

Dynamic magnetic response of magnetic multicore particles: Competing anisotropies

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Magnetic multicore nanoparticles offer a versatile route to tuning magnetic response via particle geometry and internal structure. In this work, we investigate the dynamic magnetic behavior of ellipsoidal multicore particles, focusing on the interplay between elongation, intercore dipolar interactions, and magnetic anisotropy. Using Brownian dynamics simulations with explicit Néel and Brownian relaxation, combined with a spectral reconstruction method based on non-negative least-squares fitting of autocorrelation functions, we resolve the underlying relaxation modes across a wide frequency range. To interpret the simulation results, we develop a theoretical model for the static susceptibility of multicore ellipsoids that incorporates demagnetization effects within a modified mean-field framework. We show that while elongation merely shifts the Brownian relaxation peak in weakly interacting systems, it strongly enhances dipolar correlations at higher interaction strengths, leading to spectral broadening, multiple relaxation modes, and a redistribution of dissipation towards lower frequencies. As a consequence, elongated multicores display a specific loss power at low frequencies that is improved by over an order of magnitude, while maintaining their performance at high frequencies without any decrease. This behavior is particularly relevant for magnetic hyperthermia, where operational constraints limit the accessible frequency range. Our findings provide a microscopic basis for tailoring magnetic response through particle shape and internal architecture.

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I. INTRODUCTION

Magnetic soft matter comprises a broad class of systems whose macroscopic behavior emerges from the interplay between thermal fluctuations, magnetic interactions, and particle architecture widely used nowadays for applications in technology [1–3], arts [4], and biomedicine [5–10].

Since the early theoretical description of noninteracting magnetic moments by Langevin and later Elmore [11,12] and the subsequent realization of stable ferrofluids [13,14], it has become clear that even subtle changes in particle properties—such as size [1,15–17], anisotropy [18–29], or shape [30–35]—can qualitatively alter magnetic response. Although single-core spherical nanoparticles have long served as the canonical model system, advances in synthesis now allow for precise control over particle shape [36–41] and internal structure [42–45], motivating a reexamination of the fundamental assumptions underlying magnetic self-assembly and dynamics.

One particularly striking example of the importance of particle shape arises in systems of ellipsoidal magnetic particles [46–54]. Even at the level of simple point-dipole models,

ellipsoids behave fundamentally differently from spheres: Instead of forming chainlike aggregates aligned with the magnetic field, elongated particles tend to arrange themselves into antiparallel or side-by-side configurations [55]. This behavior originates from the anisotropic demagnetizing fields and orientational constraints imposed by particle shape, and it profoundly modifies both equilibrium structures and dynamical processes. As a result, magnetic correlations, relaxation pathways, and collective response functions in ellipsoidal systems deviate markedly from those of their spherical counterparts.

At the same time, increasing attention has been directed towards multicore magnetic particles, in which several single-domain magnetic nanocrystals are embedded within a larger, typically rigid, nonmagnetic matrix [56–69]. Such particles introduce additional internal degrees of freedom: magnetic interactions between the cores, correlations mediated by the surrounding matrix, and multiple relaxation mechanisms operating on distinct length and timescales [70,71]. Magnetic multicores have already emerged as a source of innovation in the field of drug targeting [7,72], particle imaging [57,73], and immunoassays or biosensing [59,74–76]. Besides biomedical applications, multicore magnetic nanoparticles (MMNPs) also find use in nanorheology [77–80] and for the degradation of endocrine disrupting chemicals such as bisphenol A in water [81].

Previous studies have demonstrated that multicore architecture can significantly enhance magnetic losses and modify relaxation spectra compared to single-core particles, even when the overall particle size is comparable [60,82–84]. Overall, the architecture and magnetic properties of MMNPs are

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closely linked to their synthesis process [85,86]. Tomography [87], scattering experiments [88,89], and the first-order reversal curves diagram method [90–92], among others, are of significant aid for a detailed analysis of internal structure. It has recently been shown that changes in the shape and architecture of multicore magnetic nanoparticles significantly affect their thermomagnetic response, opening up broad prospects for various applications [56,93]. Examples of shape modification include ring-shaped [94] and cubic [41,95] MMNPs.

In multicore magnetic ellipsoids, however, the two sources of anisotropy—geometrical shape and internal magnetic architecture—are expected to interact in a nontrivial manner. The elongated shape not only affects the external magnetic interactions between particles but may also influence the spatial correlations between magnetic cores within a single particle, biasing their relative orientations and collective response. Such internal correlations are anticipated to leave distinct signatures in the dynamic magnetic susceptibility, altering both the characteristic relaxation times and the spectral weight associated with different relaxation modes.

In this work, we investigate the dynamic magnetic response of multicore magnetic ellipsoids with a particular focus on their zero-field susceptibility spectra. Using Brownian dynamics simulations combined with a microscopic description of magnetic relaxation at the level of individual cores, we analyze how particle shape and multicore architecture jointly determine magnetic correlations and relaxation mechanisms. By contrasting the behavior of ellipsoidal multicores with that of spherical particles and simple point-dipole models, we aim to clarify how shape-induced anisotropy reshapes magnetic dynamics. Our results provide insight into the fundamental processes governing the magnetodynamic response of complex magnetic particles and establish a framework for tailoring susceptibility spectra through controlled particle design, thus opening new avenues for controlled magnetic heating.

The structure of the paper is as follows. First, we describe the model and the set of parameters used to simulate magnetic multicore ellipsoidal particles. We begin Results with a discussion of ellipsoids carrying a point dipole and possessing an infinite magnetic anisotropy. Next, in the second part under Results, we analyze the impact of ellipsoidal elongation on the dynamic susceptibility spectra of multicore ellipsoids with finite anisotropy, with particular emphasis on the number and positions of the dissipation maxima. In the third part under Results, we elucidate this impact by calculating the demagnetization fields and examining their influence on intercore correlations, varying magnetic anisotropy and intercore interactions. The paper concludes with a brief summary and an outlook.

II. MODEL AND METHODS

A. Multicore ellipsoid

We consider a multicore magnetic nanoparticle modelled as a rigid composite object, as shown in Fig. 1(a). The shape of the modelled ellipsoid of revolution is characterized by the semiaxes ratio [Fig. 1(b)],

$$X_0 = \frac{b}{a}.$$

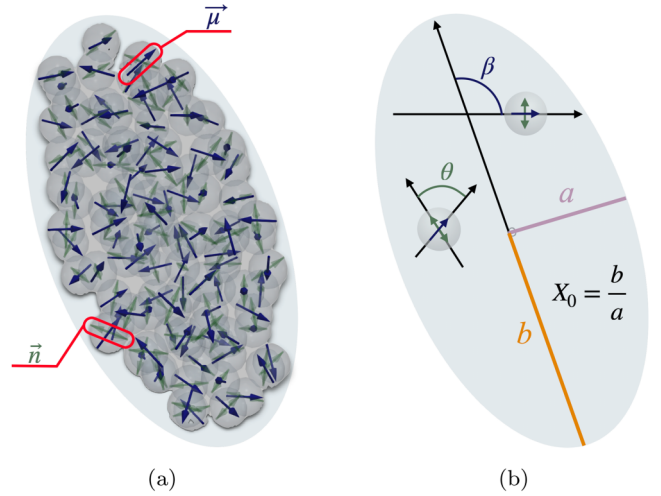


FIG. 1. (a) Snapshot of a multicore ellipsoidal particle. It contains $N_c = 100$ magnetic cores. The blue arrows denote the magnetic moments of the individual cores, while the green double-sided arrows indicate their corresponding magnetic anisotropy axes. (b) The overall multicore is modelled as an ellipsoid of revolution with semi-axes a and b , defining the aspect ratio $X_0 = b/a$. Each core moment forms an angle β with the long axis of the ellipsoid and an angle θ with its core magnetic anisotropy axis.

