Electric dipole moments and disalignment of interstellar dust grains

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ABSTRACT

The degree to which interstellar grains align with respect to the interstellar magnetic field depends on disaligning as well as aligning mechanisms. For decades, it was assumed that disalignment was due primarily to the random angular impulses a grain receives when colliding with gas-phase atoms. Recently, a new disalignment mechanism has been considered, which may be very potent for a grain that has a time-varying electric dipole moment and drifts across the magnetic field. We provide quantitative estimates of the disalignment times for silicate grains with size $>\sim 0.1 \mu m$. These appear to be shorter than the time-scale for alignment by radiative torques, unless the grains contain superparamagnetic inclusions.

Key words: dust, extinction – ISM: magnetic fields

1 INTRODUCTION

Observations of starlight polarization have revealed that some interstellar dust grains are non-spherical and aligned. The degree of alignment, and hence the polarization, depends on both aligning processes (e.g., radiative torques and paramagnetic dissipation) and disaligning processes (e.g., random torques arising from collisions with gas atoms). See Whittet (2004) for a review of polarization observations and Lazarian (2003), Roberge (2004), and Lazarian (2007) for reviews of alignment theory.

Recently, Weingartner (2006, hereafter W06) proposed an alternative disalignment mechanism for a grain that has a time-varying electric dipole moment $p$ and drifts across the interstellar magnetic field. The potency of this mechanism is sensitive to the magnitude and time-scale of fluctuations in $p$. W06 considered highly simplified models for the fluctuating dipole moment and associated disalignment in §2 and present results in §3 and conclusions in §6.

2 DISALIGNMENT ASSOCIATED WITH TIME-VARYING ELECTRIC DIPOLE MOMENTS

When a gas atom collides with a grain, it imparts an angular impulse to the grain. If no other mechanisms excite rotation, then the energy in rotation about any axis is $\sim \frac{1}{2} k_B T_{\text{gas}}$, where $k_B$ is Boltzmann’s constant and $T_{\text{gas}}$ is the gas temperature. Such motion is called ‘thermal rotation’. The thermal rotation rate for a sphere with radius $a$ is given by

$$\omega_T = \left( \frac{15k_B T_{\text{gas}}}{8\pi \rho a^3} \right)^{1/2}$$

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

where $\rho$ is the density of the grain material. In general, grains are subjected to additional torques that may drive them to suprathermal rotation, with angular speed $\omega > \omega_T$ (Purcell 1975, 1979; Draine & Lazarian 1998). For thermally rotating grains, the random collisional impulses constitute an important disalignment mechanism.

A spinning grain with non-zero electric charge acquires a magnetic dipole moment $\mu \parallel \omega$ (Martin 1971). Dolginov...
Mytrophanov (1976) showed that the Barnett effect (i.e., the tendency for a spinning paramagnetic solid to acquire a magnetization parallel or anti-parallel to ω) can provide a much larger moment. Specifically, the Barnett magnetic moment $\mathbf{\mu}_{\text{B}} = \chi_0 V/\gamma_g$, where $\chi_0$ is the static magnetic susceptibility, $\gamma_g$ is the gyromagnetic ratio of the microscopic magnetic dipoles that are responsible for the grain’s paramagnetism, and $V$ is the grain volume. The susceptibility depends on the number density of paramagnetic ions or nuclei in the grain material and is thus rather uncertain. We will adopt $\chi_0 \sim 5 \times 10^{-3} (T_\gamma/15 \text{ K})^{-1}$, where $T_\gamma$ is the grain temperature (Draine 1996; W06). With this estimate, the Barnett magnetic moment for silicate grains is

$$\mathbf{\mu}_{\text{B}}(\text{sil}) \approx 1.2 \times 10^{-19} \left(\frac{T_\gamma}{15 \text{ K}}\right)^{-1} \left(\frac{a}{0.1 \mu\text{m}}\right)^3 \times \left(\frac{\omega}{10^3 \text{ s}^{-1}}\right) \text{ statC cm.} \quad (2)$$

Suppose $\mu$ is parallel or anti-parallel to the grain’s angular momentum vector $\mathbf{J}$: $\mu = \mu_{\parallel} \hat{\mathbf{J}}$. The magnetic torque $\Gamma_\mu = \mu \times \mathbf{B}$ causes $\mathbf{J}$ to precess about the interstellar magnetic field $\mathbf{B}$ at rate

$$\Omega_{\text{q}} = \frac{|\mu| B}{J} \approx 314 \left(\frac{|\mu|}{10^{-19} \text{ statC cm}}\right) \left(\frac{\rho}{3 \text{ g cm}^{-3}}\right)^{-1} \times \left(\frac{B}{5 \mu\text{C}}\right)^{-5} \left(\frac{\rho}{0.1 \mu\text{m}}\right)^{\frac{1}{3}} \left(\frac{\omega}{10^3 \text{ s}^{-1}}\right)^{\frac{1}{3}} \text{ yr}^{-1}. \quad (3)$$

Since $\mu \propto \omega$, $\Omega_{\text{q}}$ is independent of $\omega$. The combination of an aligning torque (e.g., the radiative torque) and the magnetic torque drives the grain towards rapid precession with a constant precession angle $\theta_{\text{align}}$ (i.e., $\theta_{\text{align}}$ is the angle between $\mathbf{B}$ and $\mathbf{J}$). A large ensemble of grains will be characterized by a uniform distribution in precession phase. As a result, the observed starlight polarization is either parallel or anti-parallel to $\mathbf{J}$. (If $\theta_{\text{align}} = 0$ and $\mathbf{J} \parallel \hat{\mathbf{a}}_1$, the grain principal axis of greatest moment of inertia, then the polarization $\parallel \mathbf{B}$.) Note that alignment of the grain body with respect to $\mathbf{J}$ is also a necessary condition for polarization.

If a grain has an electric dipole moment $\mathbf{p}$ and drifts with velocity $\mathbf{v}$ across $\mathbf{B}$, then it experiences a torque $\Gamma_p = \mathbf{p} \times (\mathbf{v} \times \mathbf{B})/c$ in addition to the magnetic torque ($c$ is the speed of light). If $\mathbf{p} = p_J \hat{\mathbf{J}}$, then the grain precesses about an axis tilted at angle $\delta = \tan^{-1} |T|$ relative to $\mathbf{B}$ and the precession rate is increased by the factor $(1 + \gamma^2)^{1/2}$, where

$$\gamma \equiv \frac{p_J \omega_{\perp}}{\mu_{\parallel} c}, \quad (4)$$

with $v_{\perp}$ the component of $\mathbf{v}$ transverse to $\mathbf{B}$ (W06).

If $\mu$ and $\mathbf{p}$ are not parallel or anti-parallel to $\mathbf{J}$, then the magnetic and electric torques must be averaged over the extremely rapid grain rotation. The resulting dynamics is identical to that for $\mathbf{J}$, $\mu$, and $\mathbf{p}$ all lie along $\hat{\mathbf{a}}_1$, except with the following substitutions in equation (4):

$$\mu_{\parallel} = \frac{\mu}{\omega}, \quad (5)$$

$$p_J = \pm (p \cdot \hat{\mathbf{a}}_1) f_i(q), \quad (6)$$

with $f_i$ the moment of inertia along $\hat{\mathbf{a}}_i$ (W06). Both $\mu_{\parallel}$ and $p_J$ depend on the grain’s rotational state through the parameter $q \equiv 2I_{\parallel} E/J^2$ ($E$ is the rotational energy). In equation (6), the $+$ ($-$) sign is selected when $\mathbf{J} \cdot \hat{\mathbf{a}}_i > 0 \,(< 0)$ and the factor $f_i(q)$ is given in eq. 9 of W06. (The choice of $i$ is also discussed following eq. 9 in W06.) If the Barnett effect is responsible for the magnetic dipole moment, then $(\mu/\omega) = \chi_0 V/\gamma_g$.

If $\Gamma$ is constant in time, then the only consequence of the electric dipole is to tilt the precession axis relative to the magnetic field direction. However, $\Gamma$ can vary on relatively short time-scales. W06 discussed two sources of variation: 1. Upon each discrete charging event (e.g., the capture of an electron from the gas or photoelectric emission of an electron), $p_J$ changes. 2. When the grain’s rotational state ($q$ and/or flip state) varies, $p_J/\mu_{\parallel}$ varies (eqs. (5) and (6)).

