduced rate” $\tilde{J}$:

$$J_c = ns\sqrt{\frac{8kT_{\text{gas}}}{\pi m}}\pi a^2 \tilde{J}. \quad (3.29)$$

The sticking coefficient ($s$) is defined as the probability that the particle sticks to the grain and depends on the charge of the grain, the particle attenuation length, and the grain size [71]. For the grain model under consideration, we adopt $s \approx 0.5$. 


The $\tilde{J}$ term modifies the geometrical collisional cross section, to account for other Coulomb effects that either enhance or diminish the rate of collision. The reduced rate was first calculated by Spitzer in 1941 [64] for a charged grain in the ISM, where the charge is given by $Q_{\text{grain}}$:

$$\tilde{J} = \begin{cases} 
1 - \gamma_i & \gamma_i < 0 \\
\exp(-\gamma_i) & \gamma_i > 0 
\end{cases}$$ \hspace{1cm} (3.30)

where

$$\gamma_i = \frac{q_i Q_{\text{grain}}}{ak_B T_{\text{gas}}} = \frac{q_i U}{k_B T_{\text{gas}}}$$ \hspace{1cm} (3.31)

$$E_i = \frac{k_B T_{\text{gas}}}{2}$$ \hspace{1cm} (3.32)

and $q_i$ is the charge of the colliding particle, $U$ is the grain potential. Note that when $\gamma_i < 0$ the grain and colliding particle are of opposite charge and the collisional rate increases, as expected due to Coulomb attraction, and $J_c$ decreases when $\gamma_i > 0$ and the particle is repelled.

Draine and Sutin [16] considered the collisional charging, deriving $\tilde{J}$ for a conducting grain. They included the polarization of the grain due to the colliding charge, in their determination of capture rates, finding that the polarization had a significant effect on these rates for small grains. For large grains, such as those considered here with $a = 0.1\mu m$, the polarization interaction becomes negligible, and so we ignore the image potential in determining $J_c$. We do however, need to consider the effect that the electric dipole $p$ has on the capture rate, specifically on $\tilde{J}$. In addition, the trajectories of incoming charged particles may be bent toward the grain surface at the end of the dipole of opposite charge, or deflected away from the grain surface at the end of the dipole with the same charge, acting in both cases to reduce $p$. The following discussion describes a new calculation of these effects.
To determine the effect that a grain’s $p$ has on charged particle trajectories and capture rates, we adopt a spherical grain shape, as the calculation would be prohibitively difficult for other shapes, and use polar spherical coordinates $(\theta, \phi)$ with the origin at the grain center and with the electric dipole moment along the $z$-axis, $\hat{p} \hat{z}$. The net charge $Q$ is modelled as a point charge at the center of the grain and, similarly, $p$ is treated as a point dipole at the grain center. The trajectory of an incoming particle can be described in terms of its motion under the electric force $\mathbf{F}$ produced by the grain. The electric force experienced by the incoming particle with charge $q$ is a sum of the interactions with the grain charge $Q$ and the grain electric dipole moment $p$:

$$
\mathbf{F} = \frac{Qq}{r^2} \hat{r} + \frac{qp}{r^3} \left( 2 \cos \theta \hat{r} + \sin \theta \hat{\theta} \right). \tag{3.33}
$$

Using the expressions for kinetic $T$ and potential energy $U$, the Lagrangian of the particle is

$$
L = T - U = \frac{1}{2} m \dot{r}^2 + \frac{1}{2} mr^2 \dot{\theta}^2 + \frac{1}{2} m r^2 \sin^2 \theta \dot{\phi}^2 - \frac{Qq}{r} - \frac{qp \cos \theta}{r^2} \tag{3.34}
$$

where $m$ is the mass of the particle, and the equations of motion for the particle approaching the charged grain are:

$$
\frac{\partial L}{\partial r} - \frac{d}{dt} \frac{\partial L}{\partial \dot{r}} = 0 \tag{3.35}
$$

$$
m \ddot{r} = m r \dot{\theta}^2 + m r \sin^2 \theta \dot{\phi}^2 + \frac{Qq}{r^2} + \frac{2qp \cos \theta}{r^3} \tag{3.36}
$$

$$
\frac{\partial L}{\partial \theta} - \frac{d}{dt} \frac{\partial L}{\partial \dot{\theta}} = 0 \tag{3.37}
$$

$$
m r \ddot{\theta} = -2 m \dot{r} \dot{\theta} + m r \sin \theta \cos \theta \dot{\phi}^2 + \frac{qp \sin \theta}{r^3} \tag{3.38}
$$

$$
\frac{\partial L}{\partial \phi} - \frac{d}{dt} \frac{\partial L}{\partial \dot{\phi}} = 0 \tag{3.39}
$$
\[ mr \sin \theta \ddot{\phi} = -2m \dot{r} \sin \theta \dot{\phi} - 2mr \cos \theta \dot{\phi}, \quad (3.40) \]

where the dots denote time differentiation. In order to obtain conserved quantities (over the particle trajectory), Hamilton-Jacobi theory is used. The Hamiltonian in spherical coordinates is:

\[ H = \frac{1}{2m} \left[ p_r^2 + \frac{p_\theta^2}{r^2} + \frac{p_\phi^2}{r^2 \sin^2 \theta} \right] + U \quad (3.41) \]

\[ U(r, \theta, \phi) = U_r + \frac{U_\theta}{r^2} + \frac{U_\phi}{r^2 \sin^2 \theta} \quad (3.42) \]

\[ U_r = \frac{Qq}{r}; U_\theta = qp \cos \theta; U_\phi = 0. \quad (3.43) \]

The generalized momenta, \( p_r, p_\theta, p_\phi \) are obtained from the Lagrangian:

\[ p_r = \frac{\partial L}{\partial \dot{r}} = m \dot{r} \quad (3.44) \]

\[ p_\theta = \frac{\partial L}{\partial \dot{\theta}} = m \dot{r}^2 \dot{\theta} \quad (3.45) \]

\[ p_\phi = \frac{\partial L}{\partial \dot{\phi}} = m \dot{r}^2 \sin^2 \theta \dot{\phi} \quad (3.46) \]

The Hamilton-Jacobi equation, in spherical coordinates is,

\[ E = \frac{1}{2m} \left[ \frac{\partial S}{\partial r} \right]^2 + U_r + \frac{1}{2mr^2} \left[ \frac{\partial S^2}{\partial \theta} + 2mU_\theta \right] + \frac{1}{2mr^2 \sin^2 \theta} \left[ \frac{\partial S^2}{\partial \phi} + 2mU_\phi \right] \quad (3.47) \]

where the partial derivatives of Hamilton’s principal function, \( S \), correspond to the generalized momenta defined above:

\[ \frac{\partial S}{\partial r} = p_r; \quad \frac{\partial S}{\partial \theta} = p_\theta; \quad \frac{\partial S}{\partial \phi} = p_\phi. \quad (3.48) \]
The following conserved quantities result from this approach:

\[ p_\phi \equiv m r^2 \sin^2 \theta \dot{\phi} \]  
(3.49)

\[ \beta \equiv m^2 r^4 \dot{\theta}^2 + 2mqp \cos \theta + \frac{p_\phi^2}{\sin^2 \theta} \]  
(3.50)

\[ E \equiv \frac{m r^2}{2} + \frac{Q q}{r} + \frac{\beta}{2mr^2}. \]  
(3.51)

Figure 3.3.1 shows the parameters used to describe the trajectory of a particle with velocity

\[ \mathbf{v}_\infty = -v (\cos \theta_0 \mathbf{\hat{z}} + \sin \theta_0 \mathbf{\hat{x}}) \]  
(3.52)

far from the grain, where the negative sign indicates that the particle is traveling toward the grain. While the line \( x = \tan \theta_0 z \) passes through the center of the grain, the particle is traveling along a trajectory that is offset from this line by a distance \( b \), the impact parameter. \( r_0 \) is the length of a vector, lying within the x-z plane, that intersects a plane containing \( b \). The position of \( b \) in that plane is described by the angle \( \alpha \), with the x-z plane. Any incoming particle position far from the grain can now be described in this spherical coordinate system centered in the grain, in terms of \( r_0, \theta_0, b, \) and \( \alpha \). When the particle whose trajectory passes through the origin is located at distance \( r_0 \) from the origin, the coordinates of the other particles are

\[ (r, \theta, \phi) \approx \left( r_0, \theta_0 + \frac{b \cos \alpha}{r_0}, \frac{b \sin \alpha}{r_0 \sin \theta_0} \right). \]  
(3.53)

Therefore, the coordinates and the components of the velocity are

\[ \dot{r} \approx -v \]  
(3.54)
Figure 3.1: Parameters describing the trajectories of incoming charged particles.

\[ r \dot{\theta} \approx v \cos \alpha \frac{b}{r_0} \]  
\hspace{1cm} (3.55)

\[ r \sin \theta \dot{\phi} \approx v \sin \alpha \frac{b}{r_0}. \]  
\hspace{1cm} (3.56)

When these approximations are inserted into the equations for conserved quantities (3.50 and 3.51), those equations now become descriptions of the momentum and energy for an incoming charge infinitely far from the grain:

\[ p_\phi = mv b \sin \theta_0 \sin \alpha \]  
\hspace{1cm} (3.57)

\[ \beta = m^2 v^2 b^2 + 2mqp \cos \theta_0 \]  
\hspace{1cm} (3.58)

\[ E = \frac{mv^2}{2} + \frac{Qq}{r_0} + \frac{m^2 v^2 b^2}{2mr_0^2} + \frac{2mqp \cos \theta_0}{2mr_0^2} \]  
\hspace{1cm} (3.59)

\[ E = \frac{mv^2}{2} + \frac{Qq}{r_0}, \quad \text{as } r_0 \to \infty. \]  
\hspace{1cm} (3.60)
In order to understand how the trajectory will change as the charge gets closer to the grain, Eqns. (3.50 and 3.51) are used, respectively, with Eqns. (3.58 and 3.60) above, to obtain the radial and angular velocities:

\[ r^2 = v^2 \left( 1 - \frac{b^2}{r^2} \right) - \frac{2q}{mr} \left( Q + \frac{p \cos \theta_0}{r} \right) \]  

(3.61)

\[ r^2 \dot{\theta}_0^2 = v^2 b^2 \left( 1 - \frac{\sin^2 \theta_0 \sin^2 \alpha}{\sin^2 \theta} \right) + \frac{2qp}{m} (\cos \theta_0 - \cos \theta) \]  

(3.62)

We select the sign for the root for Eqn. (3.61), based on the fact that the charge is traveling toward the grain, so that \( \dot{r} < 0 \). The selection of the initial sign \( S \) for \( \dot{\theta} \) is more complicated. When \( \theta_0 = 0 (\pi) \) then \( S = +1 (-1) \). Otherwise, Eqn. 3.55 yields \( \dot{\theta} = vb \cos \alpha / r^2 \) for \( r \to \infty \). Thus, \( S = +1 (S = -1) \) when \( \cos \alpha > 0 (\cos \alpha < 0) \). When \( \cos \alpha = 0 \), it is necessary to consider the second order term in the expansion for \( \dot{\theta} \): \( \sin \theta \ r \dot{\theta} = v \cos \theta_0 (b/r_0)^2 \). In this case, \( S = \cos \theta_0 / | \cos \theta_0 | \). If \( \cos \theta_0 \) and \( \cos \alpha \) both equal 0, then \( \dot{\theta} \equiv 0 \). Note that \( S \) typically changes sign at points \( \theta \) where \( \dot{\theta} = 0 \).

Depending on the potential due to the grain’s charge and electric dipole, there is a critical value for the impact parameter, \( b_{\text{crit}} \), such that only when \( b \leq b_{\text{crit}} \) the incoming charge will strike the grain surface. This critical impact parameter, \( b_{\text{crit}} \), can be determined for the case where the charge comes to rest exactly at the surface of the grain, \( r = a, \dot{r} = 0 \). When these conditions are met, Eqn. (3.61) takes the form

\[ r^2 = \frac{2qQ}{mv^2} r + \frac{2qp \cos \theta_0}{mv^2} + b^2 \]  

(3.63)

\[ r = \frac{qQ}{mv^2} \pm \sqrt{\frac{q^2Q^2}{m^2v^4} + \frac{2qp \cos \theta_0}{mv^2} + b^2} \]  

(3.64)
\[
\begin{align*}
    r &= a \left[ U \pm \sqrt{U^2 + V \cos \theta_0 + \frac{b^2}{a^2}} \right] \quad (3.65)
\end{align*}
\]

where
\[
    U \equiv \frac{qQ}{mv^2a}, \quad (3.66)
\]
\[
    V \equiv \frac{2qp}{mv^2a^2}. \quad (3.67)
\]

When \( r_+ \), the larger root of Eqn. (3.65), exceeds \( a \) and there is a positive acceleration \( (\ddot{r} > 0) \) at that point \( (r = r_+) \), the particle will not impact the grain. When the sign of the grain charge matches that of the incoming particle, then \( U > 1 \), and the particle will only strike the grain if the square root in the above equation is negative and sufficiently large that \( r \leq a \).

If \( U \geq 1 \):
\[
    \sqrt{U^2 + V \cos \theta_0 + \frac{b^2}{a^2}} < 0; \quad (3.68)
\]
\[
    \frac{b_{\text{crit}}}{a} \leq \sqrt{-U^2 - V \cos \theta_0} \quad (3.69)
\]

If \( U \leq 1 \):
\[
    \sqrt{U^2 + V \cos \theta_0 + \frac{b^2}{a^2}} \leq 1 - U. \quad (3.70)
\]

When either of Eqns. (3.69 or 3.70) result in an imaginary value, \( b_{\text{crit}} = 0 \).

Above, the assumption was made that \( \ddot{r} > 0 \) for the larger root of Eqn.(3.65), \( r_+ \), when \( b = b_{\text{crit}} \). In order to show this, \( \ddot{r} \) is obtained by differentiating Eqn. (3.51):
\[
    \frac{d}{dt} E = \frac{d}{dt} \left( \frac{m\dot{r}^2}{2} + \frac{Qq}{r} + \frac{\beta}{2mr^2} \right) \quad (3.71)
\]
\[ 0 = \ddot{r} \left( \dot{r} - \frac{qQ}{mr^2} - \frac{\beta}{m^2 r^3} \right). \tag{3.72} \]

When \( \dot{r} \) is non-zero,

\[ \ddot{r} = \frac{qQ}{mr^2} + \frac{\beta}{m^2 r^3}. \tag{3.73} \]

Using the term for \( r \) derived in Eqn. (3.65), the radial acceleration \( \ddot{r} \) can be expressed in terms of \( U \) and \( V \):

\[ \ddot{r} = \frac{a^2 v^2}{r^3} \left[ U^2 + V \cos \theta_0 + \frac{b^2}{a^2} + U \sqrt{U^2 + V \cos \theta_0 + \frac{b^2}{a^2}} \right]. \tag{3.74} \]

We use the impact parameter \( b \), determined above in Eqns. (3.69 and 3.70), to find the mean collision cross section (averaged over the angle \( \theta_0 \)) for a grain at rest with respect to the surrounding gas.

\[ \bar{\sigma} = \int_{1}^{b^2} d \cos \theta_0. \tag{3.75} \]

Next, we use \( |V| \) to rule out cases where \( b_{\text{crit}} < 0 \), and consider first the case where \( U \leq 1 \):

\[ \bar{\sigma} = -\frac{1}{|V|} \int_{1}^{x} dx; \quad x = (1 - 2U - |V| \cos \theta_0); \quad \frac{dx}{d \cos \theta_0} = -|V| \tag{3.76} \]

\[ \bar{\sigma} = \frac{1}{2|V|} \left[ -(1 - 2U - |V|)^2 + (1 - 2U + |V|)^2 \right]. \tag{3.77} \]

At \( 1 - 2U = |V| \):

\[ \bar{\sigma} = \frac{1}{2(1 - 2U)} \left[ 0 + (2(1 - 2U))^2 \right] = \pi a^2 (1 - 2U) \tag{3.78} \]
and, at $1 - 2U = -|V|$:  

$$\bar{\sigma} = \frac{1}{2(1 - 2U)} \left[ 0 + (2(1 - 2U))^2 \right] = \pi a^2 (1 - 2U). \quad (3.79)$$

When $(1 - 2U) < |V| < -(1 - 2U)$ (in all cases other than the two listed above):  

$$\bar{\sigma} = \frac{1}{2|V|} \left[ (1 - 2U + |V|)^2 \right]. \quad (3.80)$$

In the case where $U \geq 1$:  

$$\bar{\sigma} = -\frac{1}{|V|} \int_1^{-1} x \, dx; \quad x = -(U^2 - |V| \cos \theta_0); \quad \frac{dx}{d \cos \theta_0} = -|V| \quad (3.81)$$

$$\bar{\sigma} = \frac{|V|}{2} \left[ - \left( -\frac{U^2}{|V|} - 1 \right)^2 + \left( -\frac{U^2}{|V|} + 1 \right)^2 \right] \quad (3.82)$$

At $|V|^{-1}U^2 = 1$:  

$$\bar{\sigma} = \frac{|V|}{2} \left[ -(-2)^2 + 0 \right] = 0, \quad (-\bar{\sigma} \text{ is eliminated}) \quad (3.83)$$

and, when $|V|^{-1}U^2 > 1$, the root in Eqn. (3.70) is imaginary, therefore $b = 0$ and $\bar{\sigma} = 0$. The remaining solution for this case is when $|V|^{-1}U^2 < 1$,  

$$\bar{\sigma} = \frac{|V|}{2} \left[ \left( -\frac{U^2}{|V|} + 1 \right)^2 \right] \quad (3.84)$$

Now that the collisional cross section has been determined for each of the cases in question, we integrate over the Maxwell speed distribution to obtain $\tilde{J}$ from Eqn. (3.29). For a grain
not drifting relative to the gas,

\[ \tilde{J}(\gamma, |\eta|) = 1 - \gamma, \quad qQ < 0 \text{ and } |\eta| \leq -\gamma \]  \hspace{1cm} (3.85)

\[ \tilde{J}(\gamma, |\eta|) = \frac{1}{4|\eta|} \left( (|\eta| - \gamma)(2 + |\eta| - \gamma) + 2 \left( 1 - e^{-((\gamma + |\eta|))} \right) \right), \quad qQ < 0 \text{ and } |\eta| \geq -\gamma \]  \hspace{1cm} (3.86)

\[ \tilde{J}(\gamma, |\eta|) = e^{-\gamma} \frac{\sinh |\eta|}{|\eta|}, \quad qQ > 0 \text{ and } |\eta| \leq \gamma/2 \]  \hspace{1cm} (3.87)

\[ \tilde{J}(\gamma, |\eta|) = -\frac{1}{2|\eta|} e^{-((\gamma + |\eta|))} \]  

\[ + \frac{|\eta|^2 + (2 - \gamma)|\eta| + (2 - \gamma + \gamma^2/4)}{4|\eta|} e^{-\gamma/2} \]  

\[ + \frac{|\eta|}{4} \int_{\gamma^2/(4|\eta|)}^{\gamma^2/2} ds \left( 1 - \frac{\gamma^2}{4|\eta|^2 s} \right)^2 e^{-s}, \quad qQ > 0 \text{ and } |\eta| \geq \gamma/2 \]  \hspace{1cm} (3.88)

where

\[ \gamma = \frac{qQ}{ak_BT} \text{ and,} \]  \hspace{1cm} (3.89)

\[ \eta = \frac{2qp}{a^2 k_BT}. \]  \hspace{1cm} (3.90)

In Figure 3.2, calculated values of \( \tilde{J} \) vs. \( \gamma \) are shown for various values of \( |\eta| \). Note that when \( \eta = 0 \), Eqns. (3.85 and 3.87) reduce to the classic Spitzer [64] equations for \( \tilde{J} \) for a charged sphere.

