THERMAL FLIPPING OF INTERSTELLAR GRAINS

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ABSTRACT

In interstellar dust grains, internal processes dissipate rotational kinetic energy. The dissipation is accompanied by thermal fluctuations, which transfer energy from the vibrational modes to rotation. Together, these processes are known as internal relaxation. For the past several years, internal relaxation has been thought to give rise to thermal flipping, with profound consequences for grain alignment theory. I show that thermal flipping is not possible in the limit that the inertia tensor does not vary with time.

Key words: dust, extinction – ISM: magnetic fields

1. INTRODUCTION

Two processes act in concert to align grains with the interstellar magnetic field: (1) the grain’s principal axis of greatest moment of inertia \( \hat{a}_1 \) aligns with respect to its angular momentum vector \( \mathbf{J} \) and (2) \( \mathbf{J} \) aligns with respect to the magnetic field vector \( \mathbf{B} \). Purcell (1979) noted that internal mechanisms for dissipating rotational energy drive the grain to its lowest energy state for a given \( \mathbf{J} \), namely steady rotation with \( \hat{a}_1 \parallel \mathbf{J} \). This occurs on a much shorter timescale than that on which external processes align \( \mathbf{J} \) relative to \( \mathbf{B} \).

Purcell (1979) identified two internal dissipation mechanisms. Inelastic dissipation results from the periodic mechanical stresses experienced by a grain that does not rotate steadily about a principal axis. The existence of this process is fairly obvious, but calculating the dissipation rate is a challenging problem (e.g., Sharma et al. 2005 and references therein). Purcell (1979) introduced a second, subtle effect, which he termed “Barnett dissipation.” When a grain does not rotate steadily about a principal axis, the angular velocity vector \( \mathbf{\omega} \) varies periodically in a coordinate system attached to the grain. If the grain consists of a paramagnetic material, then the microscopic spins (with gyromagnetic ratio \( \gamma_\mathbf{g} \)) attempt to align with the fictitious “Barnett-equivalent” magnetic field \( \mathbf{B}_{\mathrm{BE}} = \mathbf{\omega}/\gamma_\mathbf{g} \). As the grain magnetization attempts to follow \( \mathbf{B}_{\mathrm{BE}} \), rotational kinetic energy is dissipated. This process is analogous to a magnetic resonance experiment, where the dissipated energy is provided instead by the applied radiation field.

Purcell (1979) provided a heuristic derivation of the Barnett dissipation rate for oblate grains with dynamic symmetry. “Dynamic symmetry” refers to the case that \( I_2 = I_3 \), where \( I_i \) are the moments of inertia associated with the principal axes \( \hat{a}_i \). Thus, for oblate grains with this symmetry, \( I_1 > I_2 = I_3 \). (Henceforth, the term “oblate” shall always refer to dynamic, rather than geometric, symmetry.) In this case, \( \mathbf{B}_{\mathrm{BE}} \) consists of a static component \( \omega_{\parallel}/\gamma_\mathbf{g} \hat{a}_1 \) plus a component \( \mathbf{B}_{\mathrm{BE, \text{rot}}} \) with magnitude \( \omega_{\perp}/\gamma_\mathbf{g} \) that rotates in the \( \hat{a}_2 - \hat{a}_3 \) plane with angular speed \( \omega_{\text{rot}} \). Solving the Euler equations yields

\[
\omega_{\parallel} = \frac{J}{I_1} \cos \gamma, \tag{1}
\]

\[
\omega_{\perp} = \frac{J}{I_2} \sin \gamma, \tag{2}
\]

and

\[
\omega_{\text{rot}} = \frac{J(I_1 - I_2)}{I_1 I_2} \cos \gamma, \tag{3}
\]

where \( \gamma \) is the (constant) angle between \( \mathbf{J} \) and \( \hat{a}_1 \). Assuming \( \mathbf{J} \) and \( I_1 \) are constant, it is convenient to introduce a dimensionless measure of the rotational energy \( E \):

\[
q \equiv \frac{2 I_1 E}{J^2} = 1 + (r_2 - 1) \sin^2 \gamma, \tag{4}
\]

where the final equality is for oblate grains. Note that, for oblate grains, \( q \) ranges from 1 to \( r_2 \equiv I_1/I_2 \).