Two processes can yield rapid variations in the grain rotational state: 1. Thermal fluctuations, in which energy is exchanged between grain rotation and vibrational modes (Lazarian 1994; Lazarian & Roberge 1997; Lazarian & Draine 1997, 1999a, 1999b; Weingartner 2009). 2. Collisions with gas-phase atoms, which can stick to, reflect from, or evaporate from the surface, perhaps after forming a molecule (Hoang & Lazarian 2009). The efficacy of both of these mechanisms drops off dramatically as the grain rotation becomes suprathermal.

In this paper, we will only consider variations in $p_J$ associated with discrete charging events. We will also assume $q = 1$ in equation (5) and $f_i(q) = 1$ in equation (6), which are good approximations for suprathermally rotating grains. Thus, the analysis presented here is not complete for thermally rotating grains.

Since the charging processes are stochastic processes, $\Gamma$ varies stochastically, yielding random variations in the precession axis. Each time the precession axis changes direction, the precession angle changes. When these events occur at random precession phases, $\theta_{\text{align}}$ varies stochastically. In other words, the grain experiences disalignment.

W06 considered a simple scenario in which $\Gamma$ has constant magnitude but stochastically reverses sign, on time-scale $\tau_{\text{flip}}$, finding the following approximations for the disalignment time-scale when $\tau_{\text{flip}}$ is short or long compared with the precession time-scale:

$$\tau_{\text{dis}} \sim \frac{1}{\Gamma_{\parallel}} \left(\frac{|\Omega_0|}{\tau_{\text{flip}}}\right)^{1/2}, \quad \text{if} \quad \tau_{\text{flip}} \ll |\Omega_0|^{-1}(1 + \gamma^2)^{-1/2} \quad (7)$$

$$\tau_{\text{dis}} \sim (1 + \gamma^2)^{1/2} \tau_{\text{flip}}, \quad \text{if} \quad \tau_{\text{flip}} \gg |\Omega_0|^{-1}(1 + \gamma^2)^{-1/2}. \quad (8)$$

In the following section, we will consider more detailed models for the fluctuating electric dipole moment.

### 3 Grain Charging Models

A grain charging model that follows the evolution of the electric dipole moment $\mathbf{p}$ must treat both the processes that deliver charge to the grain and those that transport charge within the grain. In the cold, neutral, interstellar medium, the dominant charge delivery mechanisms are starlight-induced photoelectric emission and sticking collisions of gas-phase electrons.


3.1 Idealizations for Charge Transport Within a Grain

Bulk, neutral silicates are good insulators, with a full valence band and empty conduction band. Observations of the 9.7 \( \mu m \) band profile indicate that interstellar silicates are predominantly amorphous (Li & Draine 2001; Kemper, Vriend, & Tielens 2004; Li, Zhao, & Li 2007). In amorphous materials, localized energy states (‘traps’) appear in the tails of the conduction and valence bands. For any realistic interstellar grain, there are also localized states associated with impurity atoms. Electrons and holes can hop from site to site with assistance from a phonon (e.g., Mott & Davis 1971; Blaise 2001), so no grain is perfectly insulating.

The rate at which an electron hops from site \( i \) to site \( j \) is typically approximated as

\[ R_{\text{hop}} = v_{\text{ph}} \exp(-2r_{ij}/d_0) \exp(-W_{i\rightarrow j}/k_b T_\text{d}) \]

(Ambegaokar et al. 1971; Mady et al. 2007), where \( v_{\text{ph}} \sim 10^{15} \text{ s}^{-1} \) is the phonon frequency (Brucato et al. 2002), \( r_{ij} \) is the distance between sites \( i \) and \( j \), \( d_0 \) is the electron localization length, \( W_{i\rightarrow j} = \max[E_j - E_i, 0] \), \( E_i \) is the electron energy when localized at site \( i \), and \( T_\text{d} \) is the dust temperature.

A completely rigorous treatment of the grain electric dipole moment would include the charges as they hop among traps. However, this approach is not feasible. First, the quantities appearing in equation (9), namely \( d_0 \) and the trap energy distribution, are poorly known. Second, even for tight binding at traps (e.g., Mott & Davis 1971; Blaise 2001), so no grain is perfectly insulating.

The trajectories of charged particles in the vicinity of a grain with non-vanishing electric dipole moment \( p \) differ from those for the \( p = 0 \) case. The distribution of arrival sites on the grain surface is such as to reduce \( p = |p| \). Except for model (2) in \[\text{(3)}\], this effect is critical for limiting \( p \). However, it is extremely difficult to treat for non-spherical grain shapes. Thus, we will always treat the grain as a sphere when computing collisional charging rates and the arrival sites of colliding particles. For further simplification in these calculations, we also neglect the motion of the grain with respect to the gas. Even though the grain’s speed is assumed to be roughly the sound speed of the gas, the speed of the light electrons is greater by a factor \( \approx (m_p/m_e)^{1/2} \) (\( m_p \) and \( m_e \) are the proton and electron mass, respectively). Thus, we do not expect this assumption to introduce serious error for electron collisional charging. In addition, we neglect ion collisional charging, which is dominated by photoelectric emission. These simplifications are justified in Appendix A.

For a grain at rest with respect to the gas, the collisional charging rate is given by

\[ R = \frac{\pi a^2 n s (8k_b T_\text{gas})^{1/2}}{\pi m} \hat{R} \]

where \( n \) is the number density of the colliding particles, \( s \) is the sticking coefficient (i.e., the probability that the particle sticks to the grain upon collision), \( m \) is the mass of colliding particle, and \( \hat{R} \) accounts for deviations of the collision cross section from the geometric cross section. For the relatively large grains under consideration here, we adopt \( s \approx 1/2 \) (Weingartner & Draine 2001, hereafter WD01). Draine & Sutin (1987) provided expressions for \( \hat{R} \) for a charged, conducting sphere, including the polarization of the grain by the charged gas-phase particle. The effect of polarization decreases with grain size (as long as \( T_\text{gas} \) does not approach zero), and can be reasonably neglected when \( a > 0.1 \mu m \).

Consider a spherical grain with radius \( a \) centered at the origin. Approximate the charge distribution within the grain as a point charge \( Q \) and point dipole \( p \hat{r} \) \((p > 0)\) located at the origin. In spherical coordinates \((r, \theta, \phi)\), the electric force on a point charge \( q \) is

\[ F = \frac{Qq}{r^2} \hat{r} + \frac{2p}{r^3} (2 \cos \theta \hat{r} + \sin \theta \hat{\theta}) \]

and the potential is

\[ U = \frac{Qq}{r} + \frac{qp \cos \theta}{r^2}. \]
The equations of motion are

\begin{align}
  m\ddot{r} &= mr^2 \dot{\theta}^2 + mr \sin^2 \theta \dot{\phi}^2 + \frac{Qq}{r^2} - \frac{2q p \cos \theta}{r^3} \\
  m\ddot{\theta} &= -2m r \dot{\theta} + mr \sin \theta \cos \theta \dot{\phi}^2 + \frac{q p \sin \theta}{r^3} \\
  m r \sin \theta \ddot{\phi} &= -2mr \sin \theta \dot{\phi} + 2m r \cos \theta \dot{\theta} \dot{\phi}
\end{align}

(13)  (14)  (15)

where dots denote differentiation with respect to time and \( m \) is the mass of the point charge \( q \).

Employing Hamilton-Jacobi theory, we find the following conserved quantities:

\[ p_\phi \equiv mr^2 \sin^2 \theta \dot{\phi} \]

(16)

\[ \beta \equiv m^2 r^4 \dot{\theta}^2 + 2mq p \cos \theta + \frac{p^2 \dot{\phi}}{\sin^2 \theta} \]

(17)

\[ E \equiv \frac{1}{2} mr^2 + \frac{Qq}{r} + \frac{\beta}{2mr^2} \]

(18)

as can be verified by direct time differentiation, substituting for the second derivatives from equations (13)–(15).