In order to determine the arrival angle \( \theta \) of the incoming particle’s position on the grain surface, Eqns. (3.61 and 3.62) are used in the relation

\[ \frac{d\theta}{dr} = \frac{\dot{\theta}}{r} \]  \hspace{1cm} (3.91)
Figure 3.2: $\tilde{J}$ (here labeled $\tilde{R}$) vs. $\gamma$ for various values of $|\eta|$, as indicated to set up the equivalent integrals:

$$\int_{\theta_0}^{\theta} \frac{d\theta}{\tilde{\theta}} = \int_{a}^{\infty} \frac{dr}{\tilde{r}} \tag{3.92}$$

The left-hand integral:

$$\int_{\theta_0}^{\theta} \frac{d\theta}{\frac{1}{r^2} \sqrt{v^2 b^2 \left(1 - \frac{\sin^2 \theta_0 \sin^2 \alpha}{\sin^2 \theta} \right) + \frac{2 m}{m} (\cos \theta_0 - \cos \theta)}} \tag{3.93}$$

can be rewritten, with $V$, as:

$$\int_{\theta_0}^{\theta} \frac{d\theta}{\frac{1}{r^2} \sqrt{\sin^2 \theta - \sin \theta_0^2 \sin^2 \alpha + \frac{V a^2}{m} \sin \theta^2 (\cos \theta_0 - \cos \theta)}} \tag{3.94}$$
The right-hand integral:

\[
\int_a^\infty \frac{dr}{\sqrt{v^2 \left( 1 - \frac{b^2}{r^2} \right) - \frac{2q}{mr} \left( Q + \frac{p \cos \theta_0}{r} \right)}}
\]  

(3.95)

is also rewritten, with \( U \) and \( V \), as:

\[
\int_a^\infty \frac{dr}{\frac{vh}{r} \sqrt{\frac{r^2}{b^2} - 1 - \frac{2UQ}{r} - \frac{V \cos \theta_0}{b^2}}}
\]  

(3.96)

Substituting \( u' \) for \( r/b \), the right-hand integral becomes:

\[
\int_{a/b}^{\infty} \frac{du'b}{\sqrt{u'^2 - 1 - \frac{2Uu'}{b} - \frac{V \cos \theta_0}{b^2}}}
\]  

(3.97)

and, finally, with

\[
A \equiv 1 + VC^2 \cos \theta_0 
\]  

(3.98)

\[
B \equiv 2UC 
\]  

(3.99)

\[
C \equiv \frac{a}{b} 
\]  

(3.100)

and by cancelling the \( v, b \) and \( r \) terms across the two integrals, the right-hand integral becomes

\[
\int_{a/b}^{\infty} \frac{du'}{u'\sqrt{u'^2 - Bu' - A}}
\]  

(3.101)

Integrating the right-hand integral leads to two solutions: first, for \( A \geq 0 \):

\[
RHS = \frac{1}{\sqrt{A}} \arcsin \left( -\frac{Bu' - 2A}{|u'|\sqrt{4A + B^2}} \right)
\]  

(3.102)
which, when evaluated at the limits $C$ and $\infty$, gives

$$\text{RHS} = \frac{1}{\sqrt{A}} \left[ - \arcsin \frac{-B}{\sqrt{4A + B^2}} + \arcsin \frac{BC + 2A}{C \sqrt{4A + B^2}} \right].$$  \hfill (3.103)

Next, for $A \leq 0$:

$$\text{RHS} = -\frac{1}{\sqrt{-A}} \ln \frac{2\sqrt{-A(-A - Bu' + u'^2) - Bu' - 2A}}{u'}$$ \hfill (3.104)

which, when evaluated, gives

$$\text{RHS} = -\frac{1}{\sqrt{-A}} \left[ \ln 2\sqrt{-A - B} + \ln \frac{2\sqrt{-A}\sqrt{A-BC+C^2-BC-2A}}{C} \right].$$ \hfill (3.105)

or

$$\text{RHS} = -\frac{1}{\sqrt{-A}} \ln \frac{2\sqrt{-A\sqrt{-A - BC + C^2 - BC - 2A}}}{C(2\sqrt{-A} - B)}.$$ \hfill (3.106)

If $2q\eta/(mv^2b^2)$, $2qQ/(mv^2b)$, $a/b$, and $\alpha$ are known, then Eqn. (3.92) can be solved for $\theta$, the charged particle arrival angle. An alternative, though less efficient, method is to numerically integrate Eqns. (3.36, 3.38), the equations of motion for the incoming particle trajectory. We have implemented both the analytical and numerical methods of solution and, for many combinations of input parameters, have found the results to be in perfect agreement.

Next, we compute a distribution of arrival angles $\theta$ for given values of $\gamma$ and $\eta$. To do this, we look at a large number of possible trajectories defined by initial parameters $\theta_0$, $u \equiv v/v_{\text{th}}$, $b/a$, and $\alpha$, where the thermal velocity of the particle gas is

$$v_{\text{th}} \equiv \left( \frac{2k_B T_{\text{gas}}}{m} \right)^{1/2}.$$ \hfill (3.107)
To create sets of initial parameters, first we select a set of $N_\theta$ equally spaced values for $\theta_0$, between 0 and $\pi$. For each $\theta_0$ in the set, we select a set of $N_v$ values of $u$, beginning with the median value of the assumed Maxwellian speed distribution, $u = 1.08765$. $(N_v - 1)/2$ are selected for $u$ above the median, and the same number are selected for $u$ below the median. Each of the two groups of values is selected so that $u$ is space in equal-probability intervals, so that

$$
\frac{4}{\sqrt{\pi}} \int_{u_1}^{u_{1+i}} du u^2 e^{-u^2} = \frac{1}{N_v + 1}.
$$

(3.108)

Then for each pair of $(\theta_0, u)$, if $b_{\text{crit}} > 0$, $N_b$ values of $b/a$ between 0 and $b_{\text{crit}}/a$ are chosen, evenly spaced in $b^2$. Lastly, given $(\theta_0, u, b/a)$, we choose $N_\alpha$ values of $\alpha$, evenly spaced between 0 and $2\pi$. For each trajectory defined by a set of initial conditions, we calculate an arrival angle $\theta$, and bin the values. Each value is weighted in proportion to $b_{\text{crit}}^2$.

In Figure 3.3, $g(\cos \theta)$, the fraction of incoming particles that strike the grain with cosine of the polar angle $\leq \cos \theta$, is shown for a single value of $\gamma = 0$ and several values of $\eta$. The arrival angle $\theta$ is the polar angle relative to the dipole moment. In constructing this figure, we adopted 40 bins in $\theta$ and set $N_\theta = N_v = N_b = N_\alpha = 31$. For $|\gamma| < 1$, the values for $g \cos \theta$ look very similar to those in Figure 3.3. Distributions for $(\gamma, -\eta)$ are the same as those for $(\gamma, \eta)$, except that instead of being referenced to $\cos \theta = 1$, they are referenced to $\cos \theta = -1$, so that, $g(\gamma, -\eta, \cos \theta) = g(\gamma, \eta, -\cos \theta)$, and $g \cos \theta$ is now the fraction of particles striking the grain with cosine of the polar angle $\geq \cos \theta$. When the grain has a large positive charge, $|\gamma|$ is large, the distribution of $\cos \theta$ (arrival angles) is uniform, as seen in Figure 3.4.

An electron striking the grain will be able to penetrate to a depth determined by the electron escape length $l_e \sim 10 \text{ Å}$ [71]. In our approach we neglect this effect since $l_e \ll a$, and place arriving electrons on the grain surface, $r = a$. 
Figure 3.3: $g(\cos \theta)$ vs. $\cos \theta$ for $\gamma = 0$ and various values of $\eta$, as indicated

Figure 3.4: $g(\cos \theta)$ vs. $\cos \theta$ for $\eta = 10^2$ and various values of $\gamma$, as indicated
3.3.2 Photoemission

We approximate the photoelectric emission rate $J_{pe}$, by adopting a simplified version of the photoelectric yield model of Weingartner and Draine in [71]. The photoelectric yield $Y$ is the probability that an absorbed photon will result in an electron being emitted. [71] describe $Y$ as the product of three factors $y_0$, $y_1$ and $y_2$. The first factor listed, $y_0$, is the photoelectric yield of the bulk material. The factor $y_1$ is a size-dependent yield enhancement factor. The grains modeled in this research are relatively large, so that $y_1 = 1$. Factor $y_2$ takes into account that electrons attempting to escape the grain may be drawn back by Coulomb attraction if $Z \geq 0$, where the grain charge $Q = Ze$ and $e$ is the proton charge. The $y_2$ factor is the fraction of electrons that escape the grain completely (to infinity),

$$y_2(\nu, Z, a) = \begin{cases} \frac{E_{\text{high}}^2}{E_{\text{high}} - 3E_{\text{low}}} / (E_{\text{high}} - E_{\text{low}})^3 & Z \geq 0 \\ 1 & Z < 0 \end{cases} \quad (3.109)$$

where $E_{\text{low}} = -(Z + 1)e^2/a$ and $E_{\text{high}} = \nu - \nu_{pet}$ ($\nu_{pet}$ is the photoelectric threshold energy). To simplify the process, we adopt a constant threshold energy $\nu_{pet} \approx 8eV$ [71] and an average ISRF energy of $\nu \approx 11eV$, so that $E_{\text{high}} = 3eV$, and is independent of $Z$ and $\nu_{pet}$.

The photoemission rate $J_{pe}$ is found by integrating the yield $Y$ times the photon absorption rate over the ISRF energies above $\nu_{pet}$. We have already approximated $y_2$ as independent of $\nu$, therefore, $J_{pe} \propto y_2$, and we need only choose a proportionality constant so that the average grain potential $\approx 0.3V$ [71].

When a photon of sufficient energy to free an electron from the valence band is absorbed, the freed electron leaves a charge hole. In a dielectric grain, if the electron is unable to escape the grain, an electron-hole pair is created, with the two charges separated in position within the grain. This might occur if the photon is not absorbed until it is too deep within the grain for the freed electron to reach the surface. Or, the freed electron could take a path directed
away from the grain surface and deeper into the grain. In either case, the separation of the two charges is small, as the electron escape length is short ($l_e \ll a$) [4]. Alternatively, the escaping electron could breach the surface of the grain and be drawn back to the surface because of a Coulombic attraction to the grain if $Z \geq 0$ (resulting in $y_2 < 1$). This could result in a more significant change to $p$, but these events are rare; $y_2 \approx 0.98$ for a grain potential of 0.3V.

3.4 Charge Transport Models

3.4.1 Introduction

In the following subsections, first the expected material characteristics of a polarizing grain are described, based on observed extinction and emission spectra. Following this is a more detailed description of the electronic nature expected of the grain, and finally, the charge transport models used in the simulation runs are specifically outlined.

3.4.2 General description of the interstellar grain

The dust grains being modeled are those presumed responsible for the observed polarized starlight that is associated with the broadened absorption features at 9.7 and 18.0 $\mu$m. The 9.7 and 18 $\mu$m absorption features have been identified with silicate Si-O stretching and O-Si-O bending energies, respectively, and the broadening of the absorption lines is indicative of non-crystalline material. Most of the interstellar silicates are thought to be non-crystalline [46] [35] [36] [48]. Absorption features observed towards the Galactic center are best fit by a mix of amorphous olivine ($\text{Mg}_{2x}\text{Fe}_{2(1-x)}\text{SiO}_4$) and pyroxene ($\text{Mg}_x\text{Fe}_{1-x}\text{SiO}_3$) silicates, with no more than 3-5% (by mass) being crystalline. Kemper, Vriend and Tielens [35] [36] also show that a best fit of the data results when more than 80% of the grains are olivine and the rest are pyroxene. As yet, no samples of interstellar dust are available for examination in the laboratory, but such samples would provide a means to evaluate grain material models.

The grains of the diffuse ISM are also expected to contain a high level of impurities,
based on the levels of elements expected in the gas of the ISM and those actually observed. When these levels are below what is expected, an element is said to be “depleted” from the gas. Solar levels of elements are used as the expected standard, where the abundance of an element is measured as its number density relative to the number density of H. Hubble Space Telescope observations of the cold diffuse clouds along the line of sight to ζ Ophi and ξ Per [62] provide elemental depletion values relative to solar abundances in the CNM. Taking these depletion levels to indicate that the missing elements have been incorporated into dust grains provides, in turn, a first approximation of the upper levels of impurity for dust grains. Using the observed depletion of Fe as the limiting element abundance, substitution of Ca for Fe at the observed depleted level would result in an impurity fraction upper limit of approximately 6%. Similarly, substitution of Ni and K would result, respectively, in approximate impurity fraction upper limits of 5% and 0.4%.

In addition to impurities resulting from atomic substitution, structural defects in the grain material would be expected (e.g. due to cosmic ray hits and X-ray absorption).

The surface of a dust grain is of particular interest for the problem considered here, as the charging processes that the grain experiences principally occur within ≈ a few ×10 Å of the surface. The nature of this surface is not well understood at this point, but some reasonable models indicate characteristics that might be expected. A dust grain in the diffuse ISM provides a surface for chemical interaction and molecular production. The surface of a dust grain in the diffuse ISM is expected to accrete hydrogen atoms, which then will be photodesorbed as discussed in Chapter 2, or diffuse and chemically react with other hydrogen atoms on the surface to form H₂. Once formed, the H₂ molecules are expected to cover a small portion of the grain surface area, ∼ 2% [67] based on the balanced rates of H accretion and evaporation. A dust grain in the diffuse ISM is also not likely to be covered by a mantle of ice, as might be expected for a grain in a dense molecular cloud, so that the grain surface would most probably be a bare silicate or graphitic material, similar in composition to the grain bulk.

The large dust grains of the diffuse ISM reach an equilibrium temperature $T_{gr}$ ≈ 15 K,
surrounded by cold neutral hydrogen gas (CNM) at an equilibrium temperature $T_{\text{gas}} \approx 100\, \text{K}$. The number density of the CNM $n_H \approx 30\, \text{atoms/cm}^3$ and, with a number density for dust grains of $0.1\, \mu\text{m}$ approximated at $10^{-13}/\text{H atom}$ [67], dust-dust interaction is of very low probability and is not considered in the simulations.

3.4.3 Charge transport properties of the grain

If the grain material is some combination of olivine-type silicates, this material can be expected to have the energy band structure of an insulator, with the valence band initially filled with electrons and the conduction band initially empty. Both the conduction and valence bands would have band tails, with an energy state density (density of states) distribution function that falls off as the energy approaches the band gap. In such an insulator, the Fermi level $E_{F0}$ is located at the end of the conduction band tail, with positive energy levels above and negative energy levels below. Like the conduction or valence bands, an impurity band can develop when the potentials produced by the impurities are strong. A significant impurity level, as described above, might be expected in a dust grain, leading to an impurity band in the overall energy band structure of the grain. In a large band gap insulator, the impurity band may be located in the band gap, and similarly to the conduction and valence band modeling, would have an energy state number density (density of states) distribution with band tails.

The amorphous nature of the grain material has consequences for the conductivity of the grain, even though the grain material may be a large band gap insulator. For a perfect solid crystalline material, the electron in the lattice structure of the material can be described as a plane wave in a periodic potential function, the Bloch wave function,

$$
\Psi_k(r) = u_k(r)e^{i\mathbf{k}\cdot\mathbf{r}} \quad (3.110)
$$

where $u_k$ is the periodic potential function representing the potential wells of lattice positions in the material and $\mathbf{k}$ is an allowed vector in reciprocal space. In a perfectly crystalline
material all energy states would be of a high enough density of states that the electron wave functions would extend throughout the material (extended states). In an amorphous material such as the silicate olivine discussed above, the potential wells that represent the lattice sites have energies that vary a small amount due to a random orientation of of “p-like” and “d-like” electron orbitals in the material [5]. (Amorphous silicate material has a short-range order and long-range disorder. The short-range order means that the SiO$_4$ tetrahedra of the silicate lattice are intact, while long-range amorphous disorder refers to the rotation of the tetrahedra with respect to one another [8].) This randomization results in a lower density of states for the energy states associated with the disordered orientation. This low density of states, in turn, results in a localization of the electron wave function, so that the wave function does not extend throughout the material. The eigenfunctions of the electron wave function decay exponentially outside the sites of localization so that there is almost no contribution to dc conductivity. When an electron wave function is localized, electron mobility is limited to thermally activated “hopping” between localized lattice sites [56]. The probability that an electron will make such a hop is [5]

$$p \approx \nu_{ph} e^{-\alpha r - \Delta E/k_B T_{gr}}$$

(3.111)

where $\nu_{ph}$ is the phonon frequency of the material, $1/\alpha$ is the extension of the electronic wave function, $\Delta E$ is the difference in potential energy between a possible hopping site and the current position of an electron, $r$ is the distance between the sites, and $T_{gr}$ is the temperature of the material. When a wave function is localized, conduction is completely blocked at a temperature of 0K and is thermally activated above that temperature. In a large band gap insulating material, such as the amorphous olivine silicate being discussed here, there is no intrinsic conduction of electrons. (The density of intrinsic free charge carriers in this type of material is very low, $\approx$ a few $\times 10^3$ cm$^{-3}$ [5], and is not treated as a contributor to the time-varying distribution of charge.) If impurities within the material do not provide donor or acceptor sources that contribute to conduction, then the only means
of electronic mobility in this material, at the low temperature (15 K) expected for a grain in the CNM (once a charge is introduced) would be that of thermally activated hopping.

In an amorphous dielectric material such as olivine, the energy states associated with localization are located in the tails of the valence and conduction bands. In addition, in impurity energy bands, where impurity randomization broadens the bands creating band tails, electrons can also be localized. If impurity atoms are located at random positions and provide a significant fraction of the material (≈ 6%), the impurity band may be entirely localized. Thermally activated hopping can occur between localization sites in the impurity band, as well as in the localized band tails of the conduction and valence bands. Both electrons and holes hop between localizations, and in addition to occupying the localizations, can recombine, neutralizing both charges. A charge occupying a localization with a large potential energy well is less likely to hop to another localization, therefore these “deep traps” are more likely to be occupied.

3.4.4 Four grain models

The above description of the material, electronic and environmental characteristics of a polarizing grain provided the basis for developing a most-likely grain model. This model would have the electronic characteristics of an amorphous olivine grain of ∼ 0.1 µm in effective radius. The model would mimic a large band gap insulator with impurities of a single unidentified type randomly distributed throughout the material. Impurities would be distributed through the grain material at what is expected to be an upper limit of 6%. The assumption of short-range order and long-range disorder in the grain silicate, similar to that found in terrestrial amorphous silicates, led to a further assumption of the possibility for a single localization per unit of material. This in turn and together with the impurity number density, provided an overall density of localizations where charges could be captured, or “deep traps”.