Purcell (1979) argued that the dissipation rate is given by

\[
\left( \frac{dE}{dt} \right)_{\text{Bar}} = -V \chi'' B_{\text{BE, rot}} \omega_{\text{rot}}, \tag{5}
\]

where \( V \) is the grain volume and \( \chi'' \) is the imaginary component of the magnetic susceptibility. It is worth noting that, although this expression (as well as a variant in Lazarian & Draine 1999b) is widely used in grain alignment theory, it has not yet been rigorously derived or experimentally verified. Purcell adopted the low-frequency susceptibility

\[
\chi'' \approx \chi_0 \omega_{\text{rot}} T_2, \tag{6}
\]

where \( \chi_0 \) is the static susceptibility and \( T_2 \) is the spin–spin relaxation time.

Combining Equations (1)–(6) yields

\[
\frac{dq}{dt} = -\tau_{\text{Bar}}^{-1}(q - 1)(r_2 - q), \tag{7}
\]

with

\[
\tau_{\text{Bar}} = \frac{\gamma_0^2 I_1 I_2^2}{2 V \chi_0 T_2 T_2^2}. \tag{8}
\]

More realistic approximations for \( \chi'' \) (e.g., Draine & Lazarian 1999) yield more complicated expressions for \( dq/dt \), but retain the linear dependence on \((q - 1) \) and \((r_2 - q) \) near \( q = 1 \) and \( q = r_2 \), respectively.

In the inverse process of Barnett dissipation, a fluctuation spontaneously transfers some energy from the thermal reservoir provided by the grain vibrational modes to the grain rotation. Lazarian & Draine (1997) showed that these thermal fluctuations can play an important role in grain alignment. They examined the classic alignment model, developed by Purcell (1975, 1979), in which a systematic torque \( T_{\text{sys}} \), fixed in grain body coordinates, spins the grain to “suprathermal” rotation. Thermal rotation, arising solely from collisions with particles from a gas
with temperature $T_{\text{gas}}$, is characterized by $J \sim J_0 \equiv \sqrt{J_0 k_B T_{\text{gas}}}$ ($k_B$ is Boltzmann’s constant). Suprathermally rotating grains, with $J \gg J_0$, are impervious to disalignment by random collisions with gas atoms. Thus, $J$ can gradually align with $B$ via the Davis & Greenstein (1951) mechanism. Purcell (1979) found that the most important systematic torque results from the formation (and subsequent ejection) of $H_2$ molecules at special sites on the grain surface.

The distribution of molecule-forming surface sites can change rapidly compared with the Davis–Greenstein alignment rate (see, e.g., Lazarian 1995). As a result of this resurfacing, $\Gamma_{\text{sys}}$, $\dot{a}_1$ may reverse sign, sometimes spinning the grain down to thermal rotation. (In inertial coordinates, $\Gamma_J$ limits the minimum value of $J$.) Suprathermal thermal fluctuations cause the angle of thermal flipping and thermal trapping. For an oblate grain, in–alignment. Lazarian & Draine (1999a) introduced the concepts $\dot{a}_1$ with temperature $T$.

Information (and subsequent ejection) of $H_2$ molecules at special $\sim J$.

Thus, for oblate grains, the thermal equilibrium distribution function is

$$S(q) = A f - \frac{1}{2} d(f D) dq$$

(Equation 5.2.8 in Gardiner 2004).