Our goals are to find (1) the rate at which incoming charged particles strike the grain surface and (2) the distribution of their arrival angles \( \theta \), given \( Q \), \( p \) and \( T_{\text{gas}} \). First, we describe the trajectory of the incoming particle when it is still far from the grain (see Fig. 1). Suppose its velocity is

\[ v_\infty = -v (\cos \theta_0 \hat{x} + \sin \theta_0 \hat{z}). \]

(19)

The trajectory is offset from the line \( x = \tan \theta_0 z \), which passes through the grain center, by impact parameter \( b \); angle \( \alpha \) specifies the displacement of the trajectory from the \( x - z \) plane. Consider a plane front of incoming particles. 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

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

(20)

and the components of their velocities are

\[ \dot{r} \approx -v \]

(21)

\[ r \dot{\theta} \approx v \sin \alpha \left( \frac{b}{r_0} \right) \]

(22)

\[ r \sin \theta \dot{\phi} \approx v \sin \alpha \left( \frac{b}{r_0} \right). \]

(23)

Expressing the time derivatives in equations (21)–(23) yields

\[ p_\phi = mv b \sin \theta_0 \sin \alpha \]

(24)

\[ \beta = m^2 v^2 b^2 + 2mq p \cos \theta_0 \]

(25)

\[ E = mv^2 / 2. \]

(26)

Substituting these results in equations (17) and (18), we find

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

(27)

\[ r^4 \ddot{\theta}^2 = v^4 b^2 \left( 1 - \frac{\sin^2 \theta_0 \sin^2 \alpha}{\sin^2 \theta} \right) + \frac{2q p}{m} (\cos \theta_0 - \cos \theta) \]

(28)

We are interested in the solution with \( \dot{r} < 0 \), since the particle approaches the grain. The choice of the initial sign \( S \) is more complicated for \( \dot{\theta} \). If \( \theta_0 = 0 \) (\( \pi \)), then \( S = +1 \) (\( S = -1 \)). Otherwise, equation (22) yields \( \dot{\theta} = v b \cos \alpha / r^2 \)

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 \( \dot{\theta} \): \( \sin \theta r \dot{\theta} = v \cos \theta_0 \left( b / r_0 \right)^2 \).

Thus, in this case, \( S = \cos \theta_0 / | \cos \theta_0 | \). If \( \cos \theta_0 \) and \( \cos \alpha \) both equal zero, then \( \dot{\theta} = 0 \). Note that \( S \) typically changes sign at points \( \theta \) where \( \dot{\theta} = 0 \).

Since \( \dot{r}^2 \) is a single-valued function of \( r \) (eq 27), charge \( q \) only reaches the grain surface if \( \dot{r} \) does not reverse sign when \( r > a \). From equation (27), \( \dot{r} = 0 \) when

\[ r = a \left[ U \pm \sqrt{U^2 + V \cos \theta_0 + \left( \frac{b}{a} \right)^2} \right] \]

(29)

where \( U \equiv qQ / (mv^2 a) \) and \( V \equiv 2qp / (mv^2 a^2) \). If the larger root in equation (29), \( r_+ \), exceeds \( a \) and \( \dot{r} > 0 \) at \( r = r_+ \), then charge \( q \) does not strike the grain. If \( U > 1 \), then charge \( q \) only strikes the grain if the argument of the square root in equation (29) is negative, since \( \dot{r} \) never reaches zero in this case. Assuming \( \dot{r} > 0 \) at \( r_+ \), the critical impact parameter is given by

\[ \frac{b_{\text{crit}}}{a} = \left\{ \begin{array}{ll}
  \frac{1 + \sqrt{1 - 2U - V \cos \theta_0}}{U}, & U \leq 1 \\
  \frac{1 - \sqrt{1 + 2U - V \cos \theta_0}}{U}, & U \geq 1
\end{array} \right\}. \]

(30)

Only trajectories with \( b \leq b_{\text{crit}} \) strike the grain surface. If the relevant root in equation (29) is not real, then \( b_{\text{crit}} = 0 \). Note that \( b_{\text{crit}} \) does not depend on the angle \( \alpha \). The collision cross section is \( \pi b_{\text{crit}}^2 \).

Now we justify the assumption that \( \dot{r} > 0 \) at \( r = r_+ \) when \( b = b_{\text{crit}} \). Differentiating equation (18) yields

\[ \dot{r} \left( \dot{r} - \frac{Q}{mr^2} - \frac{\beta}{m r^3} \right) = 0. \]

(31)

The term in parentheses in equation (31) must vanish for all \( r \), except where \( \dot{r} = 0 \). Continuity implies that it vanishes at these locations as well, including at \( r = r_+ \). Equations (29) and (31) yield

Figure 1. Parameters describing the trajectories of incoming charged particles.
\[ \tilde{r} = \frac{a^2 v^2}{r^4} \left[ U^2 + V \cos \theta_0 + \left( \frac{b}{a} \right)^2 + U \sqrt{U^2 + V \cos \theta_0 + \left( \frac{b}{a} \right)^2} \right] \]

at \( r = r_+ \). If either \( U > 0 \) or \( V \cos \theta_0 > 0 \), then clearly \( \tilde{r} > 0 \) at \( r = r_+ \), regardless of \( b \). If both of these quantities are negative, then setting \( b = b_{\text{crit}} \) in equation (32) yields \( \tilde{r} = |U - 1| > 0 \) for \( r = r_+ \).

Assuming no gas-grain drift, the mean collision cross section (averaged over angle \( \theta_0 \)) is

\[
\tilde{\sigma} = \begin{cases} 
\frac{\pi a^2}{2} (2 - 2U), & 2U + |V| \leq 1 \\
\frac{\pi a^2}{2} |V|^{-1}(1 - 2U + |V|)^2, & \text{otherwise} 
\end{cases} \quad (33)
\]

when \( U \leq 1 \) and

\[
\tilde{\sigma} = \begin{cases} 
\frac{4\pi a^2}{2} |V|(1 - |V|^{-1}U)^2, & |V|^{-1}U^2 < 1 \\
|V|^{-1}U^2 \geq 1 & \text{otherwise} 
\end{cases} \quad (34)
\]

when \( U \geq 1 \).

Integrating over the Maxwell speed distribution yields the factor \( \bar{R} \) from equation (10) for a grain that does not drift relative to the gas:

\[
\bar{R}(\eta, |\eta|) = 1 - \gamma, \quad qQ < 0 \quad \text{and} \quad |\eta| \leq -\gamma 
\]

\[
\bar{R}(\eta) = \frac{1}{4|\eta|} \left\{ (|\eta| - \gamma)(2 + |\eta| - \gamma) + 2 \left[ 1 - e^{-(\gamma + |\eta|)} \right] \right\}, 
\]

\[
qQ < 0 \quad \text{and} \quad |\eta| \geq -\gamma 
\]

\[
\bar{R} = e^{-\gamma \sinh |\eta| / |\eta|}, \quad qQ > 0 \quad \text{and} \quad |\eta| \leq \gamma/2 
\]

\[
\bar{R} = \frac{1}{2|\eta|} e^{-(\gamma + |\eta|)} 
\]

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

\[
+ \frac{|\eta|^2}{4} \int_{\gamma/2}^{\gamma} ds \left( 1 - \frac{\gamma^2}{4|\eta|^2} \right)^2 e^{-s}, 
\]

\[
qQ > 0 \quad \text{and} \quad |\eta| \geq \gamma/2; 
\]

\( \gamma \equiv qQ/(a k_B T_{\text{gas}}) \), and \( \gamma \equiv qQ/(a^2 k_B T_{\text{gas}}) \). Fig. 2 displays \( \bar{R} \) versus \( \gamma \) for various values of \( |\eta| \). Note that equations (30) and (31) recover the classic Spitzer (1941) expression for \( R \) for a charged sphere when \( \eta = 0 \).

Since \( d\theta/dr = \dot{\theta}/r \), equations (27) and (28) yield

\[ F_1(\theta_0, \theta, VC^2, \alpha) = F_2(A, B, C) \]

where

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

\[ B \equiv 2UC \]

\[ C \equiv a/b \]

\[ F_1(\theta_0, \theta, VC^2, \alpha) = \]

\[ \int_{\theta_0}^{\theta} \frac{d\theta'}{\sqrt{\sin^2 \theta' - \sin^2 \theta_0 \sin^2 \alpha + VC^2 \sin^2 \theta' \cos \theta_0 - \cos \theta'}} S(\theta') \]

\[ F_2(A, B, C) = \int_{-\infty}^{\infty} \frac{du}{u \sqrt{A - B u + u^2}} \]

The integrand in equation (43) is negative when \( S < 0 \), but in these cases \( \theta < \theta_0 \), so the integral remains positive.

Figure 2. \( \bar{R} \) vs. \( \gamma \) for various values of \( |\eta| \), as indicated.