In addition to the above defining characteristics, several simplifying assumptions were made to facilitate the modeling. First, the grain was assumed to be spherical and uniform
in composition. An actual grain must be asymmetric, more closely approximated by an ellipsoid than a sphere, to produce the polarized starlight observed. However, we chose a spherical shape for the grain models because calculating electron trajectories approaching a sphere is far less difficult than calculating those trajectories for non-spherical shapes.

The second assumption is that there are relatively few deep traps as a percentage of total localization positions for charges. We assume that the band tails of the grain energy band structure are fully localized, and that the band tails have a declining density of energy states towards the band gap. An extra electron (the valence band including the band tail is full) will hop to the lowest energy state it can access, so that the end of the localized conduction band tail will be populated with deep traps (the electron can get to no lower energy state).

In the same way, a hole created by photoelectric emission from the valence band will hop to the highest energy state available, so that the end of the localized valence band tail will also be a set of deep traps. Further, temperature-activated hopping will quickly result in the occupation of these deep traps by arriving charges. Models were developed that tracked the hopping of each charge through the grain lattice, and these models showed that the charge quickly (on a timescale many orders of magnitude less than the timescale associated with either charging process) came to rest at the localizations with the deepest potential energy wells, deep traps. (Refer to Appendix D for further details regarding the grain models with hopping.) Based on these findings, and because the computational requirements for tracking all the movements of the free charges in the grain was prohibitive (run time \(\sim\) simulated time), the probability of hopping was replaced with either immediate movement of a charge to the nearest deep trap, or a random walk to the nearest deep trap, for those models with deep traps.

The third assumption is that the grain surface is presumed free of \(\text{H}_2\) molecules and does not include \(\text{H}\) accretion, migration and evaporation at surface sites. Because of the low level of expected \(\text{H}_2\) surface coverage (\(\sim 2\%\)), this was not considered a factor of significance as the percentage of surface sites occupied by deep traps was \(\leq 1\%\), and a uniformly distributed reduction of deep traps on the order of 2\% would not be statistically significant.
The assumptions above and the need to establish the upper and lower limits of the effects of grain conductivity on the evolution of the electric dipole, led to the development of four grain models.

Model 1: A perfect insulator: This model set the limit of zero conductivity, with no charge movement once a charge arrives at a surface point. (An arriving charge is here understood to mean either an electron captured from the gas, or a hole created by photoemission.) There is no hopping possible in this model, no movement of the charge possible once it arrives at the initial point. In this model, all the surface positions on the grain are effectively available to an arriving charge. If an arriving charge lands in a position occupied by an opposite charge, those charges will recombine.

Model 2: A perfect conductor: This model set the limit of complete conductivity. With this model, there is no localization of free charge as all these charges exist in extended states that include the entire grain. All free charge is spread evenly over the grain surface, therefore, given a spherical grain of uniform material, no electric dipole can exist for this model. For a non-spherical grain, the electric dipole moment \( p \propto Z \) (recall that: \( Z \) is the net number of proton charges in the grain). Given the highly amorphous nature of the grain material together with the high level of impurities expected, many more “deep traps” should exist in the material than the grain charge expected (\( \sim 20 \) for a \( 0.1 \mu \text{m} \) grain in the diffuse ISM). Therefore, this model is probably not physically representative of the actual grains, but provides an upper limit to grain conductivity.

Model 3: A conducting grain with deep traps: In this model, once a charge arrives at a position on the surface, it immediately moves to the nearest deep trap. If the trap is occupied by an opposite charge the two charges recombine. If the trap is unoccupied, the arriving charge remains in this position unless an opposite charge arrives at the same location and recombines. This model effectively greatly reduces the lattice positions available to the arriving charge.

Model 4: A partially conducting grain with deep traps: For this model, an arriving charge engages in a random walk until encountering a deep trap and then the behavior is
exactly as described in Model 3 above.

The simulations of grain charging and subsequent variation of the grain dipole using these four models is described in the following section.

### 3.5 Monte Carlo Simulations

#### 3.5.1 Introduction

The simulations expose each model to the charging processes for an extended period of time, and track the grain electric dipole moment \( \mathbf{p} \), and the grain angular momentum vector \( \mathbf{J} \) for each timestep. The angular momentum vector is assumed to be aligned with the principal axis of greatest moment of inertia, which would be the case for suprathermal rotation. A constant timestep \( dt \) is used, typically 31.56 s, which was selected to be shorter than the average time between charging events. The random number generator RAN2 of Press et al.[57] is used throughout these simulations, to determine whether a charging event occurs during a specific time step, and in positioning the charges and traps in the grain. (Coordinates for traps are randomly selected, and positioning of charges is randomly selected from either, a uniform distribution in the case of photoemission, or from the distributions described in Section 3.3.1 in the case of collisional charging.)

Environmental and grain characteristics are set for the simulations. The grain radius is set for two cases, 0.1\( \mu \)m and 0.2\( \mu \)m. For each of these radii, respectively, the photon absorption rates (for an approximate average grain potential of \( \approx 0.3V \) [71] are \( J_\gamma = 2.9 \times 10^{-2}s^{-1} \) and \( J_\gamma = 5.7 \times 10^{-2}s^{-1} \). The grain temperature is \( T_{gr} = 15K \) and the surrounding gas temperature is \( T_{gas} = 100K \). The electron number density \( n_e = 4.5 \times 10^{-2}cm^{-3} \), and the sticking coefficient \( s_e = 0.5 \). Given the above \( T_{gr} \) and \( n_e \), we adopt a magnetic susceptibility for the grain \( \chi_0 = 5 \times 10^{-3} \). The bulk photoelectric yield is approximated by \( y_0 = 6 \times 10^{-2} \), for incident photon energy \( h\nu = 10eV \) [71].

The role of the grain drift velocity across \( \mathbf{B}, v_\perp \), is crucial to determining the relative importance of \( \Upsilon \) in changing the rotational characteristics of the grain, since a small value
for $v_\perp$ could render changes to $\Upsilon$ due to a time-varying $p$, insignificant. In 2004, Yan, Lazarian and Draine [73] showed that grains in the diffuse ISM could be accelerated to supersonic velocities by interstellar magnetohydrodynamic turbulence, reaching persistent velocities up to $\sim 1\text{km s}^{-1}$ perpendicular to $B$, for grains with radii $>0.05\mu m$. We adopt the value for $v_\perp = 1\text{km s}^{-1}$ as given by [73].

With the simulation constants set, we can describe the simulation algorithm for Model 2, the perfect insulator. At the beginning of the timestep we calculate the reduced rate $\tilde{R}$ [Eqn. (3.29)]. This is done through bilinear interpolation [57] of precalculated tables of values for $\tilde{J}$, in $\ln \eta$ and $\ln \gamma$ [recall that: $\eta$ is the term associated with $p$, Eqn. (3.90); and $\gamma$ is associated with the grain charge $Z$, Eqn. (3.89)]. There are 21 values of $\eta$, from $10^{-2}$ to $10^2$, and 23 values of $\gamma$, from $-3 \times 10^2$ to $3 \times 10^2$, including 0. If $\eta < 10^{-2}$ then the value for $\tilde{J}$ is the same as that for a classic charged sphere with no dipole [64], with no interpolation required. If $|\gamma| < 10^{-2}$ (essentially no charge on the grain) then a linear interpolation in $\ln \eta$ is performed to find $\tilde{J}$, with $\ln \gamma = 0$.

At each timestep, we use $\tilde{J}$ to get the probability of an electron capture $J_c dt$ and the probability of photoemission. If there is essentially no $p$ ($\eta < 10^{-2}$), the incoming electron is assigned a random position ($\theta, \phi$) on the grain surface, where $\theta$ and $\phi$ are the polar and azimuthal angles with respect to the grain axis of rotation $\hat{\omega} = \hat{z} = \hat{a}_1$, so that $\hat{\omega}$ and $z$ and the grain’s principal axis of greatest moment of inertia $\hat{a}_1$ are all aligned. If $\eta \geq 10^{-2}$ then we interpolate as described above to find the distribution function $g(\theta')$, where $\theta'$ is the polar angle of the electron trajectory relative to the dipole moment $p$. We randomly select $\theta'$ from the distribution $g(\theta')$, and randomly select $\phi$ from a uniform distribution. The following equations describe the the arrival position on the grain, where $x$, $y$ and $z$ are grain-body coordinates:

$$x = \sin \theta' \left( \cos \phi' \cos \theta_p \cos \phi_p - \sin \phi' \sin \phi_p \right) + \cos \theta' \sin \theta_p \cos \phi_p$$

(3.112)
\[ \frac{y}{a} = \sin \theta' \left( \cos \phi' \cos \theta_p \sin \phi_p + \sin \phi' \cos \phi_p \right) + \cos \theta' \sin \theta_p \sin \phi_p \]  \tag{3.113}

\[ \frac{z}{a} = \cos \theta' \cos \theta_p - \sin \theta' \cos \phi' \sin \theta_p \]  \tag{3.114}

where \( \theta_p \) and \( \phi_p \) are the polar and azimuthal angles of the dipole moment \( \mathbf{p} \) with respect \( \hat{z} \).

We calculate the probability of the release of an electron due to photoemission \( J_{pe} dt = J_\gamma y_0 y_2 \), where \( J_\gamma \) is the rate of photon absorption given above for both grain sizes, \( y_0 \) is the bulk photoelectric yield and \( y_2 \) is the yield factor accounting for the attraction of emitted electrons for the positively charged grain, Eqn. (3.109). Since we neglect the 10\% starlight anisotropy here, the probability of photon absorption is equal over the grain surface, and the photoelectric yield is similarly uniform. Because of this, the hole that the emitted electron leaves is randomly positioned on the grain surface.

We choose initial conditions for our simulations of \( \mathbf{p} = 0 \) and \( \mathbf{Z} \) based on an average grain potential \( U = 0.3 \text{V} \). However, Draine and Lazarian [15] noted that there may be an intrinsic electric dipole moment due to the random orientation of polar constituents of the grain material, so we need to justify our choice for \( \mathbf{p} = 0 \). In order to estimate the value of \( p/ea \) for the intrinsic dipole, we assume that each polar constituent of the grain has a volume \( V_0 \) and that the dipole moment of a constituent \( p_0 = \xi e V_0^{1/3} \), where \( \xi \) is a factor used to specify the level of polarization. If each constituent is also assumed to be randomly oriented, the total intrinsic electric dipole moment \( p_{int} \sim N^{1/2} p_0 \), where the grain volume is \( 4/3 \pi a^3 = NV_0 \). Solving to remove \( N \)

\[ \frac{p}{ea} \sim \left( \frac{4 \pi}{3} \right)^{1/2} \xi \left( \frac{a}{V_0^{1/3}} \right)^{1/2} \]  \tag{3.115}

Even if we adopt a high level of polarization \( \xi \sim 0.1 \) and a high density of polar constituents \( aV_0^{-1/3} \sim 500 \), we find that \( p_{int}/ea \sim 4.6 \). This is in the same range of values that we found for \( p \) neglecting the intrinsic dipole moment (see Figure 3.5 in Section 3.6 that follows).
With the high number of traps throughout the grain material (due to its expected highly amorphous form and the high level of impurity of the grain), we expect that any intrinsic dipole moment this small will quickly be neutralized by the population of these traps with holes and electrons. So, while the net charge of the grain is small, the total number of holes and electrons in the material is large. Any dipole within the grain attracts charges in a way that tends to neutralize the dipole, and a small intrinsic dipole will do the same. Therefore, we expect that the intrinsic electric dipole moment to have no effect on our simulations, and we are justified in setting the initial dipole moment to 0.

At each time step, if an electron has been lost or captured, the dipole moment $\mathbf{p}$ and the net grain charge $Z$ are recalculated. The electric dipole moment is determined simply by the vectorial addition of all electron positions and all hole positions, relative to the grain center of mass, at a sampling time.

$$
p_x = e \left( \sum r_{h+}^x - \sum r_{e-}^x \right)
$$

$$
p_y = e \left( \sum r_{h+}^y - \sum r_{e-}^y \right)
$$

$$
p_z = e \left( \sum r_{h+}^z - \sum r_{e-}^z \right)
$$

where $r_{e-,x,y,z}$ are the displacement components for electrons, $r_{h+,x,y,z}$ are the displacement components for holes, and $e$ is the proton charge. The coordinate system used here is internal to the grain, with $\mathbf{J}$ along $\hat{z}$. The projection of $\mathbf{p}$ along $\hat{J}$, $\mathbf{p}_J$, is therefore equal to $p_z$. The charge number of the grain at any time is

$$
Z = N_{h+} - N_{e-}.
$$

We track $\theta_p$, $\phi_p$ and $p \equiv |\mathbf{p}|$

$$
p = \left( p_x^2 + p_y^2 + p_z^2 \right)^{1/2}
$$
\[ \theta_p = \arccos \frac{p_z}{p} \quad (3.121) \]

\[ \phi_p = 2 \arctan \frac{1 - p_z/p \sin \theta_p}{p_y/p \sin \theta_p} \quad (3.122) \]

We also track the direction of the grain rotation axis relative the external magnetic field \( B \), using the polar and azimuthal angles \( \theta_{\text{align}} \) and \( \phi_{\text{align}} \) as given in [68]

\[
d\theta_{\text{align}} = -\Omega_0 \Upsilon \sin (\phi_{\text{align}} + \phi_{\text{gyro}}) \, dt \quad (3.123)
\]

\[
d\phi_{\text{align}} = \Omega_0 [1 - \Upsilon \cot \theta_{\text{align}} \cos (\phi_{\text{align}} + \phi_{\text{gyro}})] \, dt \quad (3.124)
\]

where \( \Omega_0 \) is the precession angular velocity when there is no electric dipole. The gyration angle \( \phi_{\text{gyro}} \) is cumulative over time and changes with each change in grain charge \( Z \)

\[
\phi_{\text{gyro}} = \int_0^t dt' \omega_{\text{gyro}}(t') \quad (3.125)
\]

and the time-scale for gyration is

\[
\omega_{\text{gyro}}^{-1} = 2.4 \times 10^2 \left( \frac{a}{0.1 \mu m} \right)^2 \left( \frac{U}{0.3 V} \right)^{-1} \left( \frac{\rho}{3 \text{g/cm}^3} \right)^{-1} \left( \frac{B}{5 \mu G} \right)^{-1} \text{yr.} \quad (3.126)
\]

From Eqns. (3.123 and 3.124) above, gyration can be seen as a potential source of disalignment. However, in early testing with and without gyration, we found no difference in the disalignment times. This was the same result for each \( \omega/\omega_T \). Because of this, we subsequently omitted gyration and \( \omega_{\text{gyro}} \) from our simulations.

For simulations with Model 2, the perfect conductor, we use the same simulation algorithm, except that there is no need to track the arriving electron trajectories. All charge is completely and immediately delocalized, so that incoming electrons are randomly positioned on the grain surface. Instead, we take the electric dipole moment \( \mathbf{p} = p_z \mathbf{\hat{z}} \) and
\( p_z = 0.1 \text{ Zea}. \)

For simulations using the models with deep traps, Models 3 and 4, the two types of traps, those for holes and those for electrons, are separately randomly positioned throughout the grain volume. The number of each type of trap is the ratio of the grain volume to the volume per deep trap \( V_t \): \( N_t = \text{int}(4\pi a^3 / 3V_t) \). The volume per deep trap \( V_t \) is estimated based on trap levels for highly disordered (highly amorphous) materials given by Blaise [5].

In the case of simulations using Model 3, the conductivity of the grain causes an arriving electron to immediately move to the nearest appropriate deep trap. An appropriate trap would be an electron-type trap not already occupied by another electron, or a hole-type trap occupied by a hole. In the latter case, the two charges recombine. The same process applies to a hole created by photoemission, with deep traps appropriate for the hole.

For simulations using Model 4, the partially conductive grain model, an arriving electron (or just-created hole) takes a random walk from its initial position through the grain volume. The timestep \( dt \) is modified in this simulation, defined as the time \( t_{rw} \) required to move a distance \( d_{rw} = 30\, \text{Å} \). If a charge comes within \( d_{rw} \) of an appropriate deep trap, the charge is positioned in the trap and remains there until it recombines with a charge of the opposite sign. The time for each random walk step \( t_{rw} \) defined as

\[ t_{rw} = \frac{f \tau_c d_{rw}^2}{V_t^{2/3}} \]

where \( \tau_c \) is the typical time between charging events, \( f \) a factor for adjusting the timestep length. Defined this way, the typical time it takes a charge to travel between traps is \( \sim f \tau_c \). With \( f \sim 1 \), the results for Model 4 fall between the extremes of those for the perfect insulator and those for the perfect conductor with deep traps.
3.6 Results

Simulations were run for 11 different sets of input parameters and two different random number generator seeds, resulting in a total of 22 runs. Table 3.1 shows the results for those 22 runs. All four models were used in simulation runs for a grain with radius $= 0.1\mu m$, however, we ran simulations for a grain with $a = 0.2\mu m$ for Models 1 - 3, only. Model 4 was excluded because of the prohibitively long CPU time required to simulate random walks through the larger grain. The total simulated time for runs using Models 1 - 3 is $t_{tot} = 10^5$ yr, while $t_{tot}$ for simulation runs with Model 4 are orders of magnitude less.

The results of tracking the $z$ component of the electric dipole moment $p_z$ for a perfectly insulated grain are shown in Figure 3.5. The value for $p_z$ is normalized to $ea$. The dipole is seen to rapidly change direction, going through sign reversal on a very short time-scale relative to a year. Having tracked the number of sign reversals, or “flips” $N_{flip}$, that occurred over the simulation period, we arrive at the average flipping time-scale $\tau_{flip} \approx t_{tot}/N_{flip}$. We take a flip to occur each time $|p_z|$ increases beyond unity with $p_z$ having the opposite sign as it did the previous time $|p_z|$ increased past unity. The time-scale for flipping $\tau_{flip}$ is less than $10^{-3}$ yr for all three models where flipping is relevant, as shown in Table 3.1.