Weingartner & Draine (2003) defined the quantity

$$s \equiv 1 - \frac{2}{\pi} \int_0^{\alpha_{\text{max}}} d\alpha \left[ I_3(I_1 - I_2q) + I_1(I_2 - I_3) \cos^2 \alpha \right]^{1/2},$$

where

$$\alpha_{\text{max}} = \begin{cases} \pi/2, \quad q \leq I_1/I_2 \\ \cos^{-1} \left[ \frac{I_3(I_2q - I_1)}{I_1(I_2 - I_3)} \right]^{1/2}, \quad q > I_1/I_2, \end{cases}$$

and showed that the density of energy states is constant in $s$. This holds for grains with arbitrary $I_1$, $I_2$, and $I_3$. For oblate grains ($I_2 = I_3$),

$$s = 1 - \left( \frac{r_2 - q}{r_2 - 1} \right)^{1/2}.$$

Thus, for oblate grains, the thermal equilibrium distribution function is

$$f_{\text{TE}}(q) \propto \exp(-kq) \frac{ds}{dq} \propto \exp(-kq)(r_2 - q)^{-1/2},$$

where

$$k \equiv \frac{J_0^2}{2I_1 k_B T_d}.$$

The thermal equilibrium distribution function is more complicated for grains lacking dynamic symmetry, but still depends on $k$.

The impossibility of thermal flipping can be simply demonstrated by examining the relaxation at $q = r_2$ in the limit that the dust temperature $T_d \to 0$. In this limit, $k \to \infty$. As $T_d \to 0$, fluctuations cease to contribute to the probability current $S(q)$, implying that $d(f D)/dq \to 0$. This limiting
behavior must hold for all \( q \) (including \( q = r_2 \)) and for any physically realizable probability distribution \( f(q) \). Normalization of \( f(q) \) requires that any divergence at \( q = r_2 \) shall be shallower than \( f(q) \propto (r_2 - q)^{-1} \), unless \( f(q) = \delta(q - r_2) \).

Of course, the contribution of drift to the current, \( A(q)f(q) \), must also vanish at \( q = r_2 \). Evidently, it is necessary that \( A(q) \) falls off linearly or faster with \( (r_2 - q) \) near \( q = r_2 \). Note that the Barnett dissipation rate of Equation (7) does satisfy this condition. Equation (8) suggests that \( \tau_{\text{bar}} \to 0 \) as \( T_d \to 0 \), since \( \chi_0 \propto T_d^{-1} \). However, this cannot be correct, since \( A(q) = r_2 \) would be undefined rather than zero as \( T_d \to 0 \). Equation (8) does not hold for \( T_d \) lower than the Curie temperature. For such low temperatures, the material is ferromagnetic, suggesting that \( \tau_{\text{bar}} \) approaches a nonzero constant as \( T_d \to 0 \).

Focusing now on the fluctuating term at \( q = r_2 \),

\[
\lim_{(k^{-1},r_2-q) \to (0,0)} \frac{d[(k,q)D(k,q)]}{dq} = 0. \tag{16}
\]

The limit only exists if it takes the same value for all paths along which \((k^{-1},r_2-q) \to (0,0)\). Since there exist paths for which \((r_2-q) \to 0 \) arbitrarily more rapidly than \( k^{-1} \to 0 \), \( d[(f,D)/dq] \) may not contain any divergences with respect to \( q = r_2 \). Thus, for \((r_2-q) \ll 1 \), \( f \) \( D \) must either (1) be independent of \((r_2-q) \) or (2) fall off linearly or faster with \((r_2-q) \). If condition (1) holds for a particular distribution \( f_1(q) \), then it will not hold for another distribution \( f_2(q) \) having a different dependence on \((r_2-q) \) near \( q = r_2 \). Thus, condition (2) must generally obtain, implying that \( D \) must fall off as \((r_2-q)^2 \) or faster near \( q = r_2 \). This implies that \( D \) and \( dD/dq \) both vanish at \( q = r_2 \). If the diffusion coefficient is smooth with respect to \( k \) (in the sense that \( dD/dk \) exists for all \( k \)), then these conditions must be satisfied for all \( k \).