If \( \dot{\theta} \) reaches zero at \( \theta^' = \theta_1 \), then \( S \) changes sign and \( F_1 \) splits into two integrals, with limits \( \theta_0 \) to \( \theta_1 \) and \( \theta_1 \) to \( \theta \). Performing the integration in equation (43),

\[ F_2 = \frac{1}{\sqrt{A}} \sin^{-1} \left( \frac{BC + 2A}{C \sqrt{B^2 + 4A}} \right) - \sin^{-1} \left( \frac{B}{\sqrt{B^2 + 4A}} \right) \]

\[ A \geq 0 \]

\[ F_2 = \frac{1}{\sqrt{-A}} \ln \left[ \frac{2\sqrt{-A \sqrt{C^2 - BC - A} - A - BC - 2A}}{(2\sqrt{-A - B} C)} \right] \]

\[ A \leq 0 \]

Given \( 2q/(mv^2 b^2) \), \( 2q/(mv^2 b) \), \( a/b \), \( \theta_0 \), and \( \alpha \), equation (39) can be solved to efficiently find the arrival angle \( \theta \). A less efficient, but more direct, approach is to integrate the equations of motion (13) - (15). We have written FORTRAN subroutines implementing both of these methods and found perfect agreement for numerous combinations of input parameters.

To compute the distribution of arrival angles \( \theta \) for given values of \( \gamma \) and \( \eta \), we examine a large number of trajectories with initial parameters \( \theta_0, u \equiv v/v_{\text{th}}, b/a \), and \( \alpha \), where \( v_{\text{th}} \equiv (2k_B T_{\text{gas}}/m)^{1/2} \). We first select \( N_u \) values of \( \theta_0 \) from 0 to \( \pi \), uniformly spaced in \( \cos \theta_0 \). For each value of \( \theta_0 \), we select \( N_v \) values of \( u \), starting with \( u = 1.08765 \), the median value assuming the Maxwell speed distribution. We then select \( (N_u - 1)/2 \) values with \( u > 1.08765 \) spaced in equal-probability intervals, i.e., such that

\[ 4 \int_{u_i}^{u_{i+1}} du \exp(-u^2) = \frac{1}{N_u + 1} \]

(47)

Likewise for values with \( u < 1.08765 \). For each \( (\theta_0, u) \) pair, if \( b_{\text{crit}} > 0 \), then we next select \( N_v \) values of \( b/u \) between 0 and \( b_{\text{crit}}/a \), uniformly spaced in \( b^2 \). Finally, for each \( (\theta_0, b, a) \), we select \( N_v \) values of \( a \), uniformly spaced between 0 and \( 2\pi \). For each trajectory, we compute the arrival angle \( \theta \). The
results are binned, with trajectories weighted in proportion to \( b^2_{\text{grain}} \).

Fig. 3 displays \( g(\cos \theta) \) vs. \( \cos \theta \) for \( \gamma = 0 \) and various values of \( \eta \), as indicated. To construct this figure, we adopted 40 bins in \( \theta \) for \( \gamma = 0 \) and several values of \( \eta \). To see that for \( |\gamma| < 1 \), Distributions for \( (\gamma, \eta) \) and \( (\gamma, -\eta) \) are identical to those for \( (\gamma, -\eta; \cos \theta) = g(\gamma, \eta; -\cos \theta) \), with \( g(\cos \theta) \) the fraction of particles that strike with cosine of polar angle \( \geq \cos \theta \) when \( \eta < 0 \). As \( |\gamma| \) increases, the distribution in \( \cos \theta \) becomes more uniform, as seen in Fig. 4 for the case that \( \eta = 10^2 \).

Electrons arriving at the grain surface can penetrate to within the bulk of the grain, with an e-folding length \( l_e \approx 10 \) Å (see paragraph following eq. 13 in WD01). We neglect this penetration since \( l_e \ll a \); i.e., all arriving electrons are assumed to be located at \( r = a \).

### 3.3 Photoelectric Emission

We adopt a simplified version of the procedure in WD01 for calculating the rate at which photoelectrons are ejected from the grain, \( J_{\text{pe}} \). WD01 express the photoelectric yield (i.e., the probability that an electron is ejected following the absorption of a photon) as a product of three factors: the bulk yield \( g_0 \), a size-dependent yield enhancement factor \( y_1 \), and a term \( y_2 \) that accounts for the attraction of ‘attempting’ photoelectrons back to the grain when \( Z \geq 0 \). (Recall that the grain charge \( Q = Ze \), with \( e \) the proton charge.) For the relatively large grains under consideration here, \( y_1 = 1 \).

The term \( y_2 \) is given by (WD01, eq. 11)

\[
y_2 = \begin{cases} 
    E^2_{\text{high}}(E_{\text{high}} - 3E_{\text{low}})/(E_{\text{high}} - E_{\text{low}})^3, & Z \geq 0 \\
    1, & Z < 0
\end{cases}, \quad (48)
\]

with \( E_{\text{low}} = -(Z + 1)e^2/a \) and \( E_{\text{high}} = h\nu - h\nu_{\text{pet}} \) (\( h\nu_{\text{pet}} \) is the threshold photon energy for photoemission). For simplicity, we take \( E_{\text{high}} = 3 \) eV [assuming \( h\nu \approx 11 \) eV and \( h\nu_{\text{pet}} \approx 8 \) eV (WD01)], independent of \( Z \) and \( h\nu_{\text{pet}} \).

To find \( J_{\text{pe}} \), it is necessary to integrate the photon absorption rate \( R_t \) times the yield over the range of available photon energies above \( h\nu_{\text{pet}} \). Since we approximate \( y_2 \) to be independent of \( h\nu \), \( J_{\text{pe}} \propto y_2 \). We simply choose the proportionality constant so as to reproduce the average grain potential of \( \approx 0.3 \) V from WD01.

As for arriving electrons, we assume that holes produced in photemission events are located at \( r = a \). We also neglect the production of an electron-hole pair when a photon is absorbed but a photoelectron does not escape the grain. In some cases, the photon absorption occurs too deep within the grain for the photoelectron to reach the surface or the photoelectron’s velocity is directed away from the surface (resulting in \( y_0 < 1 \)). Since \( l_e \ll a \), the resulting separation of charge does not contribute significantly to the dipole moment. In other cases, a photoelectron breaches the grain surface, but returns to the grain due to an attractive Coulomb force if \( Z \geq 0 \) (resulting in \( y_2 < 1 \)). Such events could lead to a more significant change in \( p \), but are rare; \( y_2 \approx 0.98 \) when the grain potential is \( \approx 0.3 \) V.

### 4 SIMULATIONS

For each of the four charge transport models described in 3.3, we run stochastic simulations that keep track of the grain dipole moment \( p \) and the orientation in space of the grain’s rotational axis, assumed fixed with respect to the grain body (as would be appropriate for suprathermally rotating grains). We adopt \( v_{\perp} = 1 \) km s\(^{-1}\) (resulting from acceleration associated with magnetohydrodynamic turbulence; Yan et al. 2004), \( T_{\text{gas}} = 100 \) K, \( n_e = 4.5 \times 10^{-2} \) cm\(^{-3}\).
Electric dipole moments and disalignment of grains

$s_e = 0.5$, $T_d = 15$ K (hence, $\chi_0 = 5 \times 10^{-3}$), and $y_0 = 6 \times 10^{-2}$ (eq. 17 in WD01 with $h\nu = 10$ eV). We consider grains with $a = 0.1$ and 0.2 $\mu$m, for which the photon absorption rate $R_a = 2.9 \times 10^{-5}$ and $5.7 \times 10^{-4} \text{ s}^{-1}$, respectively, in order to maintain the average potential at 0.3 V. We employ a constant time step size $dt$, usually 31.56 $s$, which is smaller than the typical time between charging events.

Next, we describe the simulation algorithm for perfectly insulating grains. At the start of each time step, we find the factor $\tilde{R}$ (eq. 23) for the electron collisional charging rate by bilinear interpolation (Press et al. 1992, p. 117) in $\ln \gamma$ and $\ln \eta$, with 21 values of $\gamma$ ranging from $10^{-2}$ to $10^2$ and 11 values of $|\gamma|$ ranging from $10^{-2}$ to 3 $\times$ $10^2$ (for 23 total values of $\gamma$ in the tables, since both signs, as well as $\gamma = 0$, are included). If $|\gamma| < 10^{-2}$, then a linear interpolation is performed in $\eta$ alone (with $\gamma = 0$). If $\gamma < 10^{-2}$, then we assume the classic Spitzer (1941) expression for $\tilde{R}$ for a charged sphere (corresponding to $\eta = 0$).

