THERMAL FLIPPING AND THERMAL TRAPPING: NEW ELEMENTS IN GRAIN DYNAMICS

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ABSTRACT

Since the classical work by Purcell (1979), it has been generally accepted that most interstellar grains rotate suprathermally. Suprathermally rotating grains would be nearly perfectly aligned with the magnetic field by paramagnetic dissipation if not for “crossovers,” intervals of low angular velocity resulting from reversals of the torques responsible for suprathermal rotation. Lazarian & Draine (1997) identified thermal fluctuations within grain material as an important component of crossover dynamics. For \( a \approx 10^{-5} \) cm grains, these fluctuations ensure good correlation of angular momentum before and after crossover resulting in good alignment, in accord with observations of starlight polarization. We discuss two new processes that are important for the dynamics of \( a \approx 10^{-5} \) cm grains. “Thermal flipping” allows small grains to bypass the period of slow rotation that would otherwise occur during a crossover, thereby enhancing the alignment of small grains. “Thermal trapping” arises when thermal flipping becomes rapid enough to prevent the systematic torques from driving the grain to suprathermal rotation, thereby reducing the alignment of small grains. The observed variation of grain alignment with grain size results from a competition between thermal trapping—which suppresses suprathermal rotation of small grains—and torques due to \( \text{H}_2 \) formation and starlight—which drive large grains to suprathermal rotation rates.

Subject headings: dust, extinction — ISM: magnetic fields — polarization

1. INTRODUCTION

Suprathermal rotation is one of the essential features of grain dynamics in the diffuse interstellar medium (Purcell 1975, 1979). Purcell (1979, hereafter P79) identified three separate systematic torque mechanisms driving suprathermal rotation: inelastic scattering of impinging atoms when gas and grain temperatures differ, photoelectric emission, and \( \text{H}_2 \) formation on grain surfaces. The latter was shown to dominate the other two for typical conditions in the diffuse ISM (P79). Torques due to starlight are also important for grain radii \( a \approx 5 \times 10^{-6} \) cm (Draine & Weingartner 1996).

The arguments of P79 in favor of suprathermal rotation were so clear and compelling that other researchers were immediately convinced that grains in diffuse interstellar clouds should rotate suprathermally. Purcell’s discovery was of immense importance for grain alignment. Suprathermally rotating grains remain subject to gradual alignment by paramagnetic dissipation (Davis & Greenstein 1951), but because of their large angular momenta are essentially immune to disalignment by collisions with gas atoms.

Spitzer & McGlynn (1979, hereafter SM79) showed that suprathermally rotating grains should be susceptible to disalignment only during short intervals of slow rotation that they called “crossovers.”\(^1\) For sufficiently infrequent crossovers, suprathermally rotating grains will be well aligned with the degree of alignment determined by the time between crossovers, the degree of correlation of the direction of grain angular momentum before and after a crossover (SM79), and environmental conditions (e.g., magnetic field strength \( B \)).

The original calculations of SM79 obtained only marginal correlation of angular momentum direction before and after a crossover, but their analysis disregarded thermal fluctuations within the grain material. Lazarian & Draine (1997, hereafter LD97) showed that thermal fluctuations are very important and result in a high degree of correlation for grains larger than a critical radius \( a_c \), the radius for which the time for internal dissipation of rotational kinetic energy is equal to the duration of a crossover. Assuming internal dissipation to be dominated by Barnett relaxation (P79), LD97 found \( a_c \approx 1.5 \times 10^{-5} \) cm, in accord with observations that indicated that the dividing line between grains that contribute and those that do not contribute to starlight polarization has approximately this value (Kim & Martin 1995).

Here we report a new effect of thermal fluctuations—thermal flipping—which would lead to alignment of even the small grains with \( a \approx a_c \) if they rotate suprathermally. However, small grains are observed to not be aligned. We argue that this is caused by a related effect—thermal trapping—which causes small grains to rotate thermally much of the time, despite systematic torques that would otherwise drive suprathermal rotation.