Thus, \( A, D, \) and \( dD/dq \) all vanish at \( q = r_2 \), making this point a “natural boundary” (see Section 5.2.1e of Gardiner 2004). A system can never reach a natural boundary if it begins at a different point (i.e., with a different value of \( q \)). However, the system must reach \( q = r_2 \) and return to lower \( q \) (with a different sign for \( \cos \gamma \)) in order for a flip to occur (see Section 2.5.2 of Weingartner \\& Draine 2003). Consequently, thermal flipping is prohibited. This conclusion does not depend on the form of \( A(q) \), except that \( A(q) \) decreases as \((r_2-q) \) or faster for \( q \) near \( r_2 \). It holds for any type of internal relaxation and for grains with or without dynamic symmetry, so long as \( dD/dk \) exists for all \( k \).

If thermal flipping is truly prohibited, then this result must obtain regardless of the choice of variable. Although the current \( S \) is independent of variable, the two terms composing it, representing drift and diffusion, are not. When transforming variables in stochastic differential equations, the ordinary rules of calculus only apply for linear transformations. Otherwise, Ito’s formula must be used (see Section 4.3.3 of Gardiner 2004). When the Langevin Equation (9) is transformed to variable \( y(q) \), the result is

\[
dy = \left[ A(q) \frac{dy}{dq} + \frac{1}{2} D(q) \frac{d^2y}{dq^2} \right] dt + \sqrt{D(q)} \frac{dy}{dq} dw. \tag{17}
\]

Note the additional contribution to the drift coefficient when the Langevin equation is written in the new variable. Ito’s formula, along with the relation \( f(q)dy = f(y)dy \), yields

\[
\frac{d}{dy} [f(y)D(y)] = \frac{d}{dy} [f(q)D(q)] + f(q)D(q) \frac{d^2y/dq^2}{dy/dq}. \tag{18}
\]

If \( y(q) \propto (r_2-q)^p \) (with \( p \neq 0 \)) for \( q \) near \( r_2 \), then

\[
\frac{d^2y/dy^2}{dy/dq} \propto (r_2-q)^{-1}. \tag{19}
\]

Since \( D(q)f(q) \propto (r_2-q)^n \) with \( n > 1 \), the second term in Equation (18) vanishes at \( q = r_2 \). Thus, if the diffusion contribution to the current vanishes at the point \( q = r_2 \) for variable \( q \), then it does so for arbitrary variable.

To illustrate the above arguments in a concrete setting, I will now discuss the diffusion coefficient \( D(q) \) for an oblate grain and the approximate dissipation rate of Equation (7). Setting the probability current equal to zero for thermal equilibrium yields

\[
D(q) = \frac{1}{f_{\text{TE}}(q)} \left[ D(1)f_{\text{TE}}(1) + 2 \int_0^q A(q')f_{\text{TE}}(q') \, dq' \right]. \tag{20}
\]

Upon integrating,

\[
k^2 \tau_{\text{bar}} D(q) = \left[ 3 + 2(k-1)(r_2-q) + C(k)(r_2-q)^{1/2} \times \exp(kq) - k^{-1}[3 + 2(k-1)](r_2-q)^{1/2} \times \exp[-k(r_2-q)] \int_0^{\sqrt{k(r_2-q)}} \exp(x^2) \, dx \right] \tag{21}
\]

with

\[
C(k) = k^2 \exp(-k)(r_2-1)^{-1/2} D(q = 1, k) \tau_{\text{bar}} - 3 \exp(-k)(r_2-1)^{1/2} + k^{-1}[3 + 2k(r_2-1)] \times \exp(-kr_2) \int_0^{\sqrt{k(r_2-1)}} \exp(x^2) \, dx. \tag{22}
\]