The particle consists of N_c identical, nonoverlapping spherical cores [darker spheres in Fig. 1(a)] of diameter d , mass m_c , and individual volume,

$$v_c = \pi d^3/6.$$

The cores are randomly and uniformly distributed within the ellipsoidal volume,

$$v_p = \frac{4\pi}{3} a^2 b.$$

Once assigned, the relative positions of the cores are fixed with respect to the particle body, forming a rigid cluster that can freely move and rotate in three dimensions. The volume fraction of cores inside the multicore particle is given by

$$\varphi_c = \frac{N_c v_c}{v_p}.$$

Each core has a magnetic moment vector $\vec{\mu} = \mu \hat{\mu}$, shown with blue arrows in Figs. 1(a) and 1(b) ($\hat{\mu} = \vec{\mu}/\mu$). The length of $|\vec{\mu}| = \mu$ is fixed, but its orientation $\hat{\mu}$ is defined by the balance between the internal anisotropy field, the dipolar field created by other cores, and thermal energy $k_B T$, where k_B is the Boltzmann constant and T is the absolute temperature. We assume that each core is governed by uniaxial magnetocrystalline anisotropy with randomly orientated easy axes represented by unit vectors $\hat{n}$, shown with green double arrows in Figs. 1(a) and 1(b). The magnitude of the anisotropy field is characterized by the product of the material anisotropy constant K_m and the volume of the core. As long as entropy plays a crucial part in the behavior of nanoscale magnetic particles, it is convenient to introduce a dimensionless anisotropy parameter:

$$\sigma = \frac{K_m v_c}{k_B T}.$$

The anisotropy energy of a single core is

$$U_{\text{ani}} = -K_m v_c (\hat{\mu} \cdot \hat{n})^2. \quad (1)$$

Interactions between the cores are modelled via dipole-dipole potential. For two magnetic moments $\vec{\mu}_1$ and $\vec{\mu}_2$ separated by the vector $\vec{r}$ (with magnitude $r = |\vec{r}|$) this energy has a form:

$$U_{dd} = \frac{\mu_0}{4\pi} \left[\frac{(\vec{\mu}_1 \cdot \vec{\mu}_2)}{r^3} - \frac{3(\vec{r} \cdot \vec{\mu}_1)(\vec{r} \cdot \vec{\mu}_2)}{r^5} \right], \quad (2)$$

where μ_0 is the vacuum permeability.

The total energy of the system includes both single-core anisotropy and intercore dipole-dipole interactions, quantified by the dimensionless coupling parameter,

$$\lambda = \frac{\mu_0}{4\pi} \frac{\mu^2}{d^3 k_B T}.$$

Our model accounts for two distinct magnetization relaxation mechanisms: (i) internal Néel relaxation of individual magnetic moments $\hat{\mu}_i$ via the Landau-Lifshitz-Gilbert formalism accompanied by thermal fluctuations and (ii) Brownian rotation of the entire ellipsoidal cluster, described by the stochastic rotational dynamics of its orientation. This dual treatment captures the interplay between intraparticle dipolar reorientation and physical reorientation of the composite particle in a viscous medium.

The Brownian rotational dynamics of a single ellipsoidal particle suspended in a Newtonian fluid is governed by the overdamped (inertialess) Langevin equation for its orientation. The angular velocity $\vec{\Omega}$ of the particle is only affected by the stochastic Brownian torque $\vec{T}_B$ due to thermal fluctuations. In the body-fixed frame aligned with the particle's principal axes, this reads

$$\gamma_r \cdot \vec{\Omega} = \vec{T}_B. \quad (3)$$

The tensor γ_r depends on the particle geometry and the fluid viscosity η . For an ellipsoidal particle, it can be written as [96,97]

$$\gamma_r = \eta \mathbf{K}_r.$$

The components of $\mathbf{K}_r$ are given explicitly in terms of the semiaxes (a_1, a_2, a_3) , corresponding to (b, a, a) , as shown in Fig. 1(b), using the shape-dependent factors for each Cartesian coordinate 1, 2, or 3,

$$\varepsilon_{1(2,3)} = \int_0^\infty \frac{1}{(a_{1(2,3)}^2 + L) \sqrt{(a_1^2 + L)(a_2^2 + L)(a_3^2 + L)}} dL.$$

The diagonal components of the rotational resistance tensor for an ellipsoid are

$$\begin{aligned} \mathbf{K}_{r,11} &= \frac{16\pi}{3} \frac{a_2^2 + a_3^2}{\varepsilon_2 a_2^2 + \varepsilon_3 a_3^2}, \\ \mathbf{K}_{r,22} &= \frac{16\pi}{3} \frac{a_1^2 + a_3^2}{\varepsilon_1 a_1^2 + \varepsilon_3 a_3^2}, \\ \mathbf{K}_{r,33} &= \frac{16\pi}{3} \frac{a_1^2 + a_2^2}{\varepsilon_1 a_1^2 + \varepsilon_2 a_2^2}, \end{aligned}$$

with all off-diagonal elements equal to zero.

The stochastic torque $\vec{T}_B$ is a Gaussian random vector with zero mean, and its variance satisfies the fluctuation-dissipation theorem in a tensor form:

$$\langle \vec{T}_B(t) \otimes \vec{T}_B(s) \rangle = 2k_B T \gamma_r \delta(t - s).$$

The net magnetic moment of the composite particle, $\vec{M} = \sum_{j=1}^N \vec{\mu}_j$. The internal (Néel) dynamics of each core magnetic moment direction $\hat{\mu}_i$ is described by the overdamped Landau-Lifshitz-Gilbert equation. Neglecting fast Larmor precession and working in the laboratory reference frame, this equation for a core i can be written as

$$\frac{d\hat{\mu}_i}{dt} = \vec{\Omega}_\mu \times \hat{\mu}_i,$$

with the effective precession frequency

$$\vec{\Omega}_\mu = \vec{\Omega} + \frac{\mu_0}{\gamma_\mu} \vec{\mu}_i \times \vec{h}_i + \vec{\xi}_N.$$

Here $\vec{\xi}_N$ denotes a stochastic field accounting for thermal fluctuations in the Néel dynamics, whose components satisfy the white-noise correlation for any pair of cores i, j in a tensor form,

$$\langle \vec{\xi}_{N,i}(t) \otimes \vec{\xi}_{N,j}(s) \rangle = \mathbf{I} \frac{2k_B T}{\gamma_\mu} \delta_{ij} \delta(t - s),$$

where $\mathbf{I}$ is a unit tensor.