2. CROSSOVERS AND THERMAL FLIPPING

SM79 revealed two basic facts about grain crossovers. In the absence of external random torques, the direction of grain angular momentum \( J \) remains constant during a crossover, while the grain itself flips over. In the presence of random torques (arising, for instance, from gaseous bombardment), the degree of correlation of the direction of \( J \) before and after a crossover is determined by \( J_{\min} \), the minimum value of \( |J| \) during the crossover. Since a grain tends to rotate about its axis of maximal moment of inertia (hereafter “the axis of major inertia”), SM79 showed that the systematic torque components perpendicular to this axis are averaged out and the crossover is caused by changes in \( J_\parallel \) due to the component of the torque parallel to the axis.\(^2\) Midway through the flipover, \( J_\parallel = 0 \) and \( J_{\min} = J_\perp \).

The timescale for Barnett relaxation is much shorter than the

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\(^1\) Crossovers are caused by various grain surface processes that change the direction (in body coordinates) of the systematic torques.

\(^2\) The indices \( \parallel \) and \( \perp \) denote components parallel and perpendicular to the axis of major inertia.
time between crossovers. Thermal fluctuations cause the axis of major inertia to deviate from $J$ (Lazarian 1994). The deviations are given by a Boltzmann distribution (Lazarian & Roberge 1997) which, for an oblate grain (e.g., an $a \times b \times b$ "brick" with $b > a$) with "vibrational" temperature $T_J$ is

$$f(\beta) d\beta = \text{const} \times \sin \beta \exp \left[ -E_s(\beta)/kT_J \right] d\beta; \quad (1)$$

$$E_s(\beta) = J^2 \left[ 1 + \sin 2\beta \left( \frac{l_1}{l_2} - 1 \right) \right]$$

is the kinetic energy, and $\beta$ is the angle between the axis of major inertia and $J$. We define

$$J_f \equiv \left( \frac{l_1 l_2 kT_J}{l_1 - l_2} \right)^{1/2} \approx (2l_1 kT_J)^{1/2}, \quad (3)$$

where the approximation assumes $l_1 \approx 1.5l_2$, as for an $a \times b \times b$ brick with $b/a = \sqrt{3}$. The Barnett relaxation time is (P79)

$$t_b = 8 \times 10^{-7} a_s^2 (J_\alpha J)^2 s, \quad (4)$$

where $a_s \equiv a/10^{15}$ cm. For $J > J_b$, the most probable value of $\beta$ for distribution (1) has $J_\beta = J \sin \beta = J_\alpha$, while for $J < J_f$ the most probable value of $\beta$ is $\pi/2$. It follows from equation (1) that during suprathermal rotation ($J_f > J_f^0$), the fluctuating component of angular momentum perpendicular to the axis of major inertia ($J_f^0$) is $\approx J_f^0$.

SM79 defined the crossover time as $t_c = 2J_f/|J|$, where $J_f$ is the time derivative of $J_f$. If $t_f \ll t_c$, the Barnett fluctuations can be disregarded during a crossover, and $J_f = \text{const} \approx J_f$ (LD97). The corresponding trajectory is represented by a dashed line in Figure 1. Initially the grain rotates suprathermally with $\beta \approx 0$; $\beta$ crosses through $\pi/2$ during the crossover, and $\beta \rightarrow \pi$ as the grain spins up again to suprathermal velocities.

The condition $t_f = t_b$ was used in LD97 to obtain a critical grain size $a_c \approx 1.5 \times 10^{-5}$ cm. It was shown that $t_c < t_f$ for $a > a_c$, and paramagnetic dissipation can achieve an alignment of $\sim 80\%$ for typical values of the interstellar magnetic field. If alignment were suppressed for $a < a_c$, this would explain the observed dichotomy in grain alignment: large grains are aligned, while small grains are not.