An electron arrives with probability $R_e dt$ ($R_e$ is the electron arrival rate; eq. 23). In each time-step, we check that $R_e dt < 1$ (and likewise for the probability that a photoelectron is ejected). Here, as throughout the simulations, we use the routine ran2 from Press et al. (1992) for choosing random numbers. If $\eta < 10^{-2}$, then the electron is placed at a random location ($\theta, \phi$) on the grain surface; $\theta$ and $\phi$ are the polar and azimuthal angles, respectively, with the rotation axis $\tilde{\omega} = \tilde{z}$ as the polar axis. Otherwise, we interpolate to find the distribution function $g(\theta')$, as described in the preceding paragraph for $\tilde{R}$: $\theta'$ is the polar angle with the dipole moment $\mathbf{p}$ as the polar axis. We choose $\theta'$ randomly from the distribution $g(\theta')$ and the azimuthal angle $\phi'$ is chosen randomly from a uniform distribution. The arrival position with respect to the grain body is given by

$$x/a = \sin \theta' \cos \phi' \cos \theta_p \cos \phi_p - \sin \phi' \sin \phi_p$$

$$+ \cos \theta' \sin \theta_p \cos \phi_p \tag{49}$$

$$y/a = \sin \theta' \cos \phi' \cos \theta_p \sin \phi_p + \sin \phi' \cos \phi_p$$

$$+ \cos \theta' \sin \theta_p \sin \phi_p \tag{50}$$

$$z/a = \cos \theta' \cos \theta_p - \sin \theta' \cos \phi' \sin \theta_p \tag{51}$$

where $\theta_p$ and $\phi_p$ are the polar and azimuthal angles, respectively, of $\mathbf{p}$ relative to the grain body.

A photoelectron is ejected with probability $R_e y_0 y_2$. The resulting hole is located randomly on the grain surface.

At the start of a simulation, we set $\mathbf{p} = 0$ and choose $Z$ to correspond to the average potential of 0.3 V. Drain & Lazarian (1998) noted that a grain may have an intrinsic electric dipole moment due to the random orientations of polar constituents. Thus, our choice $\mathbf{p} = 0$ requires justification.

Consider a conducting grain with $N_{\text{hit}}$ deep traps (model 3 in W06). The largest possible magnitude of the electric dipole moment associated with excess charges (electrons and holes) occupying the deep traps is $p_{\text{max}} \sim N_{\text{hit}} ea$. If the magnitude of the intrinsic electric dipole moment $p_{\text{int}} > p_{\text{max}}$, then the intrinsic dipole could not be neutralized; thus, flipping of $p$ would not be possible. This situation is similar to that of a purely conducting grain (model 2 in W06), with $p \propto Z$ and $Z$ is always positive.

To estimate the likely magnitude of $p/ea$ associated with the intrinsic dipole, suppose each polar constituent has volume $V_0$ and dipole moment $p_0 = \zeta eV_0^{1/3}$. Assuming each constituent is randomly oriented, the total intrinsic moment $p_{\text{int}} \sim N^{1/2}p_0$, with the grain volume $(4/3)\pi a^3 = NV_0$. Eliminating $N$, we find

$$p_{\text{int}}/ea \sim \left(\frac{4\pi}{3}\right)^{1/2} \zeta \left(\frac{a}{V_0^{1/3}}\right)^{1/2}. \tag{52}$$

Even adopting relatively large values of $\zeta \sim 0.1$ and $aV_0^{-1/3} \sim 500$, we find $p_{\text{int}}/ea \sim 4.6$, comparable (in order of magnitude) to the values found in the following section, where the intrinsic electric dipole moment $p_{\text{int}}$ is neglected.

For any realistic grain, $N_{\text{hit}} \gg p_{\text{int}}/ea$; thus, we do not expect the intrinsic electric dipole moment to play any role in the long-term evolution of $p$, including the flipping of the dipole moment. Essentially, the total number of charges in the grain (the number of electrons plus the number of holes) can vastly exceed the net number of charges (number of electrons minus number of holes), and a slight asymmetry in the distribution of these charges can counter the intrinsic dipole moment.

Of all the simulations with deep traps considered in this paper, the smallest value of $N_{\text{hit}}$ is $\approx 100$, when $a = 0.1\mu$m and the volume per deep trap is $V_t = 4 \times 10^7 \text{Å}^3$. (This value of $N_{\text{hit}}$ is almost certainly much too small to be realistic, but was chosen to make the computations feasible and to, conservatively, generate a grain with low insulating capability). We ran this model 3 simulation with $p_{\text{int}} = 0$ and with $p_{\text{int}}$ as estimated above; the resulting flipping times are nearly identical, as expected.

At any time, the net charge and dipole moment are given by

$$Z = N_h - N_e \tag{53}$$

$$p = e \sum_{i=1}^{N_h} \mathbf{x}_i - e \sum_{i=1}^{N_e} \mathbf{x}_i \tag{54}$$

where $N_h$ and $N_e$ are the total number of holes and electrons, respectively, and $\mathbf{x}_i$ is the position of an electron or hole (with the origin at the grain’s center of mass, i.e., the center of the spherical grain). In each time-step, $\theta_p, \phi_p$, and $p \equiv |\mathbf{p}|$ are updated, if an electron arrives at or departs the grain. We also keep track of $\theta_{\text{align}}$ and $\phi_{\text{align}}$, the polar and azimuthal angles of the grain rotation axis with respect to the magnetic field direction, employing eqs. 14 and 15 from W06:

$$d\phi_{\text{align}} = \Omega_0 [1 - \Upsilon \cot \theta_{\text{align}} \cos(\phi_{\text{align}} + \phi_{\text{gyro}})] dt \tag{55}$$

$$d\theta_{\text{align}} = -\Omega_0 \Upsilon \sin(\phi_{\text{align}} + \phi_{\text{gyro}}) dt \tag{56}$$

where $\Omega_0$ is the precession rate for the case that $p = 0$ (eq. 33),

$$\phi_{\text{gyro}}(t) = \int_0^t dt' \omega_{\text{gyro}}(t'), \tag{57}$$

and the time-scale for gyrorotation is given by

$$\omega_{\text{gyro}}^{-1} \sim 2.4 \times 10^2 \left(\frac{\rho}{3 \text{ g cm}^{-3}}\right) \left(\frac{a}{0.1 \mu\text{m}}\right)^2 \left(\frac{U}{0.3 \text{ V}}\right)^{-1} \times \left(\frac{B}{5 \mu\text{G}}\right)^{-1}. \tag{58}$$
Note that \( \omega_{\text{gyro}} \) varies with time, since the grain potential \( U \) is not constant.

We take \( \theta_{\text{align}} = 0.1 \) and \( \phi_{\text{align}} = 0 \) initially. Within the same charging simulation, we consider several different values of \( \omega/\omega_T \) (and thus, several different values of \( \Upsilon \); recall eqs. 1, 2, and 3). In principle, gyrorotation can affect the disalignment, since \( \omega_{\text{gyro}} \) fluctuates randomly as \( Z \) does so. However, we have found that the disalignment time is identical for simulations that do (do not) include gyrorotation. Thus, we omit gyrorotation in our simulations.

The simulations for purely conducting grains are identical to those for purely insulating grains, except that it is not necessary to keep track of the electron arrival locations, since charge is immediately delocalized. Instead, we simply take \( p = p_z Z \propto Z \).

For the models containing deep traps, we first specify the average grain volume per deep trap of a given type (i.e., a trap that accommodates electrons versus one that accommodates holes), \( V_t \), then randomly place int(\( 4\pi a^3/3V_t \)) deep traps of each type throughout the grain volume. For model 3 in [35] (conducting grain with deep traps), an arriving electron is immediately moved to the accommodating trap nearest its arrival site. This nearest trap could be a vacant electron trap or an occupied hole trap; in the latter case, the charges recombine. Likewise, the hole produced in a photoemission event is immediately moved to the nearest vacant hole trap or occupied electron trap.