The characteristic Debye relaxation time is

$$\tau_D = \frac{\gamma_\mu}{2k_B T}$$

in the limit of zero anisotropy. The effective damping coefficient is $\gamma_\mu = \mu_0 \mu (1 + \alpha^2) / (\alpha \gamma_{\text{LLG}})$, incorporating the gyromagnetic ratio γ_{LLG} and the dimensionless Gilbert damping parameter α from the Landau-Lifshitz-Gilbert equation. Finally, $\vec{h}_i$ represents the effective magnetic field acting on the i th core, which comprises the anisotropy field derived from U_{ani} , and the dipolar field due to interactions with all other cores:

$$\vec{h}_i = -\frac{1}{\mu_0 \mu} \frac{\partial U_{\text{ani}}}{\partial \hat{\mu}_i} - \frac{1}{\mu_0 \mu} \sum_{j \neq i} \frac{\partial U_{dd}(\hat{\mu}_i, \hat{\mu}_j)}{\partial \hat{\mu}_i}.$$

The time τ_D is a prefactor of the Néel relaxation time, parallel and perpendicular to the core easy axis, defined as

$$\tau_N^\parallel = \tau_D \frac{e^\sigma - 1}{2\sigma} \left[\frac{1}{1 + 1/\sigma} \sqrt{\frac{\sigma}{\pi}} + 2^{-\sigma-1} \right]^{-1}, \quad (4)$$

$$\tau_N^\perp = 2\tau_D \frac{1 - G}{2 + G}. \quad (5)$$

The order parameter G quantifies the average alignment of the particle magnetic moment with its easy axis in the absence of an external field. It can be expressed as [25]

$$G = \frac{3}{2} \langle (\vec{e} \cdot \vec{n})^2 \rangle - \frac{1}{2} = \frac{3}{4} \frac{1}{\sigma} \left[\frac{\sqrt{\sigma}}{\text{Da}(\sqrt{\sigma})} - 1 \right] - \frac{1}{2},$$

where

$$\text{Da}(x) = e^{-x^2} \int_0^x e^{y^2} dy$$

is the Dawson integral.

The technical details related to the coupling of the cores magnetodynamics to the particle Brownian dynamics can be found in Ref. [98].

B. Simulation parameters

The particle aspect ratio was varied within the range $X_0 \in [1, 8]$, allowing us to continuously transform the particle shape from a sphere to a highly elongated ellipsoid of revolution. For the spherical case, the ratio between the magnetic torque coefficient and the rotational friction coefficient was fixed to

$$\frac{\gamma_\mu}{\gamma_{r,11}} = \frac{1}{200}. \quad (6)$$

This ratio implies that the rotational Brownian relaxation of the multicore particle is approximately 200 times slower than the Debye relaxation of an individual core. For magnetite, however, the Brownian relaxation time of a 10-nm core is typically about two orders of magnitude larger than the corresponding Debye relaxation time, making the ratio defined by Eq. (6) unrealistically large. Nevertheless, in the present work we retain this ratio by artificially reducing the viscosity of the implicit solvent, a common computational strategy employed to accelerate Brownian dynamics simulations while preserving the qualitative behavior of the system [99]. It is possible to do it for a single multicore in a zero applied field, as the rotation of the multicore and the internal magnetization rotation are fully decoupled.

The volume of the overall multicore, as well as the number of cores were preserved, $N_c = 100$. The volume fraction of the cores was set to $\phi_c = 0.25$. We explored interaction strengths $\lambda = 1, 3, 5$ and $\sigma = 1, 3, 5, 7$.

All equations of motion were solved numerically using the software package ESPRESSO 4.2 [100,101]. Each simulation started with a warm-up phase of 5000 integration steps. The integration time step was set to $\delta t = 0.005$. Statistical data for the autocorrelation functions (ACF) were recorded every five integration steps, while the statistics for the orientational correlations, $\cos \theta$ and $\cos \beta$, Fig. 1(b), were sampled every 100 steps. The total simulation length was 2×10^6 integration steps, except for the most elongated particles ($X_0 = 8$), for which simulations were extended up to 5×10^6 steps to ensure sufficient statistical sampling.

In order to assure independence from the placement of the cores inside the ellipsoid, four independent configurations have been simulated for every set of magnetic anisotropy, dipolar coupling constant, and ellipsoidal elongation.

C. Theory for zero-field static magnetic susceptibility

Assuming a homogeneous distribution of cores and random orientations of their easy axes within the ellipsoid, we can estimate its static susceptibility, $\chi(0)$, using the following continuous approximation. In general, the initial susceptibilities of a linearly magnetisable ellipsoidal body along ($\parallel$) and perpendicular ($\perp$) to its major axis are given by

$$\chi_{\parallel} = \frac{\chi_{\text{in}}}{1 + \chi_{\text{in}} \mathcal{N}_{\parallel}}, \quad \chi_{\perp} = \frac{\chi_{\text{in}}}{1 + \chi_{\text{in}} \mathcal{N}_{\perp}}, \quad (7)$$

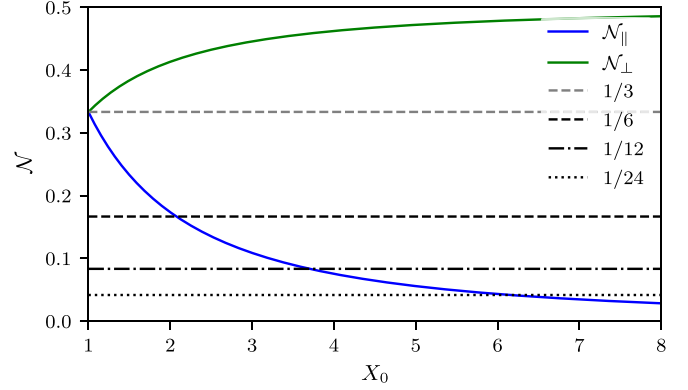


FIG. 2. Demagnetization factors parallel, $\mathcal{N}_{\parallel}$ (blue, solid line), and perpendicular, $\mathcal{N}_{\perp}$ (green, solid line), to the main axis of the ellipsoidal multicore particle as functions of particle elongation, X_0 . Horizontal lines indicate the value for spheres $\mathcal{N}_{\parallel} = \mathcal{N}_{\perp} = 1/3$ (gray dashed line), $1/6$ (black dashed line), $1/12$ (black dash-dotted line), and $1/24$ (black dotted line).

where χ_{in} denotes the intrinsic susceptibility of the material and $\mathcal{N}_{\parallel}$ and $\mathcal{N}_{\perp}$ are the corresponding demagnetization factors. For elongated particles ($X_0 > 1$), these factors are given by [102]

$$\mathcal{N}_{\parallel} = \frac{1}{X_0^2 - 1} \left(\frac{X_0}{\sqrt{X_0^2 - 1}} \operatorname{arccosh} X_0 - 1 \right), \quad \mathcal{N}_{\perp} = \frac{1 - \mathcal{N}_{\parallel}}{2}. \quad (8)$$

For χ_{in} , we adopt the second-order modified mean-field theory [103]:

$$\chi_{\text{in}} = \chi_L \left(1 + \frac{\chi_L}{3} + \frac{\chi_L^2}{144} \right). \quad (9)$$

Here χ_L is the Langevin susceptibility, i.e., the equilibrium susceptibility of an ideal gas of magnetic cores,

$$\chi_L = \frac{\mu_0 \mu^2 N_c}{3 k_B T v_p}. \quad (10)$$

To account for the random mechanical rotation of the ellipsoid due to Brownian motion, the susceptibility must be averaged over all possible orientations of the major axis:

$$\chi(0) = \frac{1}{3} \chi_{\parallel} + \frac{2}{3} \chi_{\perp}. \quad (11)$$

This approach generalizes the theory developed and validated in Refs. [68,104] for spherical multicore particles, corresponding to $X_0 = 1$ and $\mathcal{N}_{\parallel} = \mathcal{N}_{\perp} = 1/3$.