What spoils this nice picture is that sufficiently strong thermal fluctuations can assist crossovers: fluctuations in $\beta$ span $[0, \pi]$ and therefore have a finite probability to flip a grain over for an arbitrary value of $J$. The probability of such fluctuations is small for $J_f^0 > J_f^0$, but becomes substantial when $|J|$ approaches $J_f$. Indeed, it is obvious from equation (1) that in the latter case, the probability of $\beta \sim \pi/2$ becomes appreciable.

LD98 show that the probability per unit time of a flipover due to fluctuations is

$$t_f^{-1} \approx t_b^{-1} \exp \left[ -(1/2)(J/J_\alpha)^2 - 1 \right]. \quad (5)$$

Whether the grain trajectory is approximately a straight line in Figure 1 (a "regular crossover") or two lines connected by an arc (a "thermal flip") depends on the efficacy of the Barnett relaxation. Roughly speaking, thermal flipping happens when $t_f \ll J/J_\alpha$. If $J \approx J_f$, the ratio of the flipping and crossover time $t_f/t_c \approx t_b/t_c$. The latter ratio was found in LD97 to be equal to $(a/a_c)^{3/2}$. Therefore, flipping was correctly disregarded in LD97, in which only grains larger than $a_c$ were considered, but should be accounted for if $a < a_c$.

The last issue is the problem of multiple flips; a grain with $\beta > \pi/2$ can flip back. Thermal flips do not change $J$. Therefore, after a flip (from quadrant $\beta < \pi/2$ to quadrant $\beta > \pi/2$ in Fig. 1), the grain has the same $J$ as before the flip. For $J > J_f$, the thermal distribution (eq. [1]) has two most probable values of $\beta$: $\beta_+ = \sin^{-1}(J/J_\alpha)$ and $\beta_- = \pi - \beta_+$. For both $\beta_+$ and $\beta_-$, we have $J_f = J_f$. If we idealize the grain dynamics as consisting of systematic torques changing $J_f$ with $J_f = \text{const}$, plus the possibility of instantaneous "flips" (at constant $J$) between $\beta_+$ and $\beta_-$, then we can estimate the probability of one or more flips taking place during a crossover. Let $\phi(\beta)d\beta = t_f' dfb$ be the probability of a flip from $\beta$ to $\pi - \beta$ while traversing $d\beta$.

The probability of zero flips between $0$ and $\beta$ is $f_0(\beta) = \exp\left[ -\int_0^\beta \phi(x')dx' \right]$. The probability of a regular crossover (zero flips) is $p_{\text{reg}} = f_0(\pi) = e^{-2\alpha}$, where

$$\alpha \equiv \int_0^{\pi/2} \phi(x)dx \approx \sqrt{\frac{\pi}{2}} \frac{t_f}{t_b} \approx \sqrt{\frac{\pi}{2}} \left( \frac{a}{a_c} \right)^{3/2}. \quad (6)$$

Similarly, $d_{\alpha 0} = f_0' d\beta$ is the probability of one forward flip in the interval $d\beta$ with no prior or subsequent flips, and the probability of exactly one forward and zero backward flips during the crossover is $p_{\text{f0}} = f_0(\pi/2) = (1 - e^{-2\alpha})/2$. Therefore, the probability of one or more backward flips is $1 - p_{\text{reg}} - p_{\text{f0}} = (1 - e^{-2\alpha})/2 \rightarrow 1/2$ for $a \ll a_c$.

3. EFFICACY OF PARAMAGNETIC ALIGNMENT

SM79 showed that disalignment of suprathermally rotating grains occurs only during crossovers, whereas thermally rotating grains undergo randomization all of the time. Consider a grain subject to a damping torque $-J_t$, where $J_t$ is the rotational damping time, and random (nonsystematic) torques providing an excitation rate $\Delta^2/\Delta t$. Thermally rotating grains have $\langle J^2 \rangle = (1/2)J_t^2(\Delta^2/\Delta t)$ \equiv $J_{\text{th}}^2$. This definition of thermally rotating grains encompasses rotation excited by random $H_2$ formation, so long as the associated torques have no systematic component. For suprathermally rotating grains, $J_f > J_{\text{th}}$.