The precession time for a grain in the absence of the electric dipole-generated torque Eqn.(3.6) $|\Omega_0|^{-1} \approx 2.7 \times 10^{-3}$ yr ($1.1 \times 10^{-2}$ yr) for grains with $a = 0.1\mu m$ ($a = 0.2\mu m$). So, $\tau_{flip}$ is always $< |\Omega_0|^{-1}$ (but not always $\ll |\Omega_0|^{-1}$). To approximate the disalignment time-scale $\tau_{dis}$ using $\tau_{flip}$, we have the 2 Eqns. (3.26, 3.27) [68] in Section 3.2. Of these 2 possibilities, Eqn. (3.26) is the better fit, i.e. $\tau_{dis} \sim \Upsilon^{-2} |\Omega_0|^{-2} \tau_{flip}^{-1}$. Eqns. (3.4 and 3.13) show that $\Upsilon \propto \omega^{-1}$, therefore $\tau_{dis} \propto (\omega/\omega_T)^2$. (When $\Upsilon \ll 1$, as in the case of suprathermally rotating silicate grains, $\tau_{dis} \propto \Upsilon^{-2} \propto \omega^{-2}$ for $\tau_{flip} \gg |\Omega_0|^{-1}$ Eqn. (3.27), also.) For suprathermally rotating grains this means that very long simulation times are required in order to get a large enough $N_{flip}$ for a meaningful average $\tau_{flip}$. We came up with a strategy to work around this limitation, using the proportionality relations between $\tau_{dis}$, $\Upsilon$, and $\omega$. We ran for several values of $\omega/\omega_T$, as low as 0.1 and looked for scaling of $\tau_{dis}$ with $\omega/\omega_T$. 
Table 3.1: Simulation Parameters and Outputs

<table>
<thead>
<tr>
<th>Model</th>
<th>$\alpha^c$</th>
<th>$V^d$</th>
<th>$t_{\text{tw}}^e$</th>
<th>Run</th>
<th>$p_{\text{av}}^f$</th>
<th>$\tau_{\text{flip}}^g$</th>
<th>$t_{\text{tot}}^h$</th>
<th>$10^{-4}\text{ yr}$</th>
<th>$1.5^i$</th>
<th>$2.0^i$</th>
<th>$N_{\text{dev}}^a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.1</td>
<td>...</td>
<td>...</td>
<td>1</td>
<td>2.21</td>
<td>5.2</td>
<td>1.0E5</td>
<td>2348</td>
<td>218</td>
<td>30</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>0.1</td>
<td>...</td>
<td>...</td>
<td>2</td>
<td>2.18</td>
<td>5.2</td>
<td>1.0E5</td>
<td>2418</td>
<td>195</td>
<td>26</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>0.1</td>
<td>...</td>
<td>...</td>
<td>1</td>
<td>2.11</td>
<td>...</td>
<td>1.0E5</td>
<td>72</td>
<td>5</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>0.1</td>
<td>...</td>
<td>...</td>
<td>2</td>
<td>2.12</td>
<td>...</td>
<td>1.0E5</td>
<td>44</td>
<td>6</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0.1</td>
<td>4.0E7</td>
<td>...</td>
<td>1</td>
<td>1.77</td>
<td>6.8</td>
<td>1.0E5</td>
<td>1822</td>
<td>179</td>
<td>19</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0.1</td>
<td>4.0E7</td>
<td>...</td>
<td>2</td>
<td>1.77</td>
<td>6.2</td>
<td>1.0E5</td>
<td>1800</td>
<td>160</td>
<td>19</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0.1</td>
<td>4.0E6</td>
<td>...</td>
<td>1</td>
<td>2.11</td>
<td>5.8</td>
<td>1.0E5</td>
<td>2451</td>
<td>220</td>
<td>26</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0.1</td>
<td>4.0E6</td>
<td>...</td>
<td>2</td>
<td>2.13</td>
<td>5.8</td>
<td>1.0E5</td>
<td>2358</td>
<td>228</td>
<td>32</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.1</td>
<td>4.0E7</td>
<td>2.3</td>
<td>1</td>
<td>2.16</td>
<td>2.2</td>
<td>7.29E2</td>
<td>14</td>
<td>1</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.1</td>
<td>4.0E7</td>
<td>2.3</td>
<td>2</td>
<td>2.35</td>
<td>2.5</td>
<td>7.29E2</td>
<td>22</td>
<td>1</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.1</td>
<td>4.0E7</td>
<td>1.15</td>
<td>1</td>
<td>2.17</td>
<td>2.5</td>
<td>3.64E2</td>
<td>6</td>
<td>1</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.1</td>
<td>4.0E7</td>
<td>1.15</td>
<td>2</td>
<td>2.09</td>
<td>2.4</td>
<td>3.64E2</td>
<td>11</td>
<td>1</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.1</td>
<td>4.0E7</td>
<td>9.2</td>
<td>1</td>
<td>2.56</td>
<td>2.4</td>
<td>2.92E3</td>
<td>81</td>
<td>11</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.1</td>
<td>4.0E7</td>
<td>9.2</td>
<td>2</td>
<td>2.56</td>
<td>2.5</td>
<td>2.92E3</td>
<td>76</td>
<td>7</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.1</td>
<td>4.0E6</td>
<td>2.3</td>
<td>1</td>
<td>2.07</td>
<td>5.0</td>
<td>7.29E2</td>
<td>17</td>
<td>2</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.1</td>
<td>4.0E6</td>
<td>2.3</td>
<td>2</td>
<td>2.11</td>
<td>5.1</td>
<td>7.29E2</td>
<td>19</td>
<td>3</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0.2</td>
<td>...</td>
<td>...</td>
<td>1</td>
<td>2.23</td>
<td>2.6</td>
<td>1.0E5</td>
<td>172</td>
<td>16</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0.2</td>
<td>...</td>
<td>...</td>
<td>2</td>
<td>2.18</td>
<td>2.6</td>
<td>1.0E5</td>
<td>150</td>
<td>12</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>0.2</td>
<td>...</td>
<td>...</td>
<td>1</td>
<td>2.00</td>
<td>...</td>
<td>1.0E5</td>
<td>4</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>0.2</td>
<td>...</td>
<td>...</td>
<td>2</td>
<td>2.00</td>
<td>...</td>
<td>1.0E5</td>
<td>4</td>
<td>1</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0.2</td>
<td>4.0E7</td>
<td>...</td>
<td>1</td>
<td>2.07</td>
<td>2.9</td>
<td>1.0E5</td>
<td>164</td>
<td>17</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0.2</td>
<td>4.0E7</td>
<td>...</td>
<td>2</td>
<td>2.07</td>
<td>2.9</td>
<td>1.0E5</td>
<td>139</td>
<td>14</td>
<td>2</td>
<td></td>
</tr>
</tbody>
</table>

---

*Number of 1 rad deviations in alignment angle $\theta_{\text{align}}$.

*From section 3.4.

*Grain radius.

*Volume per deep trap.

*Average of the absolute value of the component of the electric dipole moment lying along the spin axis (normalized to $ea$, the product of the proton charge and the grain radius).

*Estimate of the electric dipole moment flipping time.

*Duration of the simulation.

*Suprathermality $\omega/\omega_T$. 

---
We found that in most cases \( \tau_{\text{dis}} \propto (\omega/\omega_T)^2 \), so that we can estimate \( \tau_{\text{dis}} \) for suprathermally rotating grains through extrapolation, instead of having to run for excessively long simulation times. Also, since \( \Upsilon^{-2} |\Omega_0|^{-2} \) is independent of the magnetic dipole moment \( \mu \), it is also independent of the magnetic susceptibility \( \chi_0 \). Since \( \chi_0 \) is uncertain for interstellar grains, as discussed in Section 3.2, the estimation of \( \tau_{\text{dis}} \) for suprathermally rotating grains benefits by independence from this source of uncertainty.

In an approach similar to that we used to estimate \( \tau_{\text{flip}} \) as an average over a simulation period, we estimate \( \tau_{\text{dis}} \) as an average over the full simulation runtime. We track the number of times, \( N_{\text{dev}} \), that \( \theta_{\text{align}} \) changes by 1 rad. We start the count when \( \theta_{\text{align}} \) differs from its initial value by 1 rad, \( \theta_{\text{align}} = \theta_{\text{align},1} \). At this point \( N_{\text{dev}} = 1 \). When \( \theta_{\text{align}} \) differs from \( \theta_{\text{align},1} \) by 1 rad, \( N_{\text{dev}} = 2 \) and so on for each successive deviation of 1 rad. When a large number of these deviations have occurred such that \( N_{\text{dev}} \gg 1 \), \( \tau_{\text{dis}} \approx t_{\text{tot}}/N_{\text{dev}} \). For the small values of \( \omega/\omega_T \) we have used for our simulations, this approximation of \( \tau_{\text{dis}} \) works. However, for much larger values, such as \( \omega/\omega_T \lesssim 10 \), we approximate the disalignment time as \( \tau_{\text{dis}} \approx t_{\text{tot}}/(N_{\text{dev}} + |\Delta \theta_{\text{align}}|) \), with \( \Delta \theta_{\text{align}} \) the difference of \( \theta_{\text{align}} \) at the end of the simulation, and \( \theta_{\text{align}} \) the last time the \( N_{\text{dev}} \) was updated. Table 3.1 shows values of \( N_{\text{dev}} \) for \( \log_{10}(\omega/\omega_T) = 1.0, 1.5 \) and \( 2.0 \). Where \( N_{\text{dev}} = 1 \), the estimate of \( \tau_{\text{dis}} \) is not very reliable.

We track \( \theta_{\text{align}} \) for seven different values of \( \log_{10}(\omega/\omega_T) \) (-1, -0.5, 0, 0.5, 1, 1.5, 2), in each simulation run. In Figure 3.6 we show \( \cos \theta_{\text{align}} \) for a perfectly insulated grain with \( a = 0.1 \mu m \) spinning at \( \omega/\omega_T = 10^2 \), over a simulation period of \( 10^5 \) yr.

Figure 3.7 shows how disalignment time measured through simulation compares to disalignment time calculated using Eqn. (3.26), for grains of 2 different radii. The log of disalignment time \( \log_{10}(\tau_{\text{dis}}/\text{yr}) \) is shown for each of the seven rotation rates, for perfectly insulated grains of two different sizes (\( a = 0.1 \mu m \) and \( a = 0.2 \mu m \)). Disalignment time \( \tau_{\text{dis}} \) is averaged over both realizations (runs with new random number generator seeds). The dashed line shows the results of calculating \( \tau_{\text{dis}} \) using Eqn. (3.26) for \( a = 0.2 \mu m \), and the solid line shows the same calculation results for \( a = 0.1 \mu m \). For the calculation, we use...
\( \tau_{\text{flip}} \) and the average of \( |p_z| \) as determined in the simulation. The agreement between the measured and calculated values is surprisingly good. The expected relation \( \tau_{\text{dis}} \propto (\omega/\omega_T) \) is well confirmed.

Both the disalignment time calculated with Eqn. (3.26) and the flipping timescale \( \tau_{\text{flip}} \) found in the simulations are significantly shorter than those of [68] (figures 2 and 3 in [68]). The differences are greater than two orders of magnitude for a grain with \( a = 0.1 \mu m \). Our simulations result in much larger values for the average of \( |p_z| \) than those estimated by [68], and \( \tau_{\text{dis}} \propto |p_z|^{-2} \). Our findings for the flipping timescale \( \tau_{\text{flip}} \) are also substantially shorter than those estimated by [68]. When Eqn. (3.26) is used (\( \tau_{\text{dis}} \propto \tau_{\text{flip}} \)), this partially compensates for the difference in \( p_z \) estimates. However, [68] used Eqn. (3.27) for a grain of \( a = 0.1 \mu m \), because of the larger value of \( \tau_{\text{flip}} \); in this case \( \tau_{\text{dis}} \) is larger by a factor \( \approx 2 \) when Eqn. (3.27) is used instead of Eqn. (3.26).

In Figure 3.8, disalignment timescale \( \tau_{\text{dis}} \) results are shown for variations of Models 3 and 4, as a ratio with the disalignment timescale for Model 1, the perfectly insulating grain. The simulation runs are those shown in Table 3.1 for a 0.1 \( \mu m \) radius grain. In Figure 3.8, the results of the two realizations, for the same simulation initial conditions, are averaged together to get \( \tau_{\text{dis}} \). Models 3 and 4 were set for various deep trap densities, as indicated by the volume per deep trap \( V_t \) variable, and the random walk time \( t_{\text{rw}} \) was varied for Model 4. All ratios \( \tau_{\text{dis}} / \tau_{\text{ins}} \) show values within \( \approx 50\% \) of 1, with somewhat more spread for rotation rates \( \omega/\omega_T > 10 \). The \( \tau_{\text{dis}} \) values for these higher rotation rates are less reliable, given the low number of deviations, \( N_{\text{dev}} \), as seen in Table 3.1. The \( \tau_{\text{dis}} / \tau_{\text{ins}} \) results for Model 3 with a 0.2 \( \mu m \) radius grain, were also within \( \approx 50\% \) of 1.

In Figure 3.9, the disalignment timescale for the perfect conductor \( \tau_{\text{cond}} \) over \( \tau_{\text{ins}} \) results are shown for Model 2, for both \( a = 0.1 \mu m \) and \( a = 0.2 \mu m \) grain sizes. We made the assumption that \( p_z \propto 0.1 Zea \), a seemingly conservative choice for a grain asymmetric enough to produce the observed level of polarization. However, to confirm this choice for \( p_z \) would require a solution to the electrostatic boundary value problem for a model aspherical grain. The \( \tau_{\text{cond}} \) for suprathermally rotating grains is between 1 and 2 orders of
Figure 3.5: The component of the grain dipole moment (normalized to $\varepsilon a$, the proton charge times the grain radius) lying along the spin axis vs. time, from a simulation of a perfectly insulating grain with $a = 0.1 \, \mu$m.

magnitude greater than that for the perfectly insulating grain. Since $Z$ doesn’t change sign in our simulations, although it does fluctuate in small positive values, $p_z$ doesn’t change sign either. Again, the low number of deviations, $N_{\text{dev}}$ (Table 3.1) for $\omega/\omega_T > 10$, lowers the reliability of the $\tau_{\text{dis}}$ values.
Figure 3.6: $\cos \theta_{\text{align}}$ vs. time from a simulation of a perfectly insulating grain with $a = 0.1 \, \mu m$ and $\omega/\omega_T = 10^2$; $N_{\text{dev}} = 30$ for this case.

Figure 3.7: Disalignment time vs. suprathermality for perfectly insulating grains
Figure 3.8: Ratio of disalignment time $\tau_{\text{dis}}$ of various models to that for a perfectly insulating grain, $\tau_{\text{ins}}$, for $a = 0.1 \, \mu m$. Model number from Section 3.4.4.; volume per deep trap; $V_t$; and random walk time, $t_{\text{rw}}$, are indicated.

Figure 3.9: Ratio of disalignment time for a perfectly conducting grain, $\tau_{\text{cond}}$, to that for a perfectly insulating grain, $\tau_{\text{ins}}$, for $a = 0.1$ and $0.2 \, \mu m$, as indicated.
3.7 Conclusions

With this research, we expanded the research done by [68], conducting a more detailed analysis of the effects of a time-varying electric dipole moment on grain disalignment. We used four models of charge movement for our examination: a perfectly insulating grain, a conductor with deep traps, a partial conductor with deep traps, and a perfect conductor. We focused our analysis on dielectric silicate grains and suprathermal rotation rates.

For the perfect insulator and the two models with deep traps, the disalignment time results are highly consistent, as shown in Figure 3.8. The perfect conductor model exhibited disalignment times that were up to two orders of magnitude greater than those of the perfect insulator, as depicted in Figure 3.9. We expect real interstellar grain disalignment times to fall within those of Figure 3.8, as the insulator and deep trap models more closely approximate expected actual grain characteristics, while the perfect conductor model appears unrealistic for interstellar grains.

We did not include the effects of gas-grain drift on collisional charging of the grain. A non-rotating grain drifting in the gas might be expected to accumulate charge in the direction of the grain drift velocity, creating a stable contribution to $p$. A drifting rotating grain, with the rotation axis in line with the principal axis of the greatest moment of inertia $\hat{a}_1$, might also accumulate a charge distribution dependent on the grain’s latitude that would reduce the flipping of $p_z$. In Appendix E we examine these effects and conclude that gas-grain drift produces no significant effect on grain flipping rates and can be neglected.

Radiative torque alignment seems to occur typically for suprathermally rotating grains with $\omega/\omega_T \approx 100$ and on a time-scale of $\tau_{\text{rad}} \gtrsim 10^5$ yr [18] [43] [28]. Additional research is needed to confirm these results, though. For $\omega/\omega_T \approx 100$, we have found that the timescale for disalignment due to the time-varying dipole $\tau_{\text{dis}} \lesssim 10^5$ yr, as shown in Figures 3.7 and 3.8. For the models we selected, the disalignment times associated with a grain’s time-varying electric dipole moment are shorter than the direct radiative torque alignment times and present a severe challenge to that model.

More detailed examination of the physics behind the disalignment process described here
could show that the disalignment magnitude has been overestimated. The specifics of the
grain charging process and charge transport, as well as the magnetic turbulence-induced
grain drift velocity have not been directly verified in the laboratory or by observation.
Also, interstellar grains may contain superparamagnetic inclusions, which would increase
their magnetic susceptibility. This would result in an increased magnetic moment for the
grain and a decreased value for $\Upsilon$. This, in turn, would result in longer disalignment times
as $\tau_{\text{dis}} \propto \Upsilon^{-2}$ for $\Upsilon \ll 1$. Superparamagnetic inclusions may also enhance radiative torque
alignment, as recently found by Lazarian and Hoang [44]. Superparamagnetic inclusions
could be found to reverse our finding that the disalignment time-scale due to a time-varying
electric dipole is shorter than the radiative torque alignment time-scale.
Chapter 4: Afterword: Broader Context of Work

Grain alignment seems to result from a complicated mix of processes. Contributing processes may include radiative torques, the Barnett effect, photoemission, collisional charging, acceleration due to magnetohydrodynamic (MHD) turbulence in the gas, collisions with gas atoms, magnetic field torques associated with grain magnetic moment (varying with the magnetic susceptibility of the material, as in the case of superparamagnetic inclusions), magnetic field torques associated with the electric dipole moment, various grain surface chemical processes, and more.

In order to make progress, given the complexity of the grain alignment problem, we will follow an overall strategy of running detailed simulations of grain rotational dynamics for a wide variety of grain shapes and interstellar environments. For each simulation, we will track the degree of alignment as a function of time. The model will allow for selective exclusion of processes such as those listed above for a given simulation run, allowing for the isolation of grain alignment/disalignment effects due to each process.

Observational data provide the constraints on the degree of alignment as a function of the interstellar environment. These observational data include the polarization of starlight and IR dust emission as a function of wavelength, the overall extinction curve correlation with polarization (including the polarization of the broadened 9.8\,\mu m and 18\,\mu m absorption features and the lack of polarization of the 2175\,Å feature), and the decreasing level of polarization with increasing optical depth into dense clouds. These observational data will be used to determine which simulation runs best replicate the physical reality, and will provide the means to determine which of the above processes are most important to grain alignment.

The results of this thesis work have provided valuable input to the discovery strategy described above. Recently, DDSCAT simulations were run to find the radiative torques on
10-20 different grain shapes. Attempting to include calculations of the photoemission and photodesorption torques for these simulations would have required enormous computational time and effort. By determining through the work described here that these torques can be neglected, that time and effort can be invested in other aspects of the overall problem.