Inspection of the demagnetization factors shown in Fig. 2 reveals a systematic reduction with increasing elongation. In particular, the longitudinal demagnetization factor is approximately halved at $X_0 = 2$, as indicated by the intersection of the blue solid curve with the dashed black line. As X_0 increases further to around 4, $\mathcal{N}_{\parallel}$ decreases to slightly below one quarter of its spherical value, corresponding to the crossing with the dash-dotted line. For strongly elongated particles ($X_0 = 8$), the demagnetization factor falls well below one eighth of the spherical value. These trends highlight the significant reduction of internal demagnetizing fields with increasing particle

elongation. Below we shall examine the impact of these demagnetization fields on all aspects of the dynamic magnetic response of ellipsoidal multicore particles.

D. Zero-field dynamic magnetic susceptibility

The dynamic magnetic response of the multicore ellipsoid is analyzed in the limit of an infinitesimally weak external magnetic field using the fluctuation-dissipation theorem [39]. In this framework, the key quantity is the ACF of the total magnetic moment, defined as

$$C_M(t) = \frac{\langle \vec{M}(t) \cdot \vec{M}(0) \rangle}{\langle \vec{M}^2(0) \rangle}, \quad (12)$$

where $\vec{M}(t)$ denotes the sum over all core magnetic moments at time t and the angular brackets indicate averaging over independent realizations.

The normalized dynamic magnetic susceptibility is obtained from the Fourier transform of the ACF,

$$\frac{\chi(\omega)}{\chi(0)} = 1 + i\omega \int_0^{+\infty} C_M(t) e^{i\omega t} dt = \frac{\chi'(\omega)}{\chi(0)} + i \frac{\chi''(\omega)}{\chi(0)},$$

where ω is the frequency of the weak probing oscillatory magnetic field, $\chi'(\omega)$ is the real part of the dynamic magnetic susceptibility, and $\chi''(\omega)$ is its imaginary part. To minimize the errors originated from the Fourier transform of the numerical ACF, the latter is fitted by a superposition of exponential functions. The details, as well as the examples of fitting are collected in the Supplemental Material (Fig. S1) [105].

E. Specific loss power

The imaginary part of the dynamic susceptibility provides an estimate for the heating efficiency of the magnetic system—a property that is of particular importance in magnetic hyperthermia applications. In the presence of a harmonically oscillating magnetic field ($H_0 \cos \omega$), the *specific loss power* (SLP), also referred to as the *specific absorption rate*, quantifies the heating rate per unit mass of magnetic material [106–108] and can be written as

$$\text{SLP} = Q \frac{v_c}{\varphi_c m_c}, \quad Q = \frac{\mu_0 H_0^2}{2} \omega \chi''(\omega). \quad (13)$$

To isolate the influence of multicore particle shape, intercore interactions, and magnetic anisotropy on the heating performance across different frequencies, we introduce the following dimensionless form of the loss power:

$$q = \omega \tau_D \chi''(\omega). \quad (14)$$

III. RESULTS

A. The impact of particle shape on Brownian relaxation

In order to isolate the effect of particle shape on rotational diffusion, we first neglect the internal magnetic degrees of freedom of the multicore particles and consider only their rigid-body rotation. This approximation corresponds to the limit of infinitely large magnetic anisotropy of the individual cores, such that all core moments are locked to the particle body. In this limit, each multicore ellipsoid can be represented

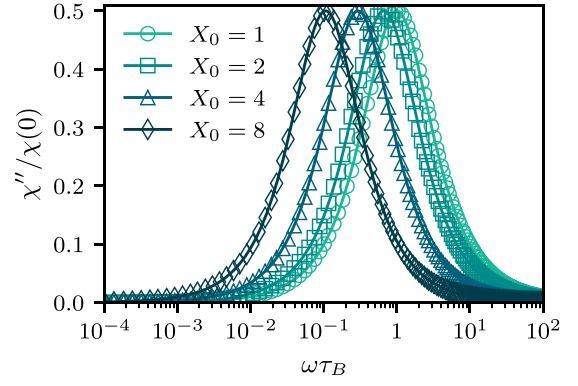


FIG. 3. For point dipoles (infinite magnetic anisotropy, Brownian relaxation only): The shift of the imaginary part of the zero-field dynamic magnetic susceptibility towards lower frequencies with growing ellipsoidal elongation. Theoretical calculations based on Eq. (16). The reference for a sphere has a maximum at unity.

by a single effective point dipole fixed in the particle frame, and magnetic relaxation occurs solely through Brownian rotation of the entire particle.

For an anisotropic body, the rotational diffusion coefficients along the principal axes, 11(22,33), are given by

$$D_{11(22,33)} = \frac{k_B T}{\gamma_{r,11(22,33)}} = \frac{\tau_{1(2,3)} k_B T}{J_{1(2,3)}}, \quad (15)$$

where $\gamma_{r,11(22,33)}$ denotes the rotational friction coefficient about axis 1,(2,3), $J_{1(2,3)}$ is the corresponding principal moment of inertia, and $\tau_{1(2,3)}$ is the angular velocity correlation time about that axis [109].

For a solid elongated ellipsoid, permanently magnetized along its principal axis, the imaginary part of the normalized dynamic susceptibility is given by a Debye-like expression [96,110],

$$\frac{\chi''(\omega)}{\chi(0)} = \frac{\omega \tau_e}{1 + \omega^2 \tau_e^2}, \quad (16)$$

where the effective relaxation time is

$$\tau_e = \frac{1}{D_{22} + D_{33}}. \quad (17)$$

In the limit $X_0 = 1$, τ_e reduces to the standard Brownian relaxation time of a sphere:

$$\tau_B = \frac{1}{2D(X_0 = 1)} = \frac{3\eta v_p}{k_B T}. \quad (18)$$

Figure 3 shows predictions from Eq. (16) for a sphere ($X_0 = 1$) and for ellipsoids with elongations up to $X_0 = 8$. In all cases, the dipole is rigidly fixed inside the particle, and relaxation is purely Brownian. With increasing elongation, a systematic shift of the peak position towards lower frequencies is observed. Quantitatively, the frequency at which $\chi''(\omega)$ reaches its maximum decreases roughly as $1/X_0$.