For \((r_2-q) \ll 1 \),

\[
k^2 \tau_{\text{bar}} D(q, k) \approx C(k) \exp(kq)(r_2-q)^{1/2} + \frac{4k^2}{(r_2-1)^2} \frac{1}{(r_2-q)^2}, \quad (r_2-q) \ll 1. \tag{23}
\]

The term containing \( C(k) \) does not fall off sufficiently quickly with \((r_2-q) \). Thus, \( C(k) = 0 \) identically (for all \( k \), if \( dD/dk \) exists for all \( k \)). The remaining term varies as \((r_2-q)^2 \), the shallowest permissible dependence. Note that the term containing \( C(k) \) satisfies condition (1) following Equation (16) for the thermal equilibrium distribution \( f_{\text{TE}}(q) \), but not the required general condition (2).

Given the above general argument prohibiting thermal flipping induced by internal relaxation, one may ask how Lazarian \\& Draine (1999a) concluded that thermal flipping is possible. Their analysis was highly approximate and did not employ any diffusion coefficient. Nevertheless, their estimate of the flipping rate agreed well with the detailed analysis of W. G. Roberge \\& K. E. S. Ford (1999, private communication), which made use of the Barnett relaxation diffusion coefficient calculated by Lazarian \\& Roberge (1997).

Lazarian \\& Roberge (1997) solved a modified version of Equation (10) for the diffusion coefficient, in which they used the angle \( \gamma \) rather than \( q \) as the variable. They considered oblate grains and the approximate Barnett dissipation rate in Equation (7). Using Equation (4) to substitute for \( q \) in terms of \( \gamma \) in Equation (7), they adopted

\[
A(\gamma) = -\frac{r_2 - 1}{2 \tau_{\text{bar}}} \sin \gamma \cos \gamma \tag{24}
\]

(see their Equations 1, 2, 4, and 16). In Purcell’s (1979) heuristic derivation of the Barnett dissipation rate, he obtained the rate at which the rotational energy \( E \) decreases. In other words, he obtained the drift coefficient \( A(E) \). Since \( q \propto E \), there is
no additional contribution to the drift coefficient arising from Ito’s formula (17) when the Langevin equation is written in the variable $q$. However, the variable in Lazarian & Roberge (1997) is the angle $\gamma$, which is a nonlinear function of $E$ (Equation (4)). The additional contribution to the drift coefficient was not included in their analysis. Despite this error, the above general argument should still yield vanishing $D$ and $dD/d\gamma$ at $\gamma = \pi/2$, and thus no thermal flipping.

In the vicinity of $\gamma = \pi/2$ (corresponding to $q = 1$), the diffusion coefficient calculated by Lazarian & Roberge (1997; their Equation (18)) is

$$
\tau_{\text{Bar}} D(\gamma) = \tau_{\text{Bar}} D(\gamma = \pi/2) + \left\{ 1 - \left( r_2 - 1 \right) k - \frac{1}{2} \right\} \times \tau_{\text{Bar}} D(\gamma = \pi/2) (\gamma - \pi/2)^2.
$$

(25)

If $D(\gamma = \pi/2)$ is taken to be zero, then $D \propto (\gamma - \pi/2)^2$, as required. In this case, thermal flipping does not occur. Lazarian & Roberge (1997) argued that $D$ should be smooth with respect to $\gamma$ and demanded that $d^2 D/d\gamma^2$ exist for all $k$. This condition is satisfied if $D(\gamma = \pi/2) = 0$ or if $D \propto k^n$ with $n \leq -1$. Lazarian & Roberge (1997) chose $D \propto k^{-1}$, which admits thermal flipping but is inconsistent with the requirement that $D(\gamma)$ falls off at least as quickly as $(\gamma - \pi/2)^2$ for $\gamma$ near $\pi/2$. (There appear to be some typographical errors in Lazarian & Roberge (1997). In their Equation (19), $D \propto k^{-1/2}$ rather than $k^{-1}$. In their Equation (18), $D(\gamma = \pi/2) = 1$ rather than falling off as $k^{-1/2}$ or $k^{-1}$.)