The electric dipole portion of this thesis work provided unexpected results, showing how effective the dipole disaligning mechanism can be. We were able to show how dipole disalignment should be implemented in grain alignment simulations, including the dipole’s effect on collisional charge rates and electron trajectories, as well as some simplifications associated with charge transport. Finally, the challenge to radiative torque alignment posed by dipole disalignment has shown the importance of including superparamagnetic inclusions in future simulations.
Appendix A: Separable Solution for the Scalar Wave Function in Spheroidal Coordinates

A scalar wave function ($\psi$) in spheroidal coordinates can be shown to be a separable solution to the scalar wave equation

$$\nabla^2 \psi + k^2 \psi = 0 \quad (A.1)$$

where $k$ is the wave number. The scalar wave function $\psi_{mn}$, for the prolate spheroidal coordinate system, is the product of $S_{m,n}(c, \eta)$, $R^{(i)}_{|m|,n}(c, \xi)$, and $\Phi(\phi)$ where $S_{m,n}(c, \eta)$ and $R^{(i)}_{|m|,n}(c, \xi)$ are the angular and radial spheroidal functions, respectively, as described in Chapter 2 Section 2.6. To improve readability in the following exercise, $S_{m,n}$ will be used for $S_{m,n}(c, \eta)$ and $R_{|m|,n}$ will be used for $R^{(i)}_{|m|,n}(c, \xi)$. Using the definition of the Laplacian ($\nabla^2$) in spheroidal coordinates

$$\frac{1}{h_\xi h_\eta h_\phi} \left[ \frac{\partial}{\partial \xi} \left( h_\xi h_\phi \frac{\partial}{\partial \xi} \right) + \frac{\partial}{\partial \eta} \left( h_\eta h_\phi \frac{\partial}{\partial \eta} \right) + \frac{\partial}{\partial \phi} \left( h_\phi \frac{\partial}{\partial \phi} \right) \right] \quad (A.2)$$

and employing the scale factor definitions in Chapter 2 Section 2.6, the scalar wave equation in spheroidal coordinates is (throughout, the upper sign is used for the oblate spheroidal coordinate system and the lower sign is used for the prolate coordinate system)

$$-k^2 \psi = \frac{4}{d^2 (\xi^2 \pm \eta^2)} \left[ \frac{\partial}{\partial \xi} \left( \xi^2 \pm 1 \right) \frac{\partial}{\partial \xi} \right] \psi + \frac{\partial}{\partial \eta} \left( 1 - \eta^2 \right) \frac{\partial}{\partial \eta} \psi + \frac{\partial}{\partial \phi} \left( \xi^2 \pm \eta^2 \right) \frac{\partial}{\partial \phi} \psi. \quad (A.3)$$

Multiplying both sides of the equation by $4/[d^2 (\xi^2 \pm \eta^2)]$, substituting $S_{m,n}R_{|m|,n}\Phi$ for
\[ \psi \text{ and then dividing by } S_{m,n} R_{|m|,n} \Phi, \text{ we obtain} \]

\[
\left[ \frac{1}{R_{|m|,n}} \frac{d}{d\xi} \left( (\xi^2 \pm 1) \frac{dR_{|m|,n}}{d\xi} \right) + \frac{1}{S_{m,n}} \frac{d}{d\eta} \left( (1 - \eta^2) \frac{dS_{m,n}}{d\eta} \right) \right. \\
\left. \times \frac{1}{\Phi} \left( \frac{\xi^2 \pm \eta^2}{(\xi^2 \pm 1)(1 - \eta^2)} \frac{d^2 \Phi}{d\phi^2} \right) \right] + k^2 \left( \xi^2 \pm \eta^2 \right) = 0. \quad (A.4) \]

Dividing through by \( (\xi^2 \pm \eta^2) / [(\xi^2 \pm 1)(1 - \eta^2)] \) and setting the \( \phi \) term of the equation equal to \(-m^2\) gives two equations

\[
\frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} = -m^2 \quad (A.5)
\]

\[
\frac{(\xi^2 \pm 1)(1 - \eta^2)}{(\xi^2 \pm \eta^2)} \left[ \frac{1}{R_{|m|,n}} \frac{d}{d\xi} \left( (\xi^2 \pm 1) \frac{dR_{|m|,n}}{d\xi} \right) + \frac{1}{S_{m,n}} \frac{d}{d\eta} \left( (1 - \eta^2) \frac{dS_{m,n}}{d\eta} \right) \right. \\
\left. \times \left( (1 - \eta^2) \frac{dS_{m,n}}{d\eta} \right) + k^2 \left( \xi^2 \pm \eta^2 \right) \right] = m^2. \quad (A.6)
\]

The separated \( \phi \)-dependent equation has both an even and an odd solution, that can also be expressed as an exponential:

\[
\Phi_e = \cos(m\phi), \quad \Phi_o = \sin(m\phi), \quad \Phi = e^{im\phi}. \quad (A.7)
\]

The \( \xi \) and \( \eta \)-dependent equation,

\[
\frac{1}{R_{|m|,n}} \frac{d}{d\xi} \left( (\xi^2 \pm 1) \frac{dR_{|m|,n}}{d\xi} \right) + \frac{1}{S_{m,n}} \frac{d}{d\eta} \left( (1 - \eta^2) \frac{dS_{m,n}}{d\eta} \right) \\
\times \left( (1 - \eta^2) \frac{dS_{m,n}}{d\eta} \right) + k^2 \left( \xi^2 \pm \eta^2 \right) - m^2 \frac{(\xi^2 \pm \eta^2)}{(\xi^2 \pm 1)(1 - \eta^2)} = 0, \quad (A.8)
\]
can be separated into two equations, one dependent on $\xi$ and the other dependent on $\eta$,

\[
\frac{1}{R_{|m|,n}} \frac{d}{d\xi} \left( (\xi^2 + 1) \frac{dR_{|m|,n}}{d\xi} \right) - m^2 \frac{(1 - \eta^2)}{(\xi^2 + 1)(1 - \eta^2)} + k^2 \xi^2 = \lambda_{mn} \quad (A.9)
\]

\[
\frac{1}{S_{m,n}} \frac{d}{d\eta} \left( (1 - \eta^2) \frac{dS_{m,n}}{d\eta} \right) - m^2 \frac{(\xi^2 + 1)}{(\xi^2 + 1)(1 - \eta^2)} - k^2 \eta^2 = -\lambda_{mn}. \quad (A.10)
\]

This results in two differential equations, which $S_{m,n}$ and $R_{|m|,n}$ must satisfy for the prolate coordinate solution,

\[
\frac{d}{d\xi} \left[ (\xi^2 - 1) \frac{dR_{|m|,n}}{d\xi} \right] - \left[ \lambda_{mn} - k^2 \xi^2 + \frac{m^2}{(\xi^2 + 1)} \right] R_{|m|,n} = 0 \quad (A.11)
\]

\[
\frac{d}{d\eta} \left[ (1 - \eta^2) \frac{dS_{m,n}}{d\eta} \right] + \left[ \lambda_{mn} - k^2 \eta^2 - \frac{m^2}{(1 - \eta^2)} \right] S_{m,n} = 0. \quad (A.12)
\]

Similarly, two differential equations are derived for the oblate coordinate system by transforming $c$ to $\mp ic$ and $\xi$ to $\pm i \xi$, so that $\psi$ is now a product of $S_{m,n}(-ic, \eta)$, $R_{|m|,n}^{(i)}(-ic, i \xi)$, and $\Phi(\phi)$, and then following the process outlined above:

\[
\frac{d}{d\xi} \left[ (\xi^2 + 1) \frac{dR_{|m|,n}}{d\xi} \right] - \left[ \lambda_{mn} - k^2 \xi^2 - \frac{m^2}{(\xi^2 + 1)} \right] R_{|m|,n} = 0 \quad (A.13)
\]

\[
\frac{d}{d\eta} \left[ (1 - \eta^2) \frac{dS_{m,n}}{d\eta} \right] + \left[ \lambda_{mn} + k^2 \eta^2 - \frac{m^2}{(1 - \eta^2)} \right] S_{m,n} = 0. \quad (A.14)
\]
Appendix B: Obtaining the Spheroidal Expansion Coefficients $d_{r}^{m,n}(c)$

The spheroidal expansion coefficients $d_{r}^{m,n}(c)$ are found by applying the method developed by Eide, Stammes, Stammes and Schulz [19], which reformulates the problem as a numerically solved eigenvalue problem. The method is described below.

The separation of variables method, when applied to the wave equation written in spheroidal coordinates

$$\frac{4}{d^{2}(\xi^{2}+\eta^{2})} \left[ \frac{\partial}{\partial \xi} \left( (\xi^{2}+1) \frac{\partial}{\partial \xi} \right) + \frac{\partial}{\partial \eta} \left( (1-\eta^{2}) \frac{\partial}{\partial \eta} \right) + \frac{\partial}{\partial \phi} \left( \frac{\xi^{2}+\eta^{2}}{(\xi^{2}+1)(1-\eta^{2})} \frac{\partial}{\partial \phi} \right) \right] \psi$$

$$+ k^{2} \psi = 0$$

(B.1)

with the separated scalar solution:

$$\psi = S_{m,n}(c,\eta)R_{|m|,n}(c,\xi)\text{e}^{im\phi},$$

(B.2)

results in the following two differential equations in $\eta$ and $\xi$ (written for the prolate coordinate system; replace $c$ with $-ic$, and $\xi$ with $i\xi$ for the oblate coordinate system):

$$\frac{d}{d\xi} \left( (\xi^{2}+1) \frac{d}{d\xi} \right) - \left[ \lambda_{m,n} - c^{2}\xi^{2} + \frac{m^{2}}{(\xi^{2}+1)} \right] R_{|m|,n}(c,\xi) = 0$$

(B.3)

$$\frac{d}{d\eta} \left( (1-\eta^{2}) \frac{d}{d\eta} S_{m,n}(c,\eta) \right) + R_{|m|,n}(c,\xi) \left[ \lambda_{m,n} + c^{2}\eta^{2} - \frac{m^{2}}{(1-\eta^{2})} \right] S_{m,n}(c,\eta) = 0.$$  

(B.4)

The characteristic value $c$ above is the product of the wave number $k$ of the medium through which the electromagnetic wave is traveling, and the spheroid’s semi-focal distance $f$, $c = kf$. 
The angular spheroidal function \( S_{m,n}(c,\eta) \) and the radial spheroidal function \( R^{(i)}_{|m|,n}(c,\xi) \), (again written for the prolate coordinates, with substitutions as described above for the oblate system), are expressed as expansions in associated Legendre functions and spherical Bessel, Neumann and Hankel functions \( (z^i; i = 1, 2, 3, 4) \), respectively:

\[
S_{m,n}(c,\eta) = \sum_{r=0,1}^\infty d_r^{m,n}(c) P_{m+r}^m(\eta)
\]  

\[
R^{(i)}_{|m|,n}(c,\xi) = \frac{1}{\sum_{r=0,1}^\infty d_r^{|m|,n}(c) \frac{(2|m|+r)!}{r!}} \left( \frac{(\xi^2 \pm 1)}{\xi^2} \right)^{|m|/2} \sum_{r=0,1}^\infty i^{r+|m|} d_r^{|m|,n}(c) \frac{(2|m|+r)!}{r!} \frac{z^i_r(c\xi)}{z^{|m|+r}(c\xi)}.
\]  

The prime (') over the summation symbol, in each case, indicates that only even values \( r \) are summed when \( n - m \) is even, and only odd values of \( r \) are summed when \( n - m \) is odd. The expansion coefficients are the same for both \( S_{m,n}(c,\eta) \) and \( R^{(i)}_{|m|,n}(c,\xi) \) for a given coordinate system.

Substituting function (B.5) into equation (B.4), results in the following recurrence relation [19] [22]:

\[
\alpha_r^m d_{m,n,r+2} + (\beta_r^m - \lambda_{m,n}) d_{r}^{m,n} + \gamma_r^m d_{r-2}^{m,n} = 0
\]  

with

\[
\alpha_r^m = \frac{(2m + r + 2)(2m + r + 1)}{(2m + 2r + 3)(2m + 2k + 5)} c^2
\]

\[
\beta_r^m = (m + r)(m + r + 1) + \frac{2(m + r)(m + r + 1) - 2m^2 - 1}{(2m + 2r - 1)(2m + 2r + 3)} c^2
\]
\[
\gamma_r^m = \frac{r(r-1)}{(2m + 2r - 3)(2m + 2r - 1)} c^2. \tag{B.10}
\]

The recurrence relation provides a means to generate a series of equations that can be solved for the expansion coefficients \(d_r^{m,n}\). Eide et al. [19] formulate the set of equations, for a given value of \(m\), as an algebraic eigenvalue/eigenvector problem. Two separate solutions are required for each \(m\): \(n - m\) even (resulting in even values of \(r\) starting with 0); and \(n - m\) odd (for odd values of \(r\) starting with 1). The sets of \(d_r^{m,n}\) values found for each value of \(n\) are the eigenvectors. The values for \(\lambda_{m,n}\) are the eigenvalues. The eigenvalue/eigenvector problem is shown here for \(n - m\) even:

\[
A \cdot V = 0 \tag{B.11}
\]

where \(A\) is

\[
\begin{bmatrix}
(\beta^m_0 - \lambda_m) & \alpha_0^m & 0 & 0 & \cdots & 0 & 0 & 0 \\
\gamma_2^m & (\beta^m_2 - \lambda_m) & \alpha_2^m & 0 & \cdots & 0 & 0 & 0 \\
0 & \gamma_4^m & (\beta^m_4 - \lambda_m) & \alpha_4^m & \cdots & 0 & 0 & 0 \\
\vdots & & & & & & & \vdots \\
0 & 0 & 0 & 0 & \cdots & \gamma_{2N-2}^m & (\beta_{2N-2}^m - \lambda_m) & \alpha_{2N-2}^m \\
0 & 0 & 0 & 0 & \cdots & 0 & \gamma_{2N}^m & (\beta_{2N}^m - \lambda_m)
\end{bmatrix}
\]

and \(V\) is

\[
\begin{bmatrix}
d_0^m \\
d_2^m \\
d_4^m \\
\vdots \\
d_{2N-2}^m \\
d_{2N}^m
\end{bmatrix}
\]
and $N$ is the truncation value that provides the level of precision required for the solution.

We wrote Fortran77 code to create these arrays for a range of $m$ values up to truncation term $M$, and solve for $d_r^{m,n}$ and $\lambda_{m,n}$ for both environments, the vacuum outside the grain and the grain interior. Since the array takes the form of a tri-diagonal matrix, we used the LAPACK [20] driver ZGEEVX to solve this eigenvector/eigenvalue problem for double complex values of the $d_r^{m,n}$ coefficients. (The characteristic value $c$ is complex for the interior of the grain.) We resorted the eigenvectors and eigenvalues resulting from ZGEEVX in descending order based on the real part of the eigenvalues, using a numerical recipe found in Press et al.[57]. The $d_r^{m,n}$ coefficients were then normalized using Flammer’s convention [22], for $n - m$ even,

$$
\sum_{r=0}^{\infty} \frac{(-1)^{r/2}(r + 2m)!}{2^r \left(\frac{r}{2}\right)! \left(\frac{r + 2m}{2}\right)!} d_r^{m,n} = \frac{(-1)^{\frac{n-m}{2}}(n + m)!}{2^{n-m} \left(\frac{n-m}{2}\right)! \left(\frac{n-m}{2}\right)!}
$$

and for $n - m$ odd,

$$
\sum_{r=0}^{\infty} \frac{(-1)^{r-1}(r + 2m + 1)!}{2^r \left(\frac{r-1}{2}\right)! \left(\frac{r + 2m + 1}{2}\right)!} d_r^{m,n} = \frac{(-1)^{\frac{n-m-1}{2}}(n + m)!}{2^{n-m} \left(\frac{n-m-1}{2}\right)! \left(\frac{n-m+1}{2}\right)!}
$$

and the results were stored.

Only $d_r^{m,n}$ coefficients and $\lambda_{m,n}$ for positive values of $m$ need to be calculated. The coefficients for negative values can be obtained through the relations [22],

$$\lambda_{-m,n} = \lambda_{m,n}$$

$$d_{r}^{-m,n} = \frac{(n-m)!(2m+r)}{(n+m)!r!} d_{r}^{m,n}$$

$$S_{-m,n}(c,\eta) = (-1)^{m} \frac{(n-m)!}{(n+m)!} S_{m,n}(c,\eta).$$
The radial function $R_{[m],n}^{(i)}(c,\xi)$ is defined for positive values of $m$ only.

We obtained agreement with published values of $d_{r,m,n}$, $\lambda_{m,n}(c,\eta)$, and $S'_{m,n}(c,\eta)$ in [22] and [47] for all levels of precision given (there were some errors for the complex values of $c$ in Tables 2.13 - 2.17 in [47]), using truncation values for $n$ and $m$, $N = M = 40$. The code ran quickly, requiring no more than several seconds.
Appendix C: Integration Methodology

In order to be able to efficiently perform the integration required for Barton’s method, we used several computational approaches that greatly reduced the time required to perform the integration. First, as described in Appendix B, we calculated the spheroidal function expansion coefficients \(a^{m,n}_r(c)\) for both the grain material (internal field) and the vacuum outside the grain (scattered field), for each \(m\) and \(n\) value, and stored these. Using the eigenvalue/eigenvector approach to calculate \(a^{m,n}_r(c)\), we also solved for the separation constants \(\lambda_{m,n}(c)\) and stored these, as well. Both \(a^{m,n}_r(c)\) and \(\lambda_{m,n}(c)\) are independent of position and therefore, just need to be calculated once. Next, we calculated the spheroidal radial functions:

\[
R_{|m|,n}^{(i)}(c, \xi) = \frac{1}{\sum_{r=0,1}^\infty a^{|m|,n}_r(c) \frac{(2|m|+r)!}{r!}} \left( \frac{\xi^2 \pm 1}{\xi^2} \right)^{|m|/2} \sum_{r=0,1}^\infty i^{r+|m|-n} a^{|m|,n}_r(c) \frac{(2|m|+r)!}{r!} i^{(i)}_{|m|+r}(c\xi)
\]

and their derivatives, again for the grain interior and the external vacuum. Since we are interested in the boundary conditions for only one surface \(\xi = \xi_0\), there is no integration with respect to \(\xi\) required and the radial functions need only be calculated once and stored. We calculated these first using Fortran 77 code, and then switched to Mathematica so that the precision could be increased past the double complex available on the gnu compiler.

Once we had these lookup tables of values available, we could consider how best to perform the integrations. In Barton’s method, there are a set of line integrals and a set of surface integrals. We describe our integration approach for the line integrals first. The line integrals, as described in Section 2.6, resulted from the integration of the internal and scattered vector wavefunctions [Eqns. (2.172), (2.173), (2.174), and (2.175)] and the angular
spheroidal function $S_{m,n}$ for the vacuum:

\[
I_{m,n,n'}^1 = 4\pi \int_0^1 N^{(s)}_{m,n;n'} S_{m,n'}(c, \eta) d\eta
\]

(C.2)

\[
I_{m,n,n'}^2 = 4\pi \int_0^1 M^{(s)}_{m,n;n'} S_{m,n'}(c, \eta) d\eta
\]

(C.3)

\[
I_{m,n,n'}^3 = 4\pi \int_0^1 N^{(t)}_{m,n;n'} S_{m,n'}(c, \eta) d\eta
\]

(C.4)

\[
I_{m,n,n'}^4 = 4\pi \int_0^1 M^{(t)}_{m,n;n'} S_{m,n'}(c, \eta) d\eta
\]

(C.5)

\[
I_{m,n,n'}^5 = 4\pi \int_0^1 N^{(s)}_{m,n;\phi} S_{m,n'}(c, \eta) d\eta
\]

(C.6)

\[
I_{m,n,n'}^6 = 4\pi \int_0^1 M^{(s)}_{m,n;\phi} S_{m,n'}(c, \eta) d\eta
\]

(C.7)

\[
I_{m,n,n'}^7 = 4\pi \int_0^1 N^{(t)}_{m,n;\phi} S_{m,n'}(c, \eta) d\eta
\]

(C.8)

\[
I_{m,n,n'}^8 = 4\pi \int_0^1 M^{(t)}_{m,n;\phi} S_{m,n'}(c, \eta) d\eta
\]

(C.9)

where integration of $\phi$ over the surface is completed, and integration with respect to $\eta$ is performed over only half the range and doubled, due to the symmetry of the spheroidal angular function $S_{m,n}$. There are eight integrals for each $m$, $n$, and $n'$ at this point.