This behavior directly reflects the anisotropic rotational diffusion of ellipsoids. As X_0 increases, the rotational friction about the transverse axes grows, leading to smaller effective rotational diffusion coefficients and, thus, to a longer Brownian relaxation time. Since the maximum of $\chi''(\omega)$ scales as

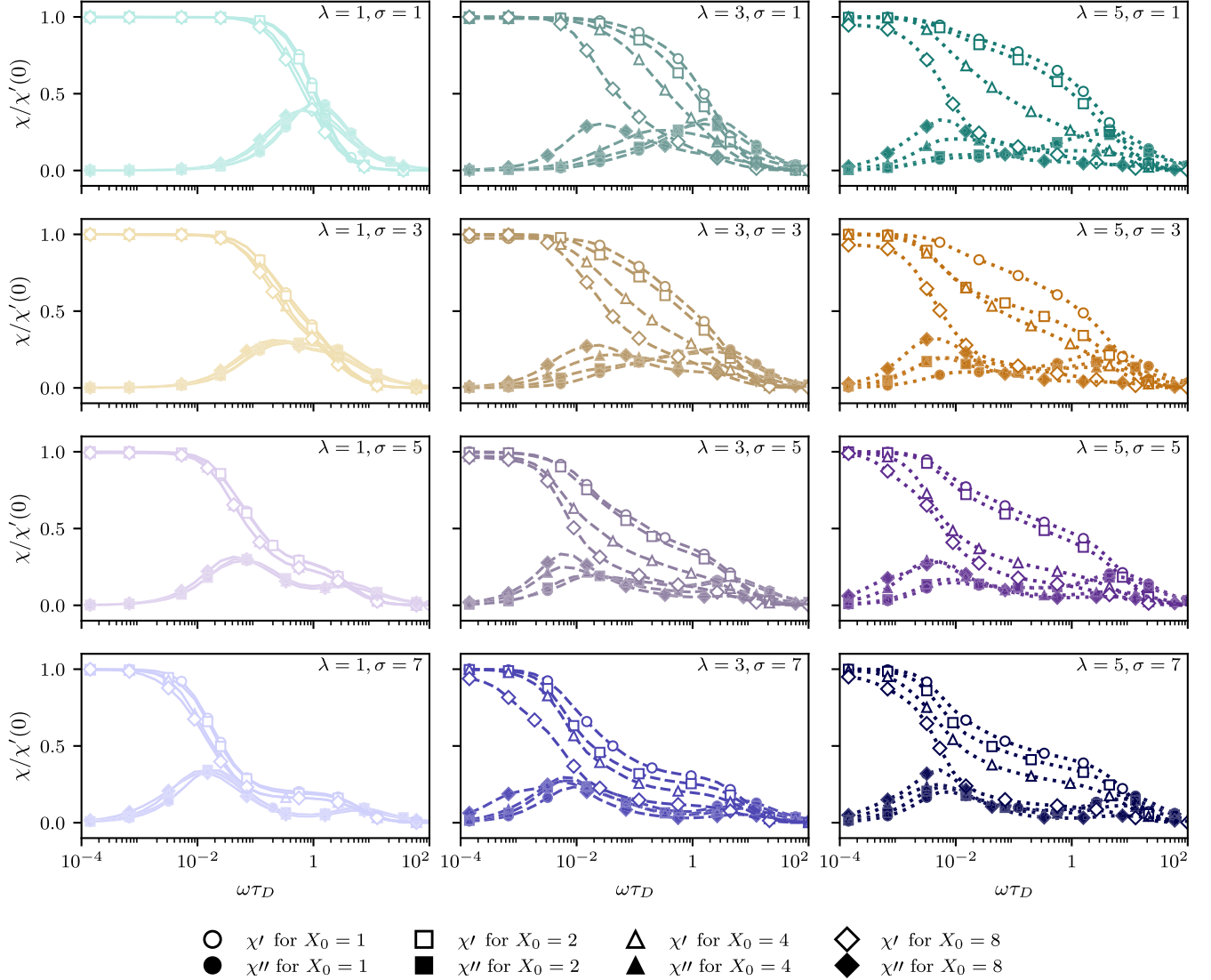


FIG. 4. The evolution of the dynamic magnetic susceptibility spectra for ellipsoids with changing elongation, core magnetic anisotropy and intercore interactions. The interaction grows from left to right as indicated by the brightness of the color; the anisotropy grows from top to bottom and is differentiated by color; the symbols are different for each elongation as shown in the legend (reference spheres are shown with circles in each subfigure); real parts of the spectra are shown with empty symbols, while the imaginary parts with filled symbols.

$\omega_{\max} \sim \tau_e^{-1}$, an increase in τ_e results in the observed shift of the dissipation peak to lower frequencies.

Importantly, while the peak position changes significantly, the overall spectral shape remains single-peaked and Debye-like. This confirms that the elongation modifies the characteristic timescale of rotational diffusion without introducing additional relaxation channels in the fixed-dipole case.

B. Combined shape and magnetic anisotropies reflected in magnetic susceptibility spectra

As the next step, we introduce finite values of both the dipolar coupling parameter λ and the magnetic anisotropy parameter σ for the cores. As noted earlier, this introduces another relaxation mechanism linked to the internal dynamics of the magnetic cores, which in turn gives rise to two additional characteristic timescales. One of these is the Debye time τ_D , which we use as the normalization factor for the

frequency axis. Consequently, when σ is small in Eqs. (4) and (5), the magnetic relaxation is governed almost exclusively by τ_D . In this limit, the maximum of the imaginary part of the susceptibility χ'' appears at unity when the horizontal axis is expressed as $\omega\tau_D$.

For finite anisotropy, however, internal relaxation of the core moments becomes relevant. The characteristic frequency associated with the Néel relaxation time from Eqs. (4) and (5) for $\sigma = 1, 3, 5, 7$ can be estimated as 0.6, 0.25, 0.07, and 0.017 respectively.

Under the same normalization, but for an infinite anisotropy, the peak corresponding to the Brownian relaxation of a spherical particle is shifted to $\omega\tau_D = 1/200 = 0.005$.

Figure 4 summarizes the frequency-dependent dynamic magnetic susceptibility of the multicore ellipsoids for different combinations of dipolar interaction strength λ , magnetic anisotropy σ , and particle elongation X_0 . The real part of the susceptibility $\chi'(\omega)$ is shown by open symbols, while

the imaginary part $\chi''(\omega)$ is indicated by filled symbols. The columns correspond to increasing dipolar coupling ($\lambda = 1, 3, 5$ from left to right), whereas the rows represent increasing magnetic anisotropy of the cores ($\sigma = 1, 3, 5, 7$ from top to bottom). Different particle elongations are distinguished by marker shape according to the legend.

For weak dipolar interactions ($\lambda = 1$) and low magnetic anisotropy ($\sigma \leq 3$), the spectra display a single relaxation process governed by the Debye time. The imaginary part $\chi''(\omega)$ shows a well-defined peak near the inverse dipolar rotational diffusion time, while $\chi'(\omega)$ decreases smoothly from its static value at low frequencies to zero at high frequencies. When the anisotropy increases, the spectra broaden and the peak of χ'' splits (see the two lower panels in the left column). One component appears at frequencies higher than $1/\tau_D$ and corresponds to the absorption peak [26], while the second shifts to considerably lower frequencies, indicating much slower relaxation processes. In this weakly interacting regime the spectra remain essentially insensitive to the particle elongation.

Increasing the dipolar interaction strength to $\lambda = 3$ (second column in Fig. 4) leads to a noticeable broadening of the spectra and a progressive shift of spectral weight towards lower frequencies. The imaginary part becomes increasingly asymmetric, reflecting a wider distribution of relaxation times. This broadening becomes stronger for larger particle elongations, indicating that both particle shape and intercore interactions contribute to slowing the magnetic response. For $\sigma \leq 3$, multicore spheres and weakly elongated ellipsoids ($X_0 = 2$) still show very similar spectra. For larger elongations, however, the spectra clearly separate into two contributions: a high-frequency component associated with fast dipolar fluctuations and a slower collective relaxation at lower frequencies.