Lazarian & Roberge (1997) tested their result for the diffusion coefficient by numerically evolving their Langevin equation for a large number of Barnett timescales and computing the average value of the internal alignment factor

$$
Q_X \equiv \frac{3}{2} \left\{ \cos^2 \gamma - \frac{1}{3} \right\}.
$$

(26)

This can also be evaluated by simple integration for a thermal distribution (their Equation (10)). The results of their simulations agreed to high accuracy with the direct calculations. They adopted the wrong Langevin equation but the correct thermal equilibrium distribution function. Their success with the test indicated that they solved Equation (10) correctly given their drift coefficient, but this drift coefficient does not describe Barnett dissipation when angle $\gamma$ is taken as the variable.

As a confidence-building check on the conclusion that thermal flipping is prohibited, I numerically evolved the Langevin equation for the case that $k = 1$ and $r_2 = 1.5$, taking $C = 0$. A fixed time step size is attempted at each step. Sometimes this results in overshooting $q = 1$; in these cases, smaller steps are tried until the resulting $q$ exceeds 1. These overshooting incidents become fractionally less common as the base step size is decreased (from $10^{-2} \tau_{\text{Bar}}$ to $10^{-5} \tau_{\text{Bar}}$). The total duration of a simulation is about $10^5 \tau_{\text{Bar}}$. At no time, for any of the base step sizes, did $q$ ever overshoot $r_2$. Incidentally, the simulations yielded the correct value for the alignment factor $Q_X$, although the convergence was slower than for the simulations in Lazarian & Roberge (1997).

The above argument that $D$ and $dD/dq$ both vanish at $q = r_2$ made no reference to the form of $A(q)$. Thus, this conclusion also holds when more realistic Barnett dissipation rates are adopted, and even for grains lacking dynamic symmetry. In all of these cases, $A(q = r_2) = 0$, since the grain is in steady rotation when $q = r_2$. Thus, $q = r_2$ is a natural boundary for the most general treatment of Barnett relaxation, if $dD/dk$ exists for all $k$. Since a grain lacking dynamic symmetry must reach (and, in general, cross) $q = r_2$ in order to flip (see Section 2.5.2 of Weingartner & Draine 2003), thermal flipping associated with Barnett relaxation is ruled out generally. The only caveat is that $dD/dk$ must exist for all $k$. Although this seems natural, a detailed model of Barnett relaxation would be needed to confirm that this condition is indeed satisfied.

The discussion here has focused on Barnett relaxation, since Barnett dissipation appears to dominate inelastic dissipation for most thermally rotating grains (Lazarian & Efroimsky 1999), especially when nuclear paramagnetism contributes. However, the argument against thermal flipping applies equally well for inelastic relaxation. Lazarian & Efroimsky (1999) did not constrain the form of the dissipation rate near $q = r_2$, but Sharma et al. (2005) found the same form as in Equation (7) for the special case of an oblate spheroid.

3. CONCLUSION

In conclusion, it appears that thermal flipping is not possible, so long as $dD/dk$ exists for all $k$ and the inertia tensor does not vary with time. A detailed model of Barnett relaxation is needed to examine the behavior of $dD/dk$.

Because of grain vibrations, the inertia tensor exhibits continual, small variations. As a result, the location of the natural boundary at $q = r_2 \equiv I_1/l_2$ wanders slightly (B. T. Draine, private communication). Further work is needed to examine whether this can give rise to flips and, if so, at what rate.

External processes (e.g., gas atom impacts) may also induce flips (with accompanying changes in $J$), but have recently been neglected in comparison with internal relaxation (e.g., Weingartner & Draine 2003). These now merit further scrutiny as well.

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