Using the definition of the angular spheroidal function $S_{m,n}$

\[
S_{m,n} = \sum_{r=0,1}^{\infty} d_r^{m,n}(c) P_{m+r}^{n}(\eta),
\]

(C.10)
each of the above integrals (for each \(m, n\), and \(n'\)) can be expanded into a double sum of integrals (one summation resulting from the expansion of \(S_{m,n}\) and the other summation for the expansion of \(S_{m,n'}\)). Each summation is over even values of \(r\) or \(r'\) if \(n - m\) is even, and over odd values of \(r\) or \(r'\) if \(n - m\) is odd. The following unique terms result.

for \(I_1\):

\[
\frac{\xi (\xi^2 - 1)}{c} \frac{dR^{(i)}_{m,n}}{d\xi} \sum_r d_r^{m,n} \sum_{r'} d_{r'}^{m,n} \int_0^1 \frac{(1 - \eta^2)^{1/2}}{(\xi^2 - \eta^2)^{3/2}} \frac{dP^m_n}{d\eta} P^m_{n'} d\eta
\]  

(C.11)

\[
\frac{R^{(i)}_{m,n}}{c} \sum_r d_r^{m,n} \sum_{r'} d_{r'}^{m,n} \int_0^1 \frac{(1 - \eta^2)^{1/2}}{(\xi^2 - \eta^2)^{3/2}} \frac{\xi^2 (\xi^2 + 1) + \eta^2 (1 - 3\xi^2)}{(\xi^2 - \eta^2)^{5/2}} \frac{dP^m_n}{d\eta} P^m_{n'} d\eta
\]  

(C.12)

\[
\frac{R^{(i)}_{m,n}}{c} \sum_r d_r^{m,n} \sum_{r'} d_{r'}^{m,n} \int_0^1 \frac{\eta (1 - \eta^2)^{1/2}}{(\xi^2 - \eta^2)^{3/2}} \left[ \lambda_{m,n} - \xi^2 c^2 - \frac{m^2}{(1 - \eta^2)} \right] P^m_n P^m_{n'} d\eta
\]  

(C.13)

\[
\frac{2\xi (\xi^2 - 1)}{c} \frac{dR^{(i)}_{m,n}}{d\xi} \sum_r d_r^{m,n} \sum_{r'} d_{r'}^{m,n} \int_0^1 \frac{\eta (1 - \eta^2)^{1/2}}{(\xi^2 - \eta^2)^{5/2}} \frac{P^m_n P^m_{n'} d\eta}{(\xi^2 - \eta^2)^{3/2}}
\]  

(C.14)

for \(I_2\):

\[
-\frac{m\xi R^{(i)}_{m,n}}{c} \sum_r d_r^{m,n} \sum_{r'} d_{r'}^{m,n} \int_0^1 \frac{1}{(\xi^2 - \eta^2)^{3/2} (1 - \eta^2)^{1/2}} P^m_n P^m_{n'} d\eta
\]  

(C.15)

for \(I_5\):

\[
\frac{m R^{(i)}_{m,n}}{c (\xi^2 - 1)^{1/2}} \sum_r d_r^{m,n} \sum_{r'} d_{r'}^{m,n} \int_0^1 \frac{(1 - \eta^2)^{1/2}}{(\xi^2 - \eta^2)} \frac{dP^m_n}{d\eta} P^m_{n'} d\eta
\]  

(C.16)

\[
\frac{m\xi (\xi^2 - 1)^{1/2}}{c} \frac{dR^{(i)}_{m,n}}{d\xi} \sum_r d_r^{m,n} \sum_{r'} d_{r'}^{m,n} \int_0^1 \frac{1}{(1 - \eta^2)^{1/2} (\xi^2 - \eta^2)} P^m_n P^m_{n'} d\eta
\]  

(C.17)
\[
\frac{im R^{(i)}_{m,n,n'}}{c (\xi^2 - 1)^{1/2}} \sum_r d^m_r \sum_{r'} d^{m'}_{r'} \int_0^1 \frac{1}{(1 - \eta^2)^{1/2}} P_m^m P^n_{n'} d\eta
\]

(C.18)

for \( I^6 \):

\[
(\xi^2 - 1)^{1/2} \xi R^{(i)}_{m,n,n'} \sum_r d^m_r \sum_{r'} d^{m'}_{r'} \int_0^1 \frac{(1 - \eta^2)^{1/2}}{(\xi^2 - \eta^2)^{1/2}} \frac{dP_m^m}{d\eta} P^n_{n'} d\eta
\]

(C.19)

\[
(\xi^2 - 1)^{1/2} \frac{dR^{(i)}_{m,n,n'}}{d\xi} \sum_r d^m_r \sum_{r'} d^{m'}_{r'} \int_0^1 \frac{\eta (1 - \eta^2)^{1/2}}{(\xi^2 - \eta^2)^{1/2}} P_m^m P^n_{n'} d\eta
\]

(C.20)

The above ten integrals involving associated Legendre functions (denoted \( I^p \)) are calculated for each unique combination of \( m, n, n', r, \) and \( r' \), up to selected truncation values for each variable, and the integral values are stored in lookup tables. The line integrals \( (I^l) \) are reconstructed using the stored integral values, \( I^p \), with the expansion coefficients \( d^m_r(c) \) and \( d^{m'}_{r'}(c) \), for both the grain interior \( c = k_t f \) and the vacuum exterior to the grain \( c = k_0 f \) where \( k_t \) is the wavenumber inside the grain, \( k_0 \) is the wavenumber of the vacuum, and \( f \) is the semifocal distance of the spheroidal grain shape. All integrals \( (I^l) \) are evaluated at \( \xi = \xi_0 \). Although there are a large number of integrals, they need only be calculated once, since they have no environment or position dependence. (Terms for line integrals \( I^3, I^4, I^7 \) and \( I^8 \) are not included, as they are the same integrals as \( I^1, I^2, I^5 \) and \( I^6 \) except that they are calculated for the internal field rather than the scattered field, and since the \( I^p \) integrals are independent of the medium, they can be reused without modification.)

Next, we consider the surface integrals in Barton’s method, at the surface defined as \( \xi = \xi_0 \). Based on the boundary conditions at the grain’s surface, as described in Chapter 2 Section 2.6
\[ A_{m,n}^{\eta} = \int_{0}^{2\pi} \int_{-1}^{1} E_{\eta}^{(i)}(c_s, \eta) e^{-im\phi} d\eta d\phi \] (C.21)

\[ A_{m,n}^{\phi} = \int_{0}^{2\pi} \int_{-1}^{1} E_{\phi}^{(i)}(c_s, \eta) e^{-im\phi} d\eta d\phi \] (C.22)

\[ B_{m,n}^{\eta} = \int_{0}^{2\pi} \int_{-1}^{1} H_{\eta}^{(i)}(c_s, \eta) e^{-im\phi} d\eta d\phi \] (C.23)

\[ B_{m,n}^{\phi} = \int_{0}^{2\pi} \int_{-1}^{1} H_{\phi}^{(i)}(c_s, \eta) e^{-im\phi} d\eta d\phi \] (C.24)

where the incident field components are (for the TE mode):

\[ E_{\text{TE}, \eta}^{(i)} = -\eta \frac{(\xi^2 \pm 1)^{1/2}}{\sqrt{(\xi^2 \pm \eta^2)^{1/2}}} \sin \phi e^{ik \cdot r} \] (C.25)

\[ E_{\text{TE}, \phi}^{(i)} = \cos \phi e^{ik \cdot r} \] (C.26)

\[ B_{\text{TE}, \eta}^{(i)} = \left( \frac{\xi (1 - \eta^2)^{1/2}}{\sqrt{(\xi^2 \pm \eta^2)^{1/2}}} \sin \theta_0 + \frac{\eta \xi^2 \pm 1)^{1/2}}{\sqrt{(\xi^2 \pm \eta^2)^{1/2}}} \cos \phi \cos \theta_0 \right) e^{ik \cdot r} \] (C.27)

\[ B_{\text{TE}, \phi}^{(i)} = \sin \phi \cos \theta_0 e^{ik \cdot r} \] (C.28)

where,

\[ k \cdot r = c_s \left[ \left( \xi^2 \pm 1 \right) \left( 1 - \eta^2 \right)^{1/2} \cos \phi \sin \theta_0 + \xi \eta \cos \theta_0 \right]. \] (C.29)

We re-write each of the surface integrals, using Euler’s formula and separating the \( \phi \) terms out for integration first.

\[ A_{m,n; \text{TE}}^{\eta} = -8 (\xi^2 - 1)^{1/2} \int_{0}^{1} \frac{\eta}{\sqrt{(\xi^2 - \eta^2)^{1/2}}} S_{m,n'} f_1 \int_{0}^{\pi/2} \sin \phi f_2 f_3 d\eta d\phi \] (C.30)
\[ A_{m,n;\text{TE}}^\phi = 8 \int_0^1 S_{m,n'} f_1 \int_0^{\pi/2} \cos \phi f_2 f_3 d\eta d\phi \] (C.31)

The integral for \( B_{m,n;\text{TE}}^\eta \) is split into two integrals \( B_{1m,n;\text{TE}}^\eta \) and \( B_{2m,n;\text{TE}}^\eta \):

\[ B_{1m,n;\text{TE}}^\eta = 8 \xi \sin \theta_0 \int_0^1 \frac{(1 - \eta^2)^{1/2}}{\left(\xi^2 - \eta^2\right)^{1/2}} S_{m,n'} f_1 \int_0^{\pi/2} f_2 f_3 d\eta d\phi \] (C.32)

\[ B_{2m,n;\text{TE}}^\eta = 8 \left(\xi^2 - 1\right)^{1/2} \cos \theta_0 \int_0^1 \frac{\eta}{\left(\xi^2 - \eta^2\right)^{1/2}} S_{m,n'} f_1 \int_0^{\pi/2} f_2 f_3 d\eta d\phi \] (C.33)

\[ B_{m,n;\text{TE}}^\phi = 8 \int_0^1 S_{m,n'} f_1 \int_0^{\pi/2} \sin \phi f_2 f_3 d\eta d\phi \] (C.34)

where,

\[ f_1 = \left[ \cos (\beta \eta) + i \sin (\beta \eta) \right] \] (C.35)

\[ f_2 = \left[ \cos (\alpha (1 - \eta^2)^{1/2} \cos \phi) + i \sin (\alpha (1 - \eta^2)^{1/2} \cos \phi) \right] \] (C.36)

\[ f_3 = (\cos m \phi - i \sin m \phi) \] (C.37)

\[ \alpha = c \left(\xi^2 - 1\right)^{1/2} \sin \theta_0 \] (C.38)

\[ \beta = c \xi \cos \theta_0 \] (C.39)

We next use the odd and even nature of \( f_2 \), and \( f_3 \) to evaluate the \( \phi \)-integrals and determine which integrals are non-zero when \( m \) is even or odd. We also use the fact that \( S_{m,n'} \) is even (odd) when \( n' - m \) is even (odd), and the odd and even nature of \( f_1 \) to evaluate the \( \eta \)-integrals, again determining which integrals are non-zero. The following integrals result when these non-zero conditions are applied.
For $A^\eta$, when $m$ is odd and $n' - m$ is even:

$$A_{m,n;\text{TE}}^\eta = -8 \left( \xi^2 - 1 \right)^{1/2} \int_0^{1} \frac{\eta}{(\xi^2 - \eta^2)^{1/2}} S_{m,n'} \sin \beta \eta$$

$$\times \int_0^{\pi/2} \sin \phi \sin m\phi \cos \left[ \alpha (1 - \eta^2)^{1/2} \cos \phi \right] d\eta d\phi \quad (C.40)$$

when $m$ is odd and $n' - m$ is odd:

$$A_{m,n;\text{TE}}^\eta = i8 \left( \xi^2 - 1 \right)^{1/2} \int_0^{1} \frac{\eta}{(\xi^2 - \eta^2)^{1/2}} S_{m,n'} \cos \beta \eta$$

$$\times \int_0^{\pi/2} \sin \phi \sin m\phi \cos \left[ \alpha (1 - \eta^2)^{1/2} \cos \phi \right] d\eta d\phi \quad (C.41)$$

when $m$ is even and $n' - m$ is even:

$$A_{m,n;\text{TE}}^\eta = -i8 \left( \xi^2 - 1 \right)^{1/2} \int_0^{1} \frac{\eta}{(\xi^2 - \eta^2)^{1/2}} S_{m,n'} \sin \beta \eta$$

$$\times \int_0^{\pi/2} \sin \phi \sin m\phi \sin \left[ \alpha (1 - \eta^2)^{1/2} \cos \phi \right] d\eta d\phi \quad (C.42)$$

when $m$ is even and $n' - m$ is odd:

$$A_{m,n;\text{TE}}^\eta = -8 \left( \xi^2 - 1 \right)^{1/2} \int_0^{1} \frac{\eta}{(\xi^2 - \eta^2)^{1/2}} S_{m,n'} \cos \beta \eta$$

$$\times \int_0^{\pi/2} \sin \phi \sin m\phi \sin \left[ \alpha (1 - \eta^2)^{1/2} \cos \phi \right] d\eta d\phi \quad (C.43)$$
For $A^{\phi}$, when $m$ is odd and $n' - m$ is even:

$$A_{m,n;\text{TE}}^{\phi} = 8 \int_{0}^{1} S_{m,n'} \cos \beta \eta \int_{0}^{\pi/2} \cos \phi \cos m \phi \cos [\alpha (1 - \eta^2)^{1/2} \cos \phi] \, d\eta \, d\phi$$  \hspace{1em} \text{(C.44)}

when $m$ is odd and $n' - m$ is odd:

$$A_{m,n;\text{TE}}^{\phi} = 8 \int_{0}^{1} S_{m,n'} \sin \beta \eta \int_{0}^{\pi/2} \cos \phi \cos m \phi \cos [\alpha (1 - \eta^2)^{1/2} \cos \phi] \, d\eta \, d\phi$$  \hspace{1em} \text{(C.45)}

when $m$ is even and $n' - m$ is even:

$$A_{m,n;\text{TE}}^{\phi} = 8 \int_{0}^{1} S_{m,n'} \cos \beta \eta \int_{0}^{\pi/2} \cos \phi \cos m \phi \sin [\alpha (1 - \eta^2)^{1/2} \cos \phi] \, d\eta \, d\phi$$  \hspace{1em} \text{(C.46)}

when $m$ is even and $n' - m$ is odd:

$$A_{m,n;\text{TE}}^{\phi} = -8 \int_{0}^{1} S_{m,n'} \sin \beta \eta \int_{0}^{\pi/2} \cos \phi \cos m \phi \sin [\alpha (1 - \eta^2)^{1/2} \cos \phi] \, d\eta \, d\phi$$  \hspace{1em} \text{(C.47)}

For $B^{\eta}$, when $m$ is odd and $n' - m$ is even:

$$B_{m,n;\text{TE}}^{\eta} = 8 \xi \sin \theta \int_{0}^{1} \frac{(1 - \eta^2)^{1/2}}{(\xi^2 - \eta^2)^{1/2}} S_{m,n'} \cos \beta \eta \int_{0}^{\pi/2} \cos m \phi \sin [\alpha (1 - \eta^2)^{1/2} \cos \phi] \, d\eta \, d\phi$$  \hspace{1em} \text{(C.48)}

when $m$ is odd and $n' - m$ is odd:

$$B_{m,n;\text{TE}}^{\eta} = -8 \xi \sin \theta \int_{0}^{1} \frac{(1 - \eta^2)^{1/2}}{(\xi^2 - \eta^2)^{1/2}} S_{m,n'} \sin \beta \eta \int_{0}^{\pi/2} \cos m \phi \sin [\alpha (1 - \eta^2)^{1/2} \cos \phi] \, d\eta \, d\phi$$  \hspace{1em} \text{(C.49)}
when $m$ is even and $n' - m$ is even:

$$B_{1,m,n;\text{TE}}^\eta = 8\xi \sin \theta_0 \int_0^1 \frac{(1 - \eta^2)^{1/2}}{\eta \sqrt{\xi^2 - \eta^2}} S_{m,n'} \cos \beta \eta \cos m\phi \cos \alpha \sqrt{1 - \eta^2} \cos \phi \, d\eta d\phi$$

when $m$ is even and $n' - m$ is odd:

$$B_{1,m,n;\text{TE}}^\eta = 8\xi \sin \theta_0 \int_0^1 \frac{(1 - \eta^2)^{1/2}}{\eta \sqrt{\xi^2 - \eta^2}} S_{m,n'} \sin \beta \eta \cos m\phi \cos \alpha \sqrt{1 - \eta^2} \cos \phi \, d\eta d\phi$$

when $m$ is odd and $n' - m$ is even:

$$B_{2,m,n;\text{TE}}^\eta = 8\xi \sin \theta_0 \int_0^1 \frac{\eta}{\eta \sqrt{\xi^2 - \eta^2}} S_{m,n'} \cos \beta \eta \times \int_0^{\pi/2} \cos \phi \cos m\phi \cos \alpha \sqrt{1 - \eta^2} \cos \phi \, d\eta d\phi$$

when $m$ is odd and $n' - m$ is odd:

$$B_{2,m,n;\text{TE}}^\eta = 8\xi \int_0^1 \frac{\eta}{\eta \sqrt{\xi^2 - \eta^2}} S_{m,n'} \cos \beta \eta \times \int_0^{\pi/2} \cos \phi \cos m\phi \cos \alpha \sqrt{1 - \eta^2} \cos \phi \, d\eta d\phi$$

when $m$ is even and $n' - m$ is even:

$$B_{2,m,n;\text{TE}}^\eta = -8\xi \sin \theta_0 \int_0^1 \frac{\eta}{\eta \sqrt{\xi^2 - \eta^2}} S_{m,n'} \sin \beta \eta \times \int_0^{\pi/2} \cos \phi \cos m\phi \sin \alpha \sqrt{1 - \eta^2} \cos \phi \, d\eta d\phi$$
when $m$ is even and $n' - m$ is odd:

$$B^\phi_{m,n'; \text{TE}} = 8t \left( \xi^2 - 1 \right)^{1/2} \cos \theta_0 \int_0^1 \frac{\eta}{(\xi^2 - \eta^2)^{1/2}} S_{m,n'} \cos \beta \eta \times \int_0^{\pi/2} \cos \phi \cos m\phi \sin [\alpha (1 - \eta^2)^{1/2} \cos \phi] d\eta d\phi \quad (C.55)$$

For $B^\phi$, when $m$ is odd and $n' - m$ is even:

$$B^\phi_{m,n'; \text{TE}} = -8t \cos \theta_0 \int_0^1 S_{m,n'} \cos \beta \eta \int_0^{\pi/2} \sin \phi \sin m\phi \cos [\alpha (1 - \eta^2)^{1/2} \cos \phi] d\eta d\phi \quad (C.56)$$

when $m$ is odd and $n' - m$ is odd:

$$B^\phi_{m,n'; \text{TE}} = 8 \cos \theta_0 \int_0^1 S_{m,n'} \sin \beta \eta \int_0^{\pi/2} \sin \phi \sin m\phi \cos [\alpha (1 - \eta^2)^{1/2} \cos \phi] d\eta d\phi \quad (C.57)$$

when $m$ is even and $n' - m$ is even:

$$B^\phi_{m,n'; \text{TE}} = 8 \cos \theta_0 \int_0^1 S_{m,n'} \sin \beta \eta \int_0^{\pi/2} \sin \phi \sin m\phi \sin [\alpha (1 - \eta^2)^{1/2} \cos \phi] d\eta d\phi \quad (C.58)$$

when $m$ is even and $n' - m$ is odd:

$$B^\phi_{m,n'; \text{TE}} = 8t \cos \theta_0 \int_0^1 S_{m,n'} \sin \beta \eta \int_0^{\pi/2} \sin \phi \sin m\phi \sin [\alpha (1 - \eta^2)^{1/2} \cos \phi] d\eta d\phi \quad (C.59)$$

In order to efficiently perform the integration over $\phi$, the $\sin [\alpha (1 - \eta^2)^{1/2} \cos \phi]$ and $\cos [\alpha (1 - \eta^2)^{1/2} \cos \phi]$ functions are each expanded in infinite series. (When integrating an expansion series, the contribution from the lower order terms often vanishes, slowing the numerical integration substantially. By considering individual terms in the expansion, we
are able to integrate symbolically on Mathematica, saving considerable time.)

\[
\sin (C \cos \phi) = \sum_{p=0}^{P} \frac{(-1)^p (C \cos \phi)^{2p+1}}{(2p+1)!} = C \cos \phi - \frac{C^3 \cos \phi^3}{3!} + \frac{C^5 \cos \phi^5}{5!} - \cdots \tag{C.60}
\]

\[
\cos (C \cos \phi) = \sum_{p=0}^{P} \frac{(-1)^p (C \cos \phi)^{2p}}{(2p)!} = 1 - \frac{C^2 \cos \phi^2}{2!} + \frac{C^4 \cos \phi^4}{4!} - \cdots \tag{C.61}
\]

where,

\[C = \alpha (1 - \eta^2)^{1/2}. \tag{C.62}\]

The integration over \(\phi\) is performed individually for each integral in the series up to a truncation number that results in the desired level of precision in the summed integral convergence (we used 80), and for each value of \(m\) up to a truncation value (again, we used 80). These individual integral values were calculated using Mathematica programs and stored for later use in reassembling the full surface integrals.