For the strongest coupling ($\lambda = 5$, right column in Fig. 4), the spectra become strongly stretched along the frequency axis. The peaks of χ'' shift to significantly lower frequencies, and the spectra broaden substantially, particularly for large X_0 . At the same time, the peak height decreases slightly, indicating that the response is distributed over several competing relaxation processes. These trends point to a pronounced slowing down of the magnetic dynamics caused by the combined action of particle shape, strong dipolar intercore coupling, and magnetic anisotropy.

Overall, Fig. 4 shows that the dynamic magnetic response of multicore ellipsoids is governed by the interplay of particle elongation, dipolar coupling, and magnetic anisotropy. While particle shape primarily sets the Brownian rotational timescale, strong intercore interactions broaden the spectra and shift the response towards slower dynamical regimes. At the same time, comparing the spectra for different values of λ at $\sigma \leq 3$ demonstrates that intercore interactions have a substantially stronger effect than in the $\sigma \geq 5$ case. Increasing anisotropy progressively hinders the reorientation of the core magnetic moments, reducing the influence of dipolar interactions on the relaxation dynamics. In this regime the particle elongation also begins to influence the internal relaxation processes.

Figure 5 summarizes the positions of the maxima of the imaginary part of the susceptibility. Each circle

corresponds to the frequency at which a maximum of $\chi''(\omega)$ occurs for a given elongation X_0 . If several maxima are present, then multiple circles appear at the same elongation. The circle size reflects the height of the corresponding peak. The columns correspond to increasing dipolar coupling ($\lambda = 1, 3, 5$ from left to right), while the rows represent increasing core anisotropy ($\sigma = 1, 3, 5, 7$ from top to bottom). The horizontal reference lines indicate the characteristic relaxation frequencies, from the inverse Brownian rotational time ($\omega\tau_D = 0.005/X_0$, solid line) to the inverse Debye time ($\omega\tau_D = 1$, dashed line), while the horizontal dash-dotted lines mark the inverse Néel relaxation times for corresponding values of σ .

For weak dipolar coupling ($\lambda = 1$), the maxima remain close to the Debye reference frequency and are basically independent of elongation. At larger anisotropy, $\sigma \geq 5$, additional maxima appear at higher frequencies, corresponding to fast internal magnetic fluctuations (absorption peak), while a slower branch emerges near the Néel timescale. As for the low anisotropy case, the elongation of an ellipsoid does not affect neither the positions, nor the heights of the maxima for $\sigma \geq 5$.

For $\lambda = 3$, even for $\sigma = 1$, we observe the shift of χ'' maximum towards lower frequencies with growing X_0 . While a multicore sphere with cores characterized by $\lambda = 3$, $\sigma = 1$ (upper plot in the middle column, Fig. 5) is clearly dominated by the combination of Debye and Néel relaxations, the maxima corresponding to ellipsoids with $X_0 \geq 4$ are found clearly below $1/\tau_N$. With increasing σ , several maxima coexist for many combinations of elongation and anisotropy, indicating the presence of multiple relaxation mechanisms. The maxima separate into two distinct branches: a high-frequency branch associated with fast internal fluctuations and a low-frequency branch related to the combination of Néel and Brownian-like relaxation, with the latter being promoted by the elongation.

For the strongest coupling ($\lambda = 5$), the separation between the relaxation branches becomes even more pronounced. The slow branch shifts further towards lower frequencies as the particle elongation increases, indicating a significant slowing down of the dominant relaxation mode. The larger circle sizes show that these slow modes increasingly dominate the response as dipolar coupling, elongation, and anisotropy grow.

Overall, Fig. 5 demonstrates that in systems with interacting magnetic cores, the elongation of the particle leads to a substantial slowing of the relaxation dynamics. Note that, in the absence of shape effects, all circles would have retained both their size and their vertical position. Instead, for the middle and right columns at $\sigma \leq 5$, we observe a decay of nearly three orders of magnitude in the dominant relaxation frequency, accompanied by an almost complete disappearance of the high-frequency maxima. This effect becomes stronger with increasing dipolar coupling. Even when the relaxation mechanism remains Néel-like, the characteristic relaxation time depends on the particle elongation, which must originate from changes in the internal arrangement of the core magnetic moments.

Figure 6(a) shows the static initial magnetic susceptibility, $\chi(0)$, as a function of the ellipsoidal elongation X_0 for different values of the intercore interaction strength λ at fixed $\sigma = 1$.