In what follows, we roughly estimate the efficacy of grain alignment for $t_f \gg t_b$, i.e., $a < a_c$. Following P79, we assume that $H_2$ torques are the dominant spin-up mechanism.

A crossover requires $N \sim J_{\text{min}}/(\Delta J)$ impulse events, where
$J_{\text{min}}$ is the minimum $J$ reached during the crossover, and the mean impulse per recombination event (see SM79) $(\Delta J)_I \approx (2n_t \nu \epsilon E/3\nu)^{1/2}$, where $\nu$ is the number of active recombination sites and $E$ is the kinetic energy per newly formed H$_2$. If $N$ is multiplied by the sum of mean squared random angular momentum impulses $(\langle \Delta J_I^2 \rangle + \langle \Delta J_{\text{th}}^2 \rangle)$, it gives the mean squared change of $J$ during a crossover. Therefore, the mean squared change of angle during a flipping-assisted crossover is

$$\langle F \rangle \approx \frac{N(\Delta J_I^2 + \Delta J_{\text{th}}^2)}{J_{\text{min}}^2} \approx \frac{\langle \Delta J_I^2 \rangle + \langle \Delta J_{\text{th}}^2 \rangle}{J_{\text{min}}^2},$$

which differs only by a factor of order unity from the expression for disorientation parameter $F$ in SM79, provided that $J_{\text{min}}$ is used instead of $J_c$. The latter is the major difference between the regular crossovers that were described by SM79 and LD97 and our present study. SM79 and LD97 dealt with the case for small grains. The critical question now is, Can the systematic torques drive small grains to large enough $J/J_0$ to suppress the thermal flipping, or is the thermal flipping sufficiently rapid to suppress the superthermality?

Consider a grain with a systematic torque $(G - 1)^{1/2}t_d/J$ along the major axis (fixed in grain coordinates). The condition $J_{\text{min}} = J \times t_d(J_{\text{min}})$ becomes

$$t_d(J_{\text{min}}) = \frac{J_{\text{min}}/J_0}{(G - 1)^{1/2}}.$$  

(11)

Thermal flipping causes the systematic torque to randomly change sign in inertial coordinates, so that

$$\langle J^2 \rangle = J_0^2 + \frac{(G - 1)J_0^2 t_d}{(t_d + t_L)},$$

(12)

giving a condition for $t_d$ in terms of $\langle F \rangle$:

$$\frac{t_d}{t_L} = \frac{\langle J(J/J_0)^2 \rangle - 1}{G - \langle J(J/J_0)^2 \rangle}.$$  

(13)

For given $a$, $G$, and $(J/J_0)^2$, equations (10) and (13) have either one or three solutions for $\langle F \rangle$. If $(G)^{1/2}$ has multiple solutions $J_1 < J_2 < J_3$, the intermediate solution $J_2$ is unstable: if $J < J_2$, then $t_d$ from equation (10) is smaller than the value required by equation (13), so $J \rightarrow J_1$; if $J > J_2$, then $J \rightarrow J_3$. In the former case, thermal flipping leads to suppression of suprathermal rotation: if the grain enters the region $J < J_2$, then it is trapped with $J \approx J_1$ until a fluctuation brings it to $J > J_2$. The timescale for such a fluctuation is $\tau_{\text{flip}} \approx t_d \exp [(J/J_0)^2]$. We refer to this phenomenon as “thermal trapping.”

As an example, consider $a(J/J_0)^2 = 5$, $G = 10^3$, and $A = 0.5$. Thermal flipping takes place during a crossover at $t_{\text{flip}} \approx 5.9J_0$. If $J^2$ drops below $J_0^2 \approx 4.5J_0^2$, the grain will be thermally trapped. For this case, thermal flipping will tend to maintain the grain at $\langle J^2 \rangle \approx J_0^2 \approx 1.02(J_0)^2$ unless thermal fluctuations succeed in getting the grain to $J > J_3$, in which case thermal flipping is unable to prevent the grain spinning up to a superthermality $(J/J_0)^2 \approx G = 10^3$. For this example, the thermal flipping time $t_{\text{flip}} \approx 50 t_D$. During this time, paramagnetic alignment will be minimal. Grains that escape the thermal trap become suprathermal and align on the timescale for paramagnetic alignment.