The integration over \(\eta\) is performed as above for the line integrals, by deconstructing the \(S_{m,n}\) function as a sum of the products of it’s expansion coefficients with the related associated Legendre functions, \(P_{m}^{n}(c, \eta)\) (refer to Eqn. (C.10)). Because of the expansion of \(\sin (C \cos \phi)\) and \(\cos (C \cos \phi)\) above, there are additional \(\eta\) integrals for each expansion term. Thus, there are \(\eta\) integrals for each value of \(m\), each value of \(2p + 1\) or \(2p\), and each value of \(r\) (where \(r\) is the summation variable for the expanded \(S_{m,n}\)). These integrals were also calculated using Mathematica code, and the reconstruction of the final integrals was done using original Fortran 77 code.

This approach to the required line and surface integration for Barton’s method may seem a bit daunting at first, due to the large number of integrals being calculated and stored, and then reassembled into the final integral forms. However, the mathematical operations are straight-forward and calculated quickly in Mathematica, and result in good convergence for all integrals. By using this approach, we have been able to avoid numerically calculating...
those integrals whose values approach zero, arrive at highly precise values, and extend Barton's previous application of this method to much more highly absorbing (complex index of refraction) materials with good results, as verified by the PMM results.
Appendix D: Grain Model with Hopping

We began the investigation of a time-varying dipole due to discrete charging events, by trying to understand the charge transport properties of the amorphous, dielectric grain material in the ISM environment. We adopted the hopping formalism of Mott and Davis [56] and Blaise [5] to describe charge transport in the highly amorphous impure grain material. In order to examine the hopping movement of charges within a grain and determine what effect this movement might have on the grain’s electric dipole moment, we developed a model to track charge hopping over time. We simulated a spherical grain with $a = 0.1 \mu m$, exposed it to the charging processes as described in section 3.3 above, and tracked the motion of each charge at each time increment. This was a computationally intensive operation, and we found that simulated time $\sim$ real runtime. Because of this, we were unable to track the charges over anything approaching the length of simulated time used for the four models above. Instead we ran the hopping model for several month-long simulations in order to understand the behavior of the charges and be able to make some simplifying assumptions that would allow for the longer simulation times using the models described in section 3.4.

We also used this model, with the hopping conduction “turned off” to independently verify the dipole flipping timescales $\tau_{\text{flip}}$ and disalignment timescales $\tau_{\text{dis}}$ found with the simulation runs above. Without hopping conduction, charges are positioned at the nearest localization position (deep trap), and this model is comparable to the models with deep traps in section 3.4.

D.1 Localized energy structure of the model

The energy band structure of the model, as discussed in Section 3.4.3, approximates that of a large band gap insulator, with the valence band initially filled with electrons and the conduction band initially empty. In our model, both the conduction and valence bands have band tails of 1 eV width, and an energy state density (density of states) distribution
function can be specified by the user. We selected a distribution function that falls off as the inverse square root of the energy as the bands approach the band gap:

\[ N(E) = C \frac{1}{\sqrt{E}}. \]  

(D.1)

The Fermi level \( E_{F0} \) is located at the end of the conduction band tail, with positive energy levels above and negative energy levels below.

A significant impurity level, as discussed earlier, might be expected in a dust grain; therefore, an impurity band is included in the energy band structure of this model. The impurity band is located in the band gap, the band center \( b = -0.5 \text{ eV} \), and the band shape is modeled with a Gaussian energy state number density (density of states) distribution (bandwidth = 0.8 eV, \( \sigma = 0.2 \text{ eV} \)).

\[ N(E) = \frac{1}{\sigma \sqrt{2\pi}} e^{-(E-b)^2/2\sigma^2}. \]  

(D.2)

The Gaussian distribution was selected as a way to represent the random positioning and orientation of a dominant impurity source, with symmetric energy band tails about the central impurity energy. The impurity band is entirely localized, due to the random positioning of the substitute atoms. Being below \( E_{F0} \), the impurity band is also initially filled with electrons.

As discussed earlier in section 3.4.3, the amorphous nature of the silicate material leads to random reorientations between larger-scale structures while maintaining short-range order [5] [8]. The assumption of short-range order and long-range disorder in the grain silicate, similar to that found in terrestrial amorphous silicates, led to the assignment of a single localization per unit of material. We used this assignment approach for impurity localizations, as well.
D.2 Setting up the model and execution timing

Computationally, a three dimensional array is used to simulate the grain material lattice, and a spherical shape for the grain is “carved” from the cubic array by designating array sites that lie beyond a selected grain radius. Each lattice site within the spherical grain represents the position of a $64.0 \, \text{Å}^3$ ($4.0 \, \text{Å}$ on a side) unit of the olivine material ($\text{Mg}_{2x}\text{Fe}_{2(1-x)}\text{SiO}_4$).

The two types of localized sites, amorphous and impurity, are then created and distributed in the spherical model. The amorphous localization level is set to that of a highly amorphous material, at 10% [5], in accordance with the observed highly broadened absorption lines. Using a density of states energy distribution function as described above, energy states equal in number to 10% of the lattice sites within the spherical model are created and randomly assigned to sites in the spherical array. In the same way, the impurity level is set to that indicated as an upper limit by observation of clouds in the diffuse ISM, at 6% [3] [62]. Using the Gaussian density of states energy distribution function above, energy states equal in number to 6% of total lattice sites within the spherical model are created and randomly distributed in the spherical array (avoiding the amorphous localization sites). The position in the lattice, the energy level, and the occupation status are stored for each of the localized sites and updated as charges are added, removed and moved through the lattice. The position and energy level of each localization site is stored during model set-up.

The distance between a position on the lattice and each lattice position within a selected range, is calculated and stored for use later when determining the probability of charge hopping. Finally, the lattice points that make up the surface of the sphere are identified and their positions are stored in an array used when determining the initial entry point for captured electrons and absorbed photons associated with photoemission. Both of these are stored to promote program efficiency, as they are used each time a charging event occurs during program execution.

The model avoids generating time steps that are based on the repeated short-term hopping of a charge between two localization positions. Such short-term hopping is caused
by the existence of two localizations of similar (or the same) energy level that are located close together. Oscillation between two such sites has almost no effect on the electric dipole moment of the grain, and results in execution inefficiency and is therefore not included in time step determination.

The model is set to execute a user-selected number of loops once the initial model setup is finished. A maximum simulated timestep is set at \( \approx 3 \) orders of magnitude below the time between charging events. After the first loop (which is pre-set to the maximum time step), each loop is a simulated time step whose length is determined by the smallest hopping time (other than short-term hopping) required by charges positioned on localization positions in the lattice. Calculated hopping times range from \( 10^{-10} \) to several \( 10^6 \) years. Computationally, if the smallest hopping time is greater than the maximum time step, then the time step length for that loop is set to the value of the maximum timestep. Because the number and position of electrons and holes is changing often in the grain model, the shortest hopping time must be dynamically determined with each loop. A variable time step length allows for resolution of individual charge movements when hopping occurs, while avoiding endless looping during periods of inactivity.

Variable time steps are integrated until the total simulated time reaches a predetermined target (usually the maximum simulated timestep), at which point the probability of electron capture or FUV photon absorption is determined. The variable time steps are also integrated continuously throughout the execution of the program and stored for use in data reporting. Because of the probabilistic and dynamic nature of time step determination, the total time required to execute all time steps varies with each execution of the program, and a sufficiently large number of steps should be chosen when setting up the program prior to execution. The number of time steps is currently set using 36000 0.1 sec increments, multiplied by a large number of hours (1000). This results in simulated total time of execution of about 75% of set simulated time.
D.3 Charging

When enough simulated time has accumulated, the probability of a charging event due either to FUV photon absorption or electron capture is calculated. (When testing for the probability of a charging event, we use an increment much smaller than the average time expected between events, $\approx 100$ s, and yet not so small as to affect computational efficiency.) One or the other event is possible at each testing increment, and whether a charging event occurs is determined by comparing the product of the simulated time increment, and either the photon absorption rate $J_\gamma$ or the electron capture rate $J_c$ to a randomly selected second number. If the product is greater than or equal to the random number, a charging event occurs.

The charging processes used to investigate charge hopping are the same as those described for the general model (section 3.3), except that the rate of photon absorption and the photoelectric yield are recalculated for each new net charge $Z$ for the grain. We use this approach to test our approximations for photoelectric yield used in Chapter 3 Section 3.3.2. We use the model for photoelectric yield developed by Weingartner and Draine [71], and describe their algorithms below.

The rate at which FUV photons irradiate an uncharged grain ($J_\gamma$) is determined by integrating the radiation energy density per energy interval ($U_E$) between the energy associated with the threshold photon energy for photoemission in silicate material, $h\nu_{pet}$ (8 eV for an uncharged grain), to just below the ionization energy of atomic hydrogen, $h\nu_{max}$ (13.6 eV):

$$J_\gamma = 4\pi a^2 \int_{h\nu_{pet}}^{h\nu_{max}} dE Q_{abs}(E) \frac{cU_E}{hE}. \quad (D.3)$$
For a charged grain \((Z = \text{charge number})\), \(h\nu_{\text{pet}}\) is modified,

\[
h\nu_{\text{pet}}(Z,a) = \begin{cases} 
  IP_V(Z,a) & , Z \geq -1 \\
  IP_V(Z,a) + E_{\text{min}}(Z,a) & , Z < -1 
\end{cases}
\]

where \(IP_V(Z,a)\) is the ionization potential of the grain material,

\[
IP_V(Z,a) = W + \left(Z + \frac{1}{2}\right) \frac{e^2}{a} + (Z + 2) \frac{e^2}{a} \frac{0.3 \text{ Å}}{a}
\]

and \(E_{\text{min}}(Z,a)\) is an estimate of the energy for which tunneling probability is \(10^{-3}\) (W&D, 2001).

\[
E_{\text{min}}(Z < 0,a) = -(Z + 1) \frac{e^2}{a} \left[1 + \left(\frac{27 \text{ Å}}{a}\right)^{0.75}\right]^{-1}.
\]

The absorption efficiency, \((Q_{\text{abs}})\), for the range of energies of interest is \(\simeq 1.2\). The radiation energy per energy interval \((u_E)\) was converted from the radiation energy per frequency interval \((u_\nu)\), using the estimate of the solar neighborhood average interstellar radiation field spectrum by [52] [50]:

\[
u u_\nu^{\text{ISRF}} = \begin{cases} 
  0 & , h\nu > 13.6 \text{ eV} \\
  3.328 \times 10^{-9} \text{ erg cm}^{-3} (h\nu/\text{ eV})^{-4.4172} & , 11.2 \text{ eV} < h\nu < 13.6 \text{ eV} \\
  8.463 \times 10^{-13} \text{ erg cm}^{-3} (h\nu/\text{ eV})^{-1} & , 9.26 \text{ eV} < h\nu < 11.2 \text{ eV} \\
  2.055 \times 10^{-14} \text{ erg cm}^{-3} (h\nu/\text{ eV})^{0.6678} & , 5.04 \text{ eV} < h\nu < 9.26 \text{ eV} \\
  (4\pi\nu/c) \sum_{i=1}^{3} w_i B_\nu(T_i) & , h\nu < 5.04 \text{ eV} ;
\end{cases}
\]
where \( w_i \) is a dilution factor and \( T_i \) is the blackbody temperature.

If photon absorption occurs, whether this absorption results in photoemission or an electron-hole pair is subsequently probabilistically determined, using the calculation for photoelectric yield [71].

\[
Y(h\nu, Z, a) = y_2(h\nu, Z, a) \min[y_0(\Theta)y_1(a, h\nu), 1] \tag{D.8}
\]

where \( y_0(\Theta)y_1(a, h\nu) \) is the yield of those electrons with sufficient energy to escape the grain surface and the image potential if the grain is negatively charged. The \( y_0 \) term is a bulk photoionization yield for silicates with a work function \( W \),

\[
y_0(\Theta) = \frac{0.5(\Theta/W)}{1 + 5(\Theta/W)} \tag{D.9}
\]

\[
\Theta = \begin{cases} 
  h\nu - h\nu_{\text{pet}} + (Z + 1)e^2/a, & Z \geq 0 \\
  h\nu - h\nu_{\text{pet}}, & Z < 0 
\end{cases} \tag{D.10}
\]

which is modified by the size-dependent geometric yield enhancement factor \( y_1(h\nu, a) \),

\[
y_1(h\nu, a) = \left( \frac{\beta}{\alpha} \right)^2 \frac{\alpha^2 - 2\alpha + 2 - 2\exp(-\alpha)}{\beta^2 - 2\beta + 2 - 2\exp(-\beta)} \tag{D.11}
\]

with \( \beta = a/l_a, \alpha = a/l_a + a/l_e \) and \( l_a \) and \( l_e \) are, respectively, the photon attenuation length and the electron mean free path. Photon attenuation length can be determined using the complex refractive index for amorphous olivine \( \text{Im}(m) \) and the FUV wavelength in vacuo,

\[
l_a = \frac{\lambda}{4\pi\text{Im}(m)}. \tag{D.12}
\]

In this model, we have adopted \( l_a = 100 \) Å and \( l_e = 10 \) Å [67].
The effect of a neutral or positively charged grain is described by the $y_2$ factor, so that $y_2 \leq 1$ is the fraction of electrons that escape the grain completely (to infinity),

$$y_2(h\nu, Z, \alpha) = \begin{cases} 
E_{\text{high}}^2 (E_{\text{high}} - 3E_{\text{low}}) / (E_{\text{high}} - E_{\text{low}})^3, & Z \geq 0 \\
1, & Z < 0
\end{cases} \quad \text{(D.13)}$$

**D.4 Initial positioning of the charge**

Captured electrons arrive at the grain surface as described in section 3.3.1, where electron trajectories are based on the electric dipole $p$ and net charge $Z$ of the grain. From the grain surface to the depth of penetration, the electron’s path is assumed to be entirely radial. Absorbed photons are assumed to be normally incident to the grain surface in this model. A point of entry on the grain model surface is randomly selected for the photon. Once an electron or photon arrives on the grain surface, it travels to a depth $d$ within the bulk material based on the probability of transmission at each layer of the material lattice from the surface to the center of the grain ($p_e(d)$ is the probability of transmission for the electron and $p_\gamma(d)$ is the probability for the photon; $d$, the depth, is an integer number of lattice layers, where a lattice layer $\simeq 4.0 \times 10^{-8}$ cm).

$$p_e(d) = e^{-d/l_e} \quad \text{(D.14)}$$

$$p_\gamma(d) = e^{-d/l_\alpha} \quad \text{(D.15)}$$

where $l_e \approx 10 \text{Å}$ is the electron escape length and $l_\alpha \approx 100 \text{Å}$ is the photon absorption length, as discussed earlier. For the electron, the point of termination determines the initial position of that charge. For the photon, the point of absorption determines the initial position of a hole and, in the case where the electron does not escape the grain, the point from which electron repositioning originates. If the point of termination/attenuation is not
a localization position, a random search for an available localization is made, beginning nearest the original point and extending through the entire material, if needed. (The assumption is made that the nearest localization would be the most probable position for an excess charge.) The charge can occupy an empty localization (within the conduction band for electrons, and within the valence and impurity bands for a hole), or recombine with an opposite charge already on a localization.

The distance traveled by an electron that is freed from a photon absorption point is based again on the electron escape length, and the direction of travel within the grain is randomly selected. If the electron lands on a lattice point that is not a localization position, the electron is moved to the nearest localization position.

D.5 Charge movement

After each charging event, the probability that a charge will hop from one localized position to another during that time step is calculated for each charge in the grain. The probabilities drive electrons toward lower energy states within the conduction band (or recombination with holes in the valence and impurity bands), and drive holes toward higher energy states in the valence and impurity bands (or recombination with electrons sitting on localization sites in the conduction band). This was briefly discussed above in reference to the determination of the length of variable time steps, and a more detailed discussion is continued here.

First, the probability per second of a charge making a thermally activated hop between any localization site and those other localization sites within a set distance is calculated for all charges in the grain at that time, and the maximum probability per second (the shortest hopping time) is used to set the variable time step.

Next, for each charge individually, the hopping probability is calculated for each localization site within the specified distance, stored in an array and summed. The summed probability is used to determine whether hopping will occur at all for the charge during the time step, and, if so, the hopping destination is randomly chosen based on the hopping
probabilities for that charge.

When a hop is indicated, a charge is moved to another localization. With the high level of localizations due to both amorphous disorder in the lattice and the random positions of impurities, hopping can (on average) be expected to occur soon after a charge arrives in the grain. We found this expectation to be true in our simulations, with hopping occurring on a time-scale many orders of magnitude less than that for charging events. Within that initial short period the charge can be expected to either hop until it settles into a position at the lowest or highest energy position available depending on whether the charge is an electron or hole, or to recombine with an opposite charge. Occasionally a charge will rapidly hop between two (or rarely, more) localizations of similar probability. During the initial start-up of the model, if it is pre-filled with a small number of charges there is considerable hopping among the pre-fill charges, resulting in much recombination. After the model has run for a period of time (determined by the size, number of pre-fill charges and how the hopping range is set) the model reaches an equilibrium average holding capacity for charge which is maintained for the remainder of execution time.