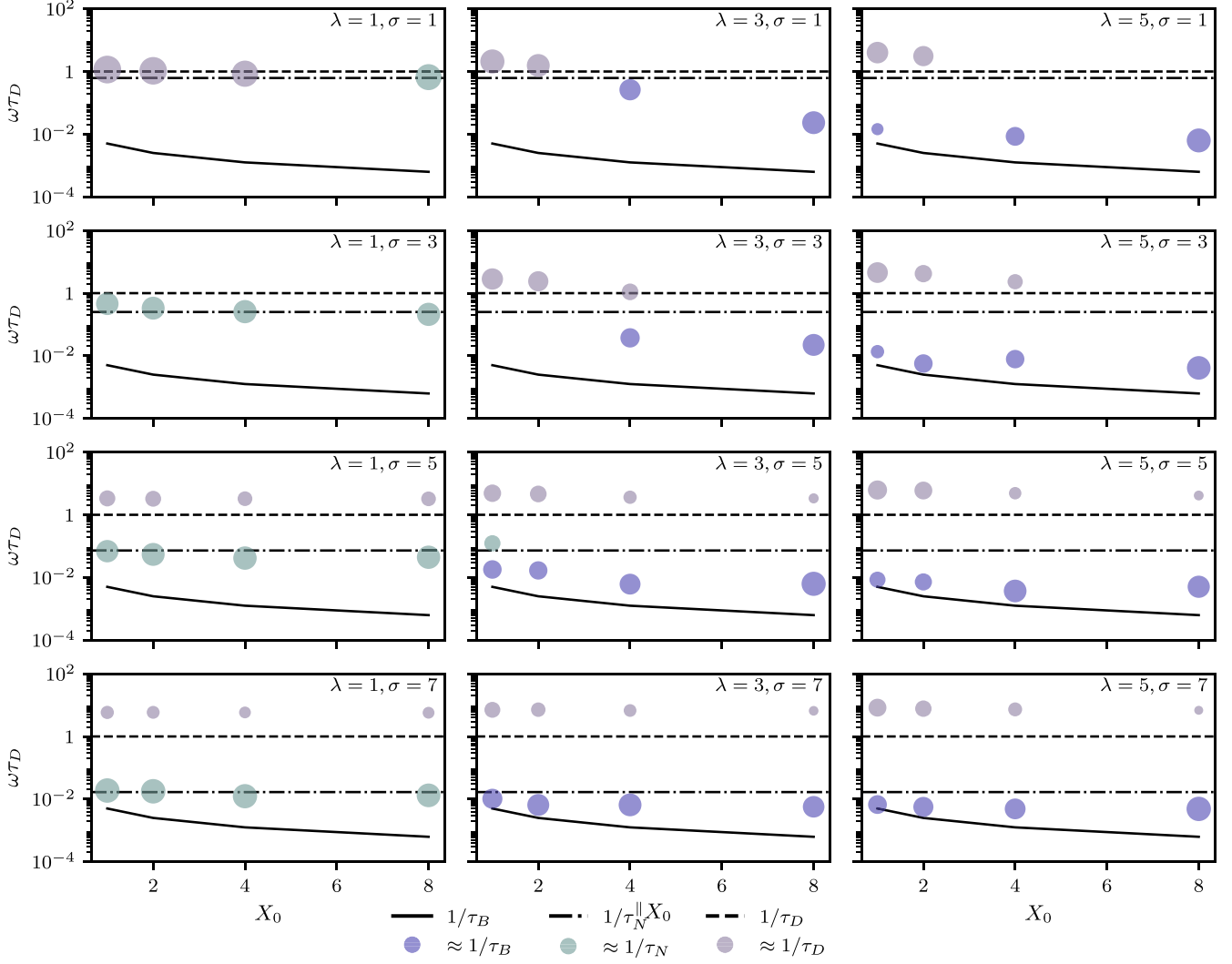


FIG. 5. Maxima positions of the imaginary part of the dynamic magnetic susceptibility spectra. Each circle corresponds to a certain frequency, at which the maximum is found for a given ellipsoidal elongation (horizontal axis). Horizontal lines in each subplot from bottom to top correspond to inverse Brownian relaxation time of the whole multicore to Debye inverse time of a single core, as shown in the legend. If the imaginary part exhibits more than one maximum there are several circles corresponding to a given elongation. The size of the circle corresponds to the height of the maximum, and their colors are chosen by calculating the distance from the circle center to reference inverse time line. The intercore interaction grows from left to right; the anisotropy of the cores grows from top to bottom.

In contrast to suspensions of single-core ellipsoids with a point dipole aligned along the main axis, where the susceptibility typically *decreases* with increasing elongation, the present results for multicore ellipsoids exhibit a strikingly different behavior: $\chi(0)$ increases strongly with X_0 .

Moreover, this growth is clearly enhanced by the interaction strength λ . For larger λ , the increase in susceptibility with X_0 becomes significantly more pronounced, indicating that elongation amplifies the effect of intercore dipolar coupling.

These findings suggest that, in multicore systems, particle elongation does not simply reduce the magnetic response through geometric effects but instead promotes stronger internal dipolar interactions, leading to an overall enhancement of the susceptibility.

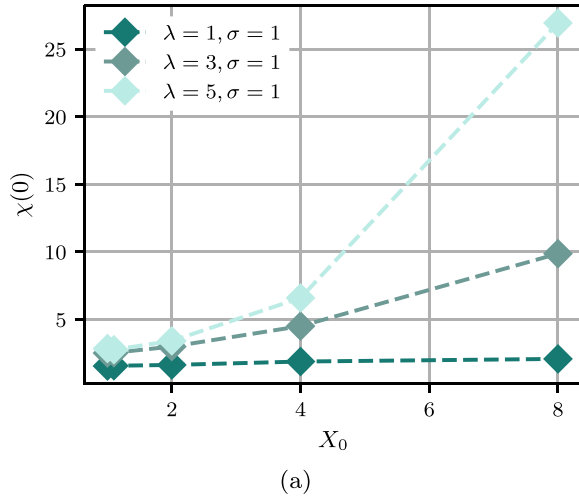
This is further confirmed by Fig. 6(b), where the normalized static magnetic susceptibility $\chi(0)/\chi_L$ is plotted versus the elongation and is compared to the modified mean-field

model, developed in Sec. II C. It turns out that mean-field level consideration of the dipolar interactions describes the behavior of highly elongated ellipsoids only for weakly interacting cores ($\lambda = 1$, dark green). With increasing intercore interactions, the deviations from the mean-field theory become evident at $X_0 \geq 4$.

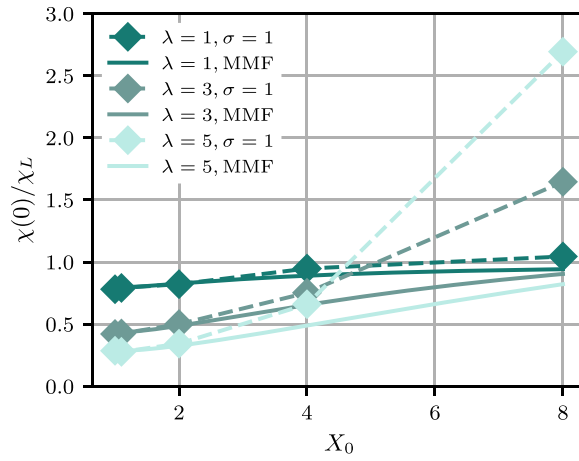
In order to provide a microscopic insight into enhanced intercore correlations with growing X_0 , we next analyze the alignment angles β and θ , introduced in Fig. 1(b).

C. Microscopic insight: Intercore correlations

Figure 7 presents the probability distributions of $\cos \beta$, where β is the angle between the magnetic moments of the cores and the long axis of the ellipsoid, for different elongations X_0 and dipolar coupling strengths λ . The upper panel corresponds to $\sigma = 1$, while the lower panel shows the case $\sigma = 3$.



(a)



(b)

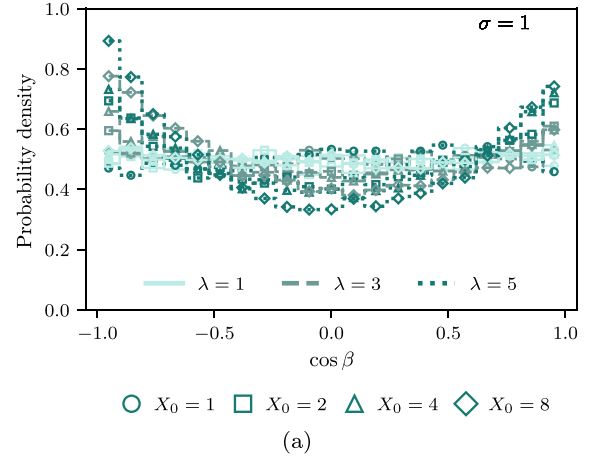
FIG. 6. (a) Static initial magnetic susceptibility, $\chi(0)$, plotted as a function of ellipsoidal elongation, X_0 . Note that these curves are σ independent [111]. (b) Normalized initial magnetic susceptibility, $\chi(0)/\chi_L$, compared to the theoretical model developed in Sec. II C.

In both cases, the distributions exhibit a clear dependence on particle elongation. As X_0 increases, the probability density becomes progressively enhanced near $\cos \beta = \pm 1$, indicating a growing tendency of the core magnetic moments to align along the major axis of the ellipsoid. Conversely, the probability of finding orientations perpendicular to the axis (i.e., $\cos \beta \approx 0$) is reduced.