For model 4 in [31] (partially conducting grain with deep traps), each electron or hole undergoes a random walk through the grain, starting at its arrival location. In each step, the charge moves distance \( d_{rw} \) (taken to be 30 \( \AA \)) in time \( t_{rw} \). Thus, for these simulations, the time step size \( dt = t_{rw} \). If a charge finds itself within distance \( d_{rw} \) of an accommodating deep trap, then it enters the trap and remains there until recombining when a charge with opposite sign arrives at the trap. The time \( t_{rw} \) is selected as follows:

\[
t_{rw} = \frac{f \tau_c d_{rw}^2}{V_t^{2/5}}
\]

with \( \tau_c \) the typical time between charging events. With this choice, the typical time for a charge to travel from one trap to another is \( \sim f \tau_c \). With \( f \sim 1 \), this model lies between the extremes of a perfect insulator and a perfect conductor with deep traps.

5 RESULTS

We ran simulations for 11 different sets of input, with 2 realizations apiece (i.e., 2 different values of the random number seed), for a total of 22 simulations. Table 1 displays input parameters for each run, as well as selected output parameters. We performed runs with models 1 through 3 of [35] for grain radii \( a = 0.1 \) and 0.2 \( \mu \)m. For model 4, only \( a = 0.1 \) \( \mu \)m is included, since the CPU time becomes prohibitive for \( a = 0.2 \) \( \mu \)m when charges execute random walks through the grain volume. For models 1 through 3, the total duration of the simulation is \( t_{\text{tot}} = 10^5 \) yr, but substantially shorter \( t_{\text{tot}} \) were obtained for model 4.

Fig. 5 displays the component of the electric dipole moment (normalized to \( e a \), the proton charge times the grain radius) lying along the spin axis vs. time, from a simulation of a purely insulating grain with \( a = 0.1 \) \( \mu \)m.

![Figure 5. The component of the grain dipole moment (normalized to ea, the proton charge times the grain radius) lying along the spin axis vs. time, from a simulation of a purely insulating grain with a = 0.1 \( \mu \)m.](image-url)
Electric dipole moments and disalignment of grains

is not typically the case when \( \omega/\omega_T \gtrsim 10 \). In general, we estimate \( \tau_{\text{dis}} \approx t_{\text{tot}}/(N_{\text{dev}} + |\Delta \theta_{\text{align}}|) \), where \( \Delta \theta_{\text{align}} \) is the value of \( \theta_{\text{align}} \) at the end of the simulation minus its value at the last time \( N_{\text{dev}} \) was incremented (which may have been the start of the simulation, if \( N_{\text{dev}} = 0 \)). Table I indicates the values of \( N_{\text{dev}} \) for \( \log_{10}(\omega/\omega_T) = 1.0, 1.5, \) and \( 2.0 \). Of course, the resulting estimate of \( \tau_{\text{dis}} \) is not very reliable for the cases where \( N_{\text{dev}} \sim 1 \).

For each simulation, we keep track of \( \theta_{\text{align}} \) for 7 different values of \( \log_{10}(\omega/\omega_T) \), evenly spaced between -1.0 and 2.0. Fig. 6 displays \( \cos \theta_{\text{align}} \) versus time from a simulation of a perfectly insulating grain with \( a = 0.1 \mu m \) and \( \omega/\omega_T = 10^2 \).

Fig. 7 displays \( \tau_{\text{dis}} \) versus \( \omega/\omega_T \) for perfectly insulating grains with \( a = 0.1 \) and \( 0.2 \mu m \). For each case, \( \tau_{\text{dis}} \) is taken to be its average over the 2 realizations. The solid (dashed) curves are \( \tau_{\text{dis}} \) from equation (7) for \( a = 0.1 \mu m \) (0.2 \mu m). We employ \( \tau_{\text{ins}} \) and the average value of \( |p_z| \) (for use in evaluating \( \Upsilon \)) as determined from the simulation. The agreement between the measured values of \( \tau_{\text{dis}} \) and those calculated with equation (7) is surprisingly good. The expectation that \( \tau_{\text{dis}} \propto (\omega/\omega_T)^2 \) is well confirmed.

The disalignment times found using equation (7) and the values of \( \tau_{\text{flip}} \) from the simulations are substantially shorter than those from W06 (see figs. 2 and 3 in W06); the discrepancy exceeds 2 orders of magnitude when \( a = 0.1 \mu m \). Our simulations yield much larger values of \( |p_z|_{\text{av}} \) than estimated by W06, and \( \tau_{\text{dis}} \propto |p_z|_{\text{av}}^2 \). The estimate of \( \tau_{\text{flip}} \) in W06 is also substantially larger than our result. When equation (7) is used \( (\tau_{\text{dis}} \propto \tau_{\text{flip}}^{-1}) \), this partially compensates for the difference associated with the \( p_z \) estimates. However, given the larger estimate for \( \tau_{\text{flip}} \), W06 employed equation (8) when \( a = 0.1 \mu m \); in this case, \( \tau_{\text{dis}} \) is larger by a factor \( \approx 2 \) when equation (8) is used instead of equation (7).

Fig. 8 shows the ratio of \( \tau_{\text{dis}} \) for several simulation runs to its value for the perfectly insulating case, \( \tau_{\text{ins}} \), for \( a = 0.1 \mu m \). All of the simulations from Table I are included, except for the perfectly conducting case. The results always lie within \( \approx 50 \) percent of unity, with somewhat greater scatter when \( \omega/\omega_T > 10 \); the results for these high-\( \omega \) cases are not particularly reliable, since the corresponding \( N_{\text{dev}} \) are small (see Table I). The ratio \( \tau_{\text{dis}}/\tau_{\text{ins}} \) also lies within 50 percent of unity for the model 3 run for \( a = 0.2 \mu m \).

Fig. 9 displays the ratio of \( \tau_{\text{dis}} \) for a perfectly conducting grain, \( \tau_{\text{cond}} \), to \( \tau_{\text{ins}} \), for \( a = 0.1 \) and \( 0.2 \mu m \). We assumed

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**Table 1. Simulation Parameters and Outputs**

| Model | \( a \) | \( V_0 \) | \( t_r \) | Run | \( |p_z|_{\text{av}} \) | \( \tau_{\text{ins}} \) | \( t_{\text{tot}} \) | \( N_{\text{dev}} \) |
|-------|---|----|----|-----|-----------------|-----------------|---------------|--------------|
| 1     | 0.1 | ... | ... | 1   | 2.21            | 5.2             | 1.0E5         | 2348         |
| 1     | 0.1 | ... | ... | 2   | 2.18            | 5.2             | 1.0E5         | 2418         |
| 1     | 0.1 | ... | ... | 1   | 2.11            | ...             | 1.0E5         | 72           |
| 1     | 0.1 | ... | ... | 2   | 2.12            | ...             | 1.0E5         | 44           |
| 1     | 0.4E7| ... | ... | 1   | 1.77            | 6.8             | 1.0E5         | 1822         |
| 1     | 0.4E7| ... | ... | 2   | 1.77            | 6.2             | 1.0E5         | 1800         |
| 1     | 0.4E6| ... | ... | 1   | 2.11            | 5.8             | 1.0E5         | 2451         |
| 1     | 0.4E6| ... | ... | 2   | 2.13            | 5.8             | 1.0E5         | 2358         |
| 1     | 0.4E7| 2.3 | 1   | 2.16 | 2.2             | 7.29E2         | 14            |
| 1     | 0.4E7| 2.3 | 2   | 2.35 | 2.5             | 7.29E2         | 22            |
| 1     | 0.4E7| 1.15| 1   | 2.17 | 2.5             | 3.64E2         | 6             |
| 1     | 0.4E7| 1.15| 2   | 2.09 | 2.4             | 3.64E2         | 11            |
| 1     | 0.4E7| 9.2 | 1   | 2.56 | 2.4             | 2.92E3         | 81            |
| 1     | 0.4E7| 9.2 | 2   | 2.56 | 2.5             | 2.92E3         | 76            |
| 1     | 0.4E6| 2.3 | 1   | 2.07 | 5.0             | 7.29E2         | 17            |
| 1     | 0.4E6| 2.3 | 2   | 2.11 | 5.1             | 7.29E2         | 19            |
| 1     | 0.2  | ... | ... | 1   | 2.23            | 2.6             | 1.0E5         | 172          |
| 1     | 0.2  | ... | ... | 2   | 2.18            | 2.6             | 1.0E5         | 150          |
| 1     | 0.2  | ... | ... | 1   | 2.00            | ...             | 1.0E5         | 4            |
| 1     | 0.2  | ... | ... | 2   | 2.00            | ...             | 1.0E5         | 4            |
| 1     | 0.2  | 4.0E7| 1   | 2.07 | 2.9             | 1.0E5          | 164           |
| 1     | 0.2  | 4.0E7| 2   | 2.07 | 2.9             | 1.0E5          | 139           |

---

\( a \): Number of 1 rad deviations in alignment angle \( \theta_{\text{align}} \).