For those charges not undergoing rapid hopping between two localizations, the probability per second of an electron making a hop to a lower energy state site is \[ p = \nu_{p} e^{-\alpha r} \] (D.16) and the probability of a hole making a hop to a lower energy state, \[ p = \nu_{p} e^{-\alpha r + \frac{\Delta E}{k T}}. \] (D.17) While the probabilities of a hop to a higher energy state are, for an electron, \[ p = \nu_{p} e^{-\alpha r - \frac{\Delta E}{k T}}. \] (D.18)
and the probability of a hole making a hop to a higher energy state,

\[ p = \nu_{ph} e^{-\alpha r}. \]  

(D.19)

In the above equations, \( \nu_{ph} \), the phonon frequency of the material, is set at \( 2.5 \times 10^{13} \text{s}^{-1} \) [7]; and \( \alpha \), the inverse of the electronic wave extension, is set between the values of 0.5 and \( 2.0 \times 10^9 \), [5], (1.5 nm is considered a large extension of the wave function). Having obtained the probability per second, that value is then multiplied by the time step to obtain the hopping probability.

For charges rapidly oscillating between two localization positions, the probability that a charge will be found on the original localization after a long (relatively) period of time (\( p_{osc} \)) is calculated using the time step (\( dt \)) and the probability per second as described above,

\[ p_{osc} = e^{-p_1 dt} \left[ \left( \frac{1}{1 + \frac{p_1}{p_2}} \right) e^{-p_1 dt} + \left( \frac{1}{1 + \frac{p_2}{p_1}} \right) e^{-p_2 dt} \right] \]  

(D.20)

where \( p_1 \) is the probability per second of being in the original localization position, and \( p_2 \) is the probability per second of being in the second localization position, both calculated for a non-oscillating charge. This formula was empirically determined by simulation, testing against expected outcomes.

We calculated the hopping probability due to the electrostatic potential between the hopping charge and other near charges (within a selected range), for each possible site the charge could hop to, to determine whether it would have a significant effect relative to the hopping probabilities calculated above. The electrostatic potential probability factor is,

\[ P_U = e^{-\Delta U e/kT_y} \]  

(D.21)

where potentials due to any charges at sites within a range of a possible hopping site are
summed for both the initial position and the possible final position,

\[ \Delta U = \sum_{\text{final}} \frac{e}{r} - \sum_{\text{initial}} \frac{e}{r}. \]  \hspace{1cm} (D.22)

### D.6 Findings

We found that after a charging event, in most cases an injected charge very quickly hopped to a nearby deep trap or recombined with a nearby opposite charge. Even when multiple hops were required, on average all charge motion was completed on a timescale \( \sim 10^{-4} \) to \( 10^{-8} \) s, orders of magnitude smaller than the average charging timescale \( \sim 100 \) s. The high density of traps associated with the highly amorphous and highly impure material, in most cases allowed the extension of the localized electron wavefunction to overlap many traps, providing a path to the deep traps. This resulted in charges tending to occupy the deep traps very soon after appearing at the grain surface, and provided the basis of our approximations for the placement of charges in deep traps for Models 3 and 4 in Chapter 3 Section 3.4.

There was no significant variation of the charge distribution caused by rapid oscillation of a charge between two traps with the same potential. Simulations showed that when this occurred, the charge oscillated between traps that were located very closely together. This appears to be an effect of the range of the localized wavefunction. If the extension of the wavefunction in the actual grain material falls within the range for disordered dielectrics described by Blaise [5], we are justified in neglecting this level of detail for charge movement in our simulations.

In early testing where we included the electrostatic potential factor, we observed no significant change in the distribution of charge in the grain, when compared to simulation runs without the electrostatic factor. Based on this finding, the electrostatic potential factor can be neglected for grain conduction.

We found that when hopping was “turned off” in this model, and the simulation was
run for $10^5$ yr, for the six rotation rates $\omega/\omega_T$, the dipole flipping timescales $\tau_{\text{flip}}$ and disalignment timescales $\tau_{\text{dis}}$ were of the same order of magnitude as those found using the deep trap models of section 3.4 above. These results justify the approximation made in placing charge on the grain surface $r = a$ for Model 1 (perfectly insulating), rather than placing it within the grain volume as was done in the hopping model, it also justifies our neglect of detailed hopping in Models 3 and 4 (models with deep traps). The results also justify our approximations of photoelectric yield, in as much as the model in [71] is accurate.

The extension of the charge wavefunction, the density of traps, the distribution functions describing the energy bandtails and the nature of the impurity band presented here are estimations made in order to approximate conduction for actual grain material. The investigation of conduction in disordered dielectric materials has not, at this point, covered the very low temperatures of the actual grain material (15 K) and the very low rate of charge injection ($\sim 1$ charge per 100 s) the grain experiences. Laboratory investigation of grain-like silicates in a low temperature, low charge-rate environment may prove that these conduction mechanisms behave differently or are dominated by other means of conduction in the actual environment.
Appendix E: Collisional Charging for a Drifting Grain

A grain drifts at a velocity $v_{gr}$ with respect to the surrounding gas. The grain rotates uniformly about the principal axis of greatest moment of inertia $\hat{a}_1$, which is inclined at an angle $\theta_{Jv}$ with respect to $v_{gr}$.

In order to describe the position and velocity of a colliding gas-phase charged particle, a large sphere is projected around the grain, with radius equal to $r_{big}$ and origin at the grain’s center of mass. A charged particle approaching the grain has a velocity $v$ components in spherical coordinates $(v, \theta_{in}, \phi_{in})$ where the polar axis for spherical coordinates is parallel to $v_{gr}$. The Maxwell speed distribution describes the expected particle velocity magnitude

$$P(v) = 4\pi \left( \frac{m}{2\pi kT_{gas}} \right)^{3/2} v^2 \exp \left( -\frac{mv^2}{2kT_{gas}} \right)$$  \hspace{1cm} (E.1)

and the rate at which particles with speeds between $v$ and $v + dv$, enter the projected sphere from within a solid angle $d\cos\theta_{in}d\phi_{in}$, where the solid angle is centered about $(\theta_{in}, \phi_{in})$, is

$$dR = \pi r_{big}^2 n \frac{1}{4\pi} d\cos\theta_{in}d\phi_{in}P(v)dv|v - v_{gr}|$$  \hspace{1cm} (E.2)

where $n$ is the number density of charged particles. By replacing $v$ with the dimensionless quantity $u = v/v_{th}$, where the thermal velocity is

$$v_{th} = \sqrt{\frac{2kT}{m}}$$  \hspace{1cm} (E.3)

and integrating over $\phi_{in}$, the incremental rate $dR$ becomes

$$dR = \pi r_{big}^2 ne \left( \frac{8kT}{\pi m} \right)^{1/2} d\tilde{R}$$  \hspace{1cm} (E.4)
where, the reduced rate increment, \( d\tilde{R} \), is

\[
d\tilde{R} = du \, d\cos \theta_{\text{in}} u_{1} e^{-u^{2}}.
\]  

(E.5)

The term \( u_{1} \) is the particle’s dimensionless speed in the rest frame of the grain

\[
u_{1} = \sqrt{u^{2} + u_{\text{gr}}^{2} + 2nu_{\text{gr}} \cos \theta_{\text{in}}}; \quad u_{\text{gr}} = v_{\text{gr}}/v_{\text{th}}.
\]  

(E.6)

Integrating the reduced rate increment over the entire sphere

\[
\tilde{R} = -\int_{0}^{\infty} du \, u^{2} e^{-u^{2}} \int_{-1}^{1} \sqrt{u^{2} + u_{\text{gr}}^{2} + 2nu_{\text{gr}} \cos \theta_{\text{in}}} d\cos \theta_{\text{in}}
\]

\[
= 1 + \frac{u_{\text{gr}}^{2}}{3} - \frac{u_{\text{gr}}^{4}}{3} \int_{0}^{1} dx \, e^{-u_{\text{gr}}^{2} x} (1 - \sqrt{x})^{3}.
\]  

(E.7)

(E.8)

The particle arrival angle with respect to the grain’s rest frame, \( \theta_{1} \), is described by the relation

\[
\cos \theta_{1} = \frac{u \cos \theta_{\text{in}} + u_{\text{gr}}}{u_{1}}.
\]  

(E.9)

When the grain’s drifting velocity relative to the gas \( v_{\perp} = 1\text{km s}^{-1} \) and the temperature of the gas is \( T_{\text{gas}} = 100 \text{ K} \), then \( u_{\text{gr}} = 0.0182 \) for electrons and \( u_{\text{gr}} = 0.778 \) for protons.

For each of these cases of \( u_{\text{gr}} \), we calculate \( u_{1} \) and \( d\tilde{R} \) using \( 10^{10} \) values for \((u, \theta_{\text{in}})\). For each of the \( 10^{5} \) values of \( u \) up to a maximum value of 4, \( 10^{5} \) values of \( \theta_{\text{in}} \) are generated, evenly distributed in probability, as described in text around equation 3.108, Section 3.3.1.

These results are used to construct probability distributions for \( u_{1} \) and for \( \cos \theta_{1} \). For \( u_{1} \), a probability \( P(u_{1}) \) that an incoming particle will have dimensionless speed \( \leq u_{1} \) is constructed, with 100 bins in \( u_{1} \). For each value of \( u_{1} \), a cumulative probability \( P(\cos \theta_{1}) \) is constructed, again with 100 bins, this time in \( \cos \theta_{1} \). Note that the minimum possible
value of $\cos \theta$ is -1 when $u > u_{gr}$ and $[1 - (u/u_{gr})^2]$ when $u < u_{gr}$.

We set the length of the time-step for our simulations to be 10 times smaller than the inverse of the rate electrons enter our large sphere (equations E.4 and E.8) to ensure good resolution for our collision events and because the electron rate is higher than the proton rate. We randomly and independently determine whether either charged particle (electron or proton) enters the large sphere, at each time-step. If so, the velocity of the incoming particle is set in the rest frame of the grain. First a value of $u_1$ is chosen randomly for the particle, then a value for $\cos \theta_1$ is randomly chosen from the distribution for $u_1$. The final component of velocity $\phi_1$, is selected, again randomly, from a uniform distribution in $0$ to $2\pi$. The impact parameter $b$ and the azimuthal angle $\alpha$ (refer to Figure 3.3.1 in Section 3.3.1) need to set for $r = r_{big}$; both are randomly selected from uniform distributions, with $b$ being chosen from a distribution in $b^2$.

We have described the incoming particle’s position and velocity in a spherical coordinate system at rest with respect to the grain, and with the polar axis along the grain’s velocity with relative to the gas, $v_{gr}$ (“$v_{gr}$ coordinates”). The velocity and position can be transformed into a Cartesian version of these coordinates, with the Cartesian axes denoted by $\hat{x}_v$, $\hat{y}_v$ and $\hat{z}_v$

$$v_1 = -v_{th}u_1 (\sin \theta_1 \cos \phi_1 \hat{x}_v + \sin \theta_1 \sin \phi_1 \hat{y}_v + \cos \theta_1 \hat{z}_v) \quad \text{(E.10)}$$

$$x_v = b \cos \alpha_1 \cos \theta_1 \cos \phi_1 - b \sin \alpha_1 \sin \phi_1 + z_{arr} \sin \theta_1 \cos \phi_1 \quad \text{(E.11)}$$

$$y_v = b \cos \alpha_1 \cos \theta_1 \sin \phi_1 - b \sin \alpha_1 \cos \phi_1 + z_{arr} \sin \theta_1 \sin \phi_1 \quad \text{(E.12)}$$

$$z_v = -b \cos \alpha_1 \sin \theta_1 + z_{arr} \cos \theta_1 \quad \text{(E.13)}$$

with $z_{arr} = \left(\frac{r_{big}^2 - b^2}{2}\right)^{1/2}$. 
Now, we define a set of Cartesian axes where the \( \hat{z} \) axis is aligned with \( \hat{a}_1 \) in the grain:

\[
\hat{z}_J = \hat{a}_1 = \hat{z}_v \cos \theta_{Jv} + \hat{x}_v \sin \theta_{Jv} \tag{E.14}
\]

\[
\hat{x}_J = (\hat{x}_v \cos \theta_{Jv} - \hat{z}_v \sin \theta_{Jv}) \cos \lambda + \hat{y}_v \sin \lambda \tag{E.15}
\]

\[
\hat{y}_J = \hat{y}_v \cos \lambda - (\hat{x}_v \cos \theta_{Jv} - \hat{z}_v \sin \theta_{Jv}) \sin \lambda \tag{E.16}
\]

with \( \lambda \) as the phase angle of the grain’s rotation. The phase angle is selected randomly. (We neglect the rotation of the grain during the approach of the particle.) Another set of Cartesian axes are defined, with the electric dipole \( \mathbf{p} \) as the polar axis this time (“\( \mathbf{p} \)-coordinates”):

\[
\hat{z}_p = \hat{p} = \hat{x}_J \sin \theta_{pJ} \cos \phi_{pJ} + \hat{y}_J \sin \theta_{pJ} \sin \phi_{pJ} + \hat{z}_J \cos \theta_{pJ} \tag{E.17}
\]

\[
\hat{x}_p = \hat{x}_J \cos \theta_{pJ} \cos \phi_{pJ} + \hat{y}_J \cos \theta_{pJ} \sin \phi_{pJ} - \hat{z}_J \sin \theta_{pJ} \tag{E.18}
\]

\[
\hat{y}_p = -\hat{x}_J \sin \phi_{pJ} + \hat{y}_J \cos \phi_{pJ} \tag{E.19}
\]

We use equations E.14 through E.19 to create dot products that we use to transform the position and velocity expression in “\( \mathbf{v}_{gr} \)-coordinates” to “\( \mathbf{p} \)-coordinates” (employing trigonometric identities to simplify the final forms):

\[
\hat{x}_p \cdot \hat{x}_v = \cos \theta_{pJ} \cos \theta_{Jv} \cos (\phi_{pJ} + \lambda) - \sin \theta_{pJ} \sin \theta_{Jv} \tag{E.20}
\]

\[
\hat{x}_p \cdot \hat{y}_v = \cos \theta_{pJ} \sin (\phi_{pJ} + \lambda) \tag{E.21}
\]

\[
\hat{x}_p \cdot \hat{z}_v = -\cos \theta_{pJ} \sin \theta_{Jv} \cos (\phi_{pJ} + \lambda) - \sin \theta_{pJ} \cos \theta_{Jv} \tag{E.22}
\]

\[
\hat{y}_p \cdot \hat{x}_v = -\cos \theta_{Jv} \sin (\phi_{pJ} + \lambda) \tag{E.23}
\]

\[
\hat{y}_p \cdot \hat{y}_v = \cos (\phi_{pJ} + \lambda) \tag{E.24}
\]
\[ \hat{y}_p \cdot \hat{z}_v = \sin \theta_J \sin (\phi_{pJ} + \lambda) \] (E.25)

\[ \hat{z}_p \cdot \hat{y}_v = \sin \theta_{pJ} \sin (\phi_{pJ} + \lambda) \] (E.26)

\[ \hat{z}_p \cdot \hat{z}_v = - \sin \theta_{pJ} \sin \theta_J \cos (\phi_{pJ} + \lambda) + \cos \theta_{pJ} \cos \theta_J \] (E.27)

Finally, the Cartesian “\(p\)-coordinates” of the incoming particle’s position and velocity are used in the following geometric relations the components of position and velocity in spherical coordinates:

\[ r = r_{\text{big}} \] (E.28)

\[ \theta = \arccos \left( \frac{z_p}{r} \right) \] (E.29)

\[ \phi = 2 \arctan \left( \frac{r_{p0} - x_p}{y_p} \right) \] (E.30)

\[ \frac{dr}{dt} = \frac{1}{r} \left( x_p \frac{dx_p}{dt} + y_p \frac{dy_p}{dt} + z_p \frac{dz_p}{dt} \right) \] (E.31)

\[ \frac{d\theta}{dt} = - \frac{1}{rr_{p0}} \left( r \frac{dz_p}{dt} - z_p \frac{dr}{dt} \right) \] (E.32)

\[ \frac{d\phi}{dt} = - \frac{1}{r_{p0}^2} \left( x_p \frac{dy_p}{dt} - y_p \frac{dx_p}{dt} \right) \] (E.33)

where \( r_{p0} = (x_p^2 + y_p^2)^{1/2} \). The critical impact parameter \( b_{\text{crit}} \) is dependent on the speed of the incoming particle \( v_1 = v_{1h} u_1 \) and \( \cos \theta_0 = -v_1^{-1} \frac{dz_p}{dt} \) Eqns. (3.69 and 3.70). If \( b \leq b_{\text{crit}} \), the equations of motion Eqns. (3.36 to 3.40), are integrated to determine where the particle hits the grain surface.

We tried various values of \( r_{\text{big}} \), and while the larger values yield higher accuracy, they also require smaller time-steps. We found that \( r_{\text{big}} = 50a \) provided a high level of accuracy while still requiring a reasonable amount of time to calculate.

We substituted the procedures described here into simulations using our model of the
perfectly insulated grain \((a = 0.1 \mu m)\), and looked at the effects for both electrons and protons. After a simulated runtime of 100 yr, we found that \(|p_z|_{\text{avg}}/ea \approx 2.5\) and \(\tau_{\text{flip}}\) ranged from \(5.8 \times 10^{-4}\) to \(6.0 \times 10^{-4}\) as \(\cos \theta_0\) ranged from 0 to 1. These results are very similar to results we obtained for collisional charging when gas-grain drift was ignored, and where we ignored the effect of proton collision with the grain as shown in Table 3.1. Due to the precession of the grain angular momentum vector \(\mathbf{J}\) about the Galactic magnetic field \(\mathbf{B}\), the time-scale for changes to \(\theta_{Jv}\) are short compared to the 100 yr simulation period (but an order of magnitude longer than the time-scale for dipole flipping \(\tau_{\text{flip}}\)). Even with this short time-scale, we show that the electric dipole moment is insensitive to \(\theta_{Jv}\). Therefore, we believe that we are justified in neglecting gas-grain drift in our calculation of incoming electron trajectories, as this introduces no significant error to those calculations.
Bibliography
Bibliography


Margaret E. Jordan graduated from the University of California at Irvine in 1987, with a Bachelors of Science in physics. Following graduation, she was employed as a systems engineer in the aerospace industry. Altogether she has more than eighteen years of professional experience in this field. Four years of her professional career were spent providing systems engineering and system test support for satellite ground system software, as well as software systems reliability analysis and software mission support. In addition, Ms. Jordan has eleven years of space hardware systems engineering, which includes low Earth orbit telecommunications support, commercial and civil space strategic planning, space systems engineering, commercial space system cost modeling and technical feasibility analysis, mission analysis and planning, commercial space business development, and microgravity materials processing experimental design and integration. The remaining 3 years of her professional career were spent providing supervision of space qualified military satellite (MILSTAR) hardware production.

Ms. Jordan returned to school in 2002, initially in graduate-level Extended Studies classes at George Mason University, then in a graduate degree program at the same university. She received a M.S. degree in Applied Physics and Engineering from GMU in 2009. Her research has focused on physics of the interstellar medium (ISM), specifically, interstellar dust grain alignment. During this research, she has created detailed three dimensional models in Fortran, designed to simulate processes occurring over 10,000 years. This work has resulted in joint publication, with her adviser Prof. Joseph Weingartner, of two professional papers and a poster presentation at the January 2010 American Astronomical Society conference in Washington, DC.

**Publications**