Let $\eta$ be the probability per crossover of becoming thermally trapped. The fraction of grains that are not thermally trapped at any time is $x = t_d/(t_d + \eta t_{\text{flip}})$. We can estimate the grain alignment by using equations (8) and (9) with $A = x$ and $C = [1 - \exp (-\langle F \rangle)][1 - (1 - x)[1 - \exp (-\langle F \rangle)]^{-1}$.

During a crossover, the first thermal flip occurs at $J \approx J_{\text{min}}$, only a bit larger than $J$, the thermal trapping boundary. We have seen above that for $a < a_\ast \approx 0.5$, for which we estimated $t_{\text{flip}} \approx 50 t_L$, we see that the fraction of grains that are not trapped, $x = J/(1 + 50\eta t_d/t_L)$, could be small if $\eta \approx 0.1$. More detailed studies of the dynamics are required to estimate $\eta$, and to provide more reliable estimates of $t_{\text{flip}}$ before we can quantitatively estimate the degree to which thermal trapping will suppress the alignment of small grains.

Inspection of Figure 2 shows that thermal trapping solutions
are only found if \( G \) is not too large (e.g., for \( G = 10^7 \), we have no thermal trapping solution in Fig. 2 for \( a_s = 0.5 \)). Such degrees of superthermality would follow from variations of accommodation coefficient and photoelectric yield, but higher values have been estimated for \( \Sigma_2 \) torques (P79, LD97).

For example, LD97 estimate \( G = 2 \times 10^7 a_s (\gamma/0.2)^2 \times (10^{11} \text{ cm}^{-2} / \alpha) \), where \( \alpha \) is the surface density of active chemisorption sites. The values of \( G \approx 10^4 \) required for thermal trapping to be possible for \( a_s \approx 0.5 \) grains would appear to require \( (\gamma/0.2)^2 / \alpha \approx 10^{-14} \text{ cm}^2 \). If essentially every surface site is an active chemisorption site, we could have \( \alpha \approx 10^{14} \text{ cm}^{-2} \); alternatively, it is conceivable that \( \gamma \ll 1 \) for very small grains. The latter idea was advocated by Lazarian (1995), who found that oxygen poisoning of catalytic sites is enhanced for grains with \( a < 10^{-3} \text{ cm} \). Recent experimental work (Pirronello et al. 1997a, 1997b) suggests that \( \gamma \) may be much smaller than is usually assumed. Moreover, recent research (Lazarian & Efroimsky 1999; Lazarian & Draine 1999) shows that faster processes of internal relaxation are possible. These processes should enable thermal trapping for larger values of \( G \).

5. CONCLUSIONS

Thermal flipping is a critical element of the dynamics of small \((a \approx 10^{-5} \text{ cm})\) grains. If small grains rotate suprathermally, then thermal flipping would promote their alignment by suppressing disalignment during "flipping-assisted" crossovers. Since small grains are observed to not be aligned, it follows that most must not rotate suprathermally.

One way for small grains to not rotate suprathermally would be for the systematic torques from \( \Sigma_2 \) formation and photoelectric emission to be much smaller than current estimates. However, we also find that thermal flipping can result in thermal trapping, whereby rapid thermal flipping can prevent systematic torques from driving small grains to suprathermal rotation rates. As a result, at any given time an appreciable fraction of small grains are thermally trapped and being disaligned by random processes.

The thermal trapping effect is of increasing importance for smaller grains and may explain the observed minimal alignment of \( a \approx 5 \times 10^{-6} \text{ cm} \) dust grains (Kim & Martin 1995).

Note added in manuscript.—After acceptance of this Letter, we learned of calculations by W. G. Roberge & K. E. S. Ford (1999, private communication) that confirm the accuracy of equation (5) for \( J / J_\star \geq 1 \).

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