\( b \): From section 3.

\( c \): Grain radius.

\( d \): Volume per deep trap.

\( e \): Duration of random walk step.

\( f \): 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).

\( g \): Estimate of the electric dipole moment flipping time.

\( h \): Duration of the simulation.

\( i \): Suprathermality \( \omega/\omega_T \).
that \( p_z = 0.1 Z e a \), which seems conservative for grains sufficiently asymmetric to produce the observed polarization. However, a solution of the electrostatic boundary value problem for model aspherical grains would be needed to confirm this choice. The disalignment times tend to be 1 to 2 orders of magnitude longer for conducting grains than for insulating grains. This is not surprising, since \( Z \), and hence \( p_z \) for conductors, does not change sign (although it does fluctuate).

Note that the data points for \( \omega/\omega_T > 10 \) are not reliable, given the small values of \( N_{\text{dev}} \) in these cases (Table I).

6 CONCLUSIONS

We have conducted a more detailed analysis of grain disalignment associated with the time-varying electric dipole...
moment than was attempted in W06, focusing on superthermally rotating silicate grains. We considered 4 idealized models for how charge is transported within the grain (§5.1): a perfect insulator, 2 models involving special sites in the grain (‘deep traps’) where electrons or holes are effectively trapped, and a perfect conductor. The resulting disalignment times $\tau_{\text{dis}}$ for the first 3 models are highly consistent (Fig. 5) and substantially shorter (up to 2 orders of magnitude) than those obtained by W06 (cf. Fig. 7 here with figs. 2 and 3 in W06). We expect the behavior of real grains to be bracketed by these 3 models. Disalignment proceeds more slowly (up to 2 orders of magnitude; Fig. 9) for conducting grains, but we do not expect this idealization to be realistic for interstellar grains.

In treating the collisional charging, we neglected the gas-grain drift. Drift can, in principle, affect the time variation of the electric dipole moment. For a non-rotating grain, there may be a stable contribution to the electric dipole moment. For a non-rotating grain, suppressing flips in the azimuthal angle $\phi_{\text{in}}$ and with speeds between $v$ and $v + dv$ is

$$dR = \pi r_{\text{big}}^2 n \frac{1}{4\pi} d \cos \theta_{\text{in}} d\phi_{\text{in}} P(v) dv |v - v_{\text{gr}}|$$

(A1)

where $P(v)$ is the Maxwell speed distribution. After integrating over $\phi_{\text{in}}$,

$$dR = \pi r_{\text{big}}^2 n \left( \frac{8k_BT}{\pi m} \right)^{1/2} dR$$

(A2)

with

$$d\tilde{R} = du d\cos \theta_{\text{in}} u^2 u_1 \exp(-u^2);$$

(A3)

the dimensionless speed $u = v/v_{\text{th}}$ and

$$u_1 = (u^2 + u_{\text{gr}}^2 + 2u_{\text{gr}} \cos \theta_{\text{in}})^{1/2}$$

(A4)

is the particle’s dimensionless speed in the rest frame of the grain ($u_{\text{gr}} = v_{\text{gr}}/v_{\text{th}}$). Integrating over the entire large sphere yields

$$\tilde{R} = 1 + \frac{u_{\text{gr}}^2}{3} \int_0^1 dx \exp(-u_{\text{gr}}^2 x)(1 - \sqrt{x})^3.$$  

(A5)

The arrival angle $\theta_1$ in the rest frame of the grain is characterized by

$$\cos \theta_1 = u \cos \theta_{\text{in}} + u_{\text{gr}}.$$  

(A6)

When $v_\perp = 1 \text{ km s}^{-1}$ and $T_{\text{gas}} = 100 \text{ K}$, $u_{\text{gr}} = 0.0182$ for electrons and 0.778 for protons. For each of these values of $u_{\text{gr}}$, we calculate $u_1$ and $d\tilde{R}$ for $10^5$ values of $(u, \theta_{\text{in}})$ (100 for each input variable) spaced evenly in probability (as described in the text surrounding eq. 17) and with a maximum value of $u = 4$. The results are used to construct the probability $P(u_1)$ that an incoming particle has dimensionless speed in the grain’s frame $\leq u_1$ (with 100 bins in $u_1$). For each value of $u_1$, the corresponding cumulative probability $P(\cos \theta_1)$ is constructed, again with 100 bins. Note that the minimum possible value of $\cos \theta_1$ is $-1$ when $u > u_{\text{gr}}$ and $[1 - (u/u_{\text{gr}})^2]^{1/2}$ when $u < u_{\text{gr}}$.

To simulate the collisional charging, we adopt a time step 10 times smaller than the inverse of the rate at which electrons enter the large sphere surrounding the grain (eqs. A2 and A5). In each step, we draw a random number to determine whether or not an electron enters the large sphere; likewise for a proton. When a charged particle enters the large sphere, a value of $u_1$ is picked randomly from its distribution. Then, $\cos \theta_1$ is chosen randomly from the distribution for the given $u_1$. The final component of the particle’s velocity in the grain’s rest frame, $\phi_{\text{in}}$, is selected randomly from a uniform distribution between 0 and $2\pi$. Two components of the incoming particle’s position remain to be determined (given $r = r_{\text{big}}$): the impact parameter $b$ and the azimuthal angle $\phi_1$. These are both chosen randomly (b from a uniform distribution in $b^2$).

At this point, the position and velocity of the incoming

**APPENDIX A: COLLISIONAL CHARGING FOR A DRIFTING GRAIN**

Consider a grain drifting with velocity $v_{\text{gr}}$ with respect to the gas. The grain rotates uniformly about $\hat{a}_1$, which is inclined at angle $\theta_{\text{in}}$ relative to $v_{\text{gr}}$.

To treat the collisional charging in this case, we first construct a large sphere with radius $r_{\text{big}}$ instantaneously centered on the grain. Adopting the rest frame of the gas and taking the direction of the drift velocity $v_{\text{gr}}$ as the polar axis for spherical coordinates, the velocity $v$ of a gas-phase particle has components $(v, \theta_{\text{in}}, \phi_{\text{in}})$. The rate at which gas-phase particles enter the large sphere from within solid angle $d \cos \theta_{\text{in}} d\phi_{\text{in}}$ about $(\theta_{\text{in}}, \phi_{\text{in}})$ and with speeds between $v$ and $v + dv$ is

$$dR = \pi r_{\text{big}}^2 n \frac{1}{4\pi} d \cos \theta_{\text{in}} d\phi_{\text{in}} P(v) dv |v - v_{\text{gr}}|$$

(A1)

where $P(v)$ is the Maxwell speed distribution. After integrating over $\phi_{\text{in}},$

$$dR = \pi r_{\text{big}}^2 n \left( \frac{8k_BT}{\pi m} \right)^{1/2} dR$$

(A2)

with

$$d\tilde{R} = du d\cos \theta_{\text{in}} u^2 u_1 \exp(-u^2);$$

(A3)

the dimensionless speed $u = v/v_{\text{th}}$ and

$$u_1 = (u^2 + u_{\text{gr}}^2 + 2u_{\text{gr}} \cos \theta_{\text{in}})^{1/2}$$

(A4)

is the particle’s dimensionless speed in the rest frame of the grain ($u_{\text{gr}} = v_{\text{gr}}/v_{\text{th}}$). Integrating over the entire large sphere yields

$$\tilde{R} = 1 + \frac{u_{\text{gr}}^2}{3} \int_0^1 dx \exp(-u_{\text{gr}}^2 x)(1 - \sqrt{x})^3.$$  

(A5)

The arrival angle $\theta_1$ in the rest frame of the grain is characterized by

$$\cos \theta_1 = u \cos \theta_{\text{in}} + u_{\text{gr}}.$$  

(A6)

When $v_\perp = 1 \text{ km s}^{-1}$ and $T_{\text{gas}} = 100 \text{ K}$, $u_{\text{gr}} = 0.0182$ for electrons and 0.778 for protons. For each of these values of $u_{\text{gr}}$, we calculate $u_1$ and $d\tilde{R}$ for $10^5$ values of $(u, \theta_{\text{in}})$ (100 for each input variable) spaced evenly in probability (as described in the text surrounding eq. 17) and with a maximum value of $u = 4$. The results are used to construct the probability $P(u_1)$ that an incoming particle has dimensionless speed in the grain’s frame $\leq u_1$ (with 100 bins in $u_1$). For each value of $u_1$, the corresponding cumulative probability $P(\cos \theta_1)$ is constructed, again with 100 bins. Note that the minimum possible value of $\cos \theta_1$ is $-1$ when $u > u_{\text{gr}}$ and $[1 - (u/u_{\text{gr}})^2]^{1/2}$ when $u < u_{\text{gr}}$.

To simulate the collisional charging, we adopt a time step 10 times smaller than the inverse of the rate at which electrons enter the large sphere surrounding the grain (eqs. A2 and A5). In each step, we draw a random number to determine whether or not an electron enters the large sphere; likewise for a proton. When a charged particle enters the large sphere, a value of $u_1$ is picked randomly from its distribution. Then, $\cos \theta_1$ is chosen randomly from the distribution for the given $u_1$. The final component of the particle’s velocity in the grain’s rest frame, $\phi_{\text{in}}$, is selected randomly from a uniform distribution between 0 and $2\pi$. Two components of the incoming particle’s position remain to be determined (given $r = r_{\text{big}}$): the impact parameter $b$ and the azimuthal angle $\phi_1$. These are both chosen randomly (b from a uniform distribution in $b^2$).

At this point, the position and velocity of the incoming

**APPENDIX A: COLLISIONAL CHARGING FOR A DRIFTING GRAIN**

Consider a grain drifting with velocity $v_{\text{gr}}$ with respect to the gas. The grain rotates uniformly about $\hat{a}_1$, which is inclined at angle $\theta_{\text{in}}$ relative to $v_{\text{gr}}$.
particle are specified relative to a coordinate system at rest with respect to the grain and with \( \mathbf{v}_g \), as the polar axis (`\( \mathbf{v}_g \)-coordinates'). Denoting Cartesian axes in this coordinate system as \( \hat{x}_v, \hat{y}_v, \) and \( \hat{z}_v \), the velocity is given by

\[
\mathbf{v}_v = -v_{1y} \mathbf{u}_1 (\hat{x}_v \sin \theta_1 \cos \phi_1 + \hat{y}_v \sin \theta_1 \sin \phi_1 + \hat{z}_v \cos \theta_1) (A7)
\]

and the position by

\[
x_v = b \cos \alpha_1 \cos \theta_1 \cos \phi_1 - b \sin \alpha_1 \sin \phi_1 + z_{\text{arr}} \sin \theta_1 \cos \phi_1 \tag{A8}
\]
\[
y_v = b \cos \alpha_1 \cos \theta_1 \sin \phi_1 + b \sin \alpha_1 \cos \phi_1 + z_{\text{arr}} \sin \theta_1 \sin \phi_1 \tag{A9}
\]
\[
z_v = -b \cos \alpha_1 \sin \theta_1 + z_{\text{arr}} \cos \theta_1 \tag{A10}
\]

where \( z_{\text{arr}} = (r_{\text{big}}^2 - b^2)^{1/2} \).

Denoting a Cartesian coordinate system attached to the grain body by \((x_j, y_j, z_j)\),

\[
\ddot{z}_j = \dddot{z}_j = \dddot{\theta}_j = \dddot{\phi}_j = 0
\]

From equations (A11)–(A14), we find the following dot products for use in transforming the position and velocity of the incoming gas-phase particle from \( \mathbf{v}_g \)-coordinates (eqs. A11–A14) to \( \mathbf{p} \)-coordinates:

\[
\ddot{x}_p \cdot \ddot{x}_v = \cos \theta_{\text{arr}} \cos \theta_{\text{arr}} \cos (\phi_{\text{arr}} + \lambda) - \sin \theta_{\text{arr}} \sin \theta_{\text{arr}} \sin \phi_{\text{arr}} \tag{A17}
\]
\[
\ddot{x}_p \cdot \ddot{y}_v = \cos \theta_{\text{arr}} \cos \theta_{\text{arr}} \sin (\phi_{\text{arr}} + \lambda) \tag{A18}
\]
\[
\ddot{x}_p \cdot \ddot{z}_v = -\cos \theta_{\text{arr}} \sin \theta_{\text{arr}} \cos (\phi_{\text{arr}} + \lambda) + \sin \theta_{\text{arr}} \cos \theta_{\text{arr}} \cos \phi_{\text{arr}} \tag{A19}
\]
\[
\ddot{y}_p \cdot \ddot{x}_v = -\cos \theta_{\text{arr}} \cos \theta_{\text{arr}} \sin (\phi_{\text{arr}} + \lambda) \tag{A20}
\]
\[
\ddot{y}_p \cdot \ddot{y}_v = \cos (\phi_{\text{arr}} + \lambda) \tag{A21}
\]
\[
\ddot{y}_p \cdot \ddot{z}_v = \sin \theta_{\text{arr}} \sin \theta_{\text{arr}} \sin (\phi_{\text{arr}} + \lambda) \tag{A22}
\]
\[
\ddot{z}_p \cdot \ddot{x}_v = \sin \theta_{\text{arr}} \cos \theta_{\text{arr}} \cos (\phi_{\text{arr}} + \lambda) + \cos \theta_{\text{arr}} \sin \theta_{\text{arr}} \sin \phi_{\text{arr}} \tag{A23}
\]
\[
\ddot{z}_p \cdot \ddot{y}_v = \sin \theta_{\text{arr}} \cos \theta_{\text{arr}} \sin (\phi_{\text{arr}} + \lambda) \tag{A24}
\]
\[
\ddot{z}_p \cdot \ddot{z}_v = -\sin \theta_{\text{arr}} \sin \theta_{\text{arr}} \cos (\phi_{\text{arr}} + \lambda) + \cos \theta_{\text{arr}} \cos \theta_{\text{arr}} \cos \phi_{\text{arr}} \tag{A25}
\]

Finally, the Cartesian \( \mathbf{p} \)-coordinates of the incoming particle’s position and velocity are used in the following geometric relations to find the components in spherical coordinates:

\[
r = r_{\text{big}} \tag{A26}
\]
\[
\theta = \cos^{-1} \left( \frac{z_p}{r} \right) \tag{A27}
\]
\[
\phi = 2 \tan^{-1} \left( \frac{r_{y0} - x_p}{y_p} \right) \tag{A28}
\]

with \( r_{y0} = (x_p^2 + y_p^2)^{1/2} \). The critical impact parameter \( b_{\text{crit}} \) depends on the particle speed \( v_1 = v_{1y} \mathbf{u}_1 \) and \( \cos \theta = -r_{y0}^{-1} z_{y0}/dt \) (eq. A30). If \( b \leq b_{\text{crit}} \), then we integrate the equations of motion (13–14) to determine where on the grain surface the particle hits.

We have tried various values of \( r_{\text{big}} \). Of course, larger values yield higher accuracy but also require smaller time steps. We found that \( r_{\text{big}} = 50a \) yields high accuracy and is not prohibitively time consuming.

Substituting the collisional charging procedure described here in our charging simulations (and including both electrons and protons), we examined a perfectly insulating grain with \( a = 0.1 \mu m \). With a duration of 100 yr, we found that \( |p_{1y}/e| \approx 2.5 \) and \( r_{\text{th}} \) ranges from \( 5.8 \times 10^{-4} \) to \( 6.0 \times 10^{-4} \) as \( \cos \theta_{\text{arr}} \) ranges from 0 to 1. These are very close to the results obtained previously, neglecting grain drift (and ignoring protons) in the treatment of collisional charging (see Table 1). Due to precession of \( \mathbf{J} \) about \( \mathbf{B} \), the angle \( \theta_{\text{arr}} \) changes on a time-scale short compared with the simulation time of 100 yr (but an order of magnitude longer than \( r_{\text{th}} \)). However, our results imply that the behavior of the electric dipole moment is insensitive to the value of \( \theta_{\text{arr}} \). Thus, we conclude that the neglect of grain drift in 13 does not yield significant error.

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