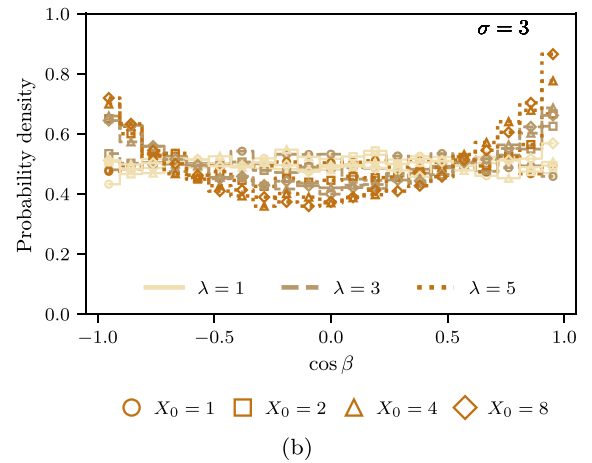
This effect is further amplified by increasing dipolar coupling λ . Stronger intercore interactions lead to more pronounced peaks at $\cos \beta = \pm 1$, demonstrating that dipolar interactions promote collective alignment of the core moments along the elongated direction.

The behavior is qualitatively similar for both values of σ , although the distributions for $\sigma = 3$ appear smoother and less sharply peaked, reflecting a broader orientational spread.

Overall, these results confirm that particle elongation enhances the internal alignment of magnetic moments and that this alignment is strongly mediated by dipolar interactions. This provides a microscopic explanation for the previously observed slowing down of the relaxation



(a)



(b)

FIG. 7. Probability density of the cosine of the angle between the magnetic moments of the cores and the long axis of the ellipsoid, $\cos \beta$; see Fig. 1(b). The color and the line type both indicate the intercore interactions, while the symbol differentiates the elongation. The probability of dipoles aligning with the ellipsoidal axis increases with elongation.

dynamics: Elongation promotes cooperative dipolar ordering within the multicore structure, which in turn hinders magnetic reorientation.

The distributions of angles θ , Fig. 1(b), turn out to be much less sensitive to the multicore elongation and show an expected transition from uniform distributions to more easy-axis-orientated ones with growing σ . The details can be found in Fig. S2 in Supplemental Material [105].

D. Specific loss power

Had the interactions between the cores inside a multicore particle been independent of the shape of the latter, the elongation of the overall multicore that preserves the total volume would not have affected the values of q , defined in Eq. (14). However, as we showed above, the intercore interactions are enhanced by the growth of X_0 , and as a result, X_0 has a clear impact on the shape of $\chi''(\omega)$.

In Fig. 8, we plot a normalized specific loss power, $q/q_{X_0=1}$, as a function of $\omega\tau_D$. This way, we can clearly visualize the impact of multicore particle shape on heat efficiency.

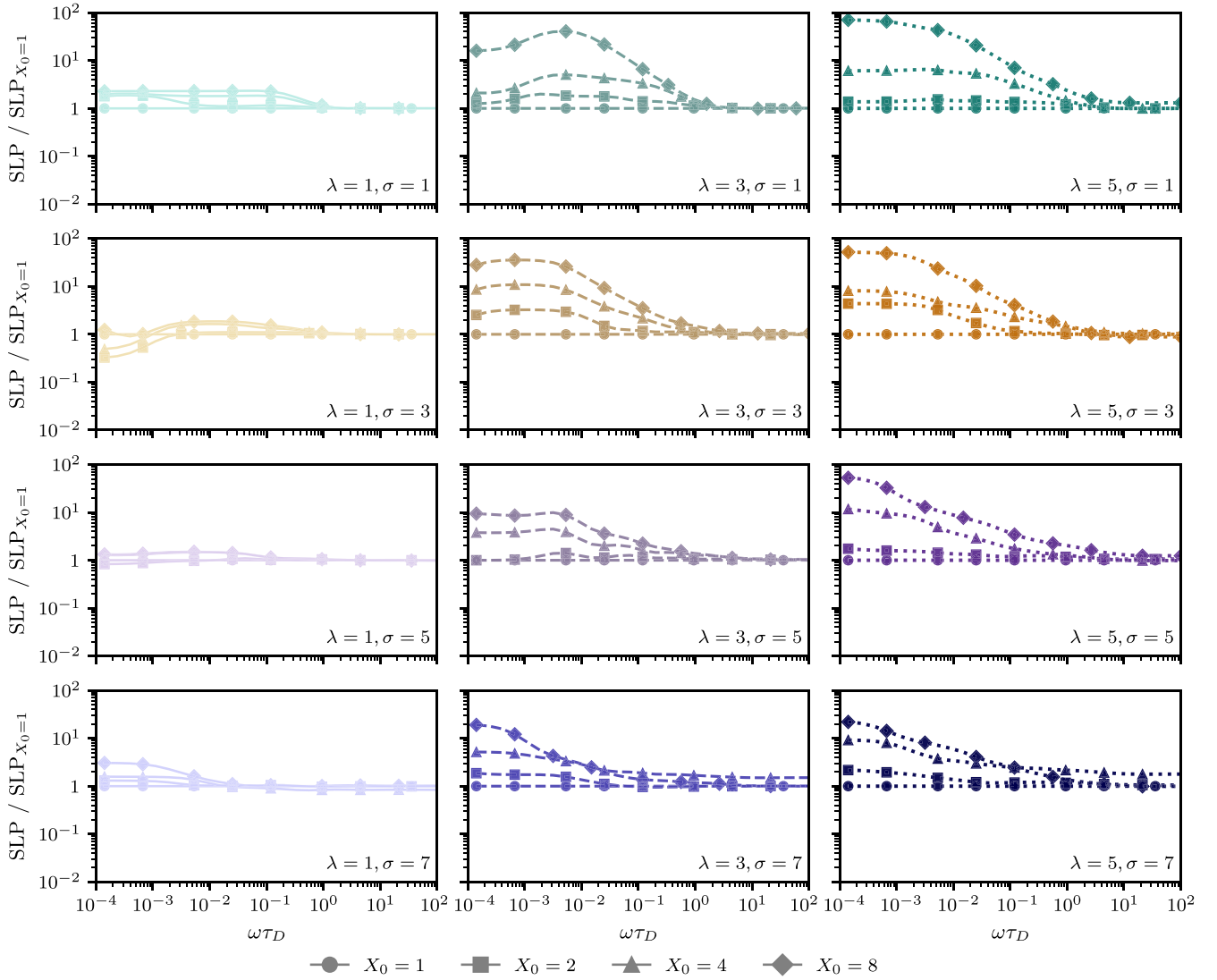


FIG. 8. Normalized specific loss power, $q/q_{x_0=1}$, as a function of $\omega\tau_D$ for different λ , σ , and x_0 . Columns correspond to $\lambda = 1, 3, 5$, rows to $\sigma = 1, 3, 5, 7$, and markers indicate $X_0 = 1, 2, 4, 8$. All values are normalized by the reference case for a spherical multicore particle, $X_0 = 1$.

For weak interactions ($\lambda = 1$, left column), the normalized loss power remains close to unity across the entire frequency range, indicating that particle elongation has only a minor effect on heating efficiency. This behavior is largely independent of σ , suggesting that in the weakly interacting regime, both anisotropy and shape play a limited role.

As the interaction strength increases ($\lambda = 3$, middle column), deviations from unity become more pronounced, particularly at low and intermediate frequencies. Elongated particles ($X_0 > 1$) exhibit an enhancement of q at low $\omega\tau_D$, followed by a reduction at higher frequencies. This reflects the growing influence of intercore dipolar interactions, which modify the spectral shape of $\chi''(\omega)$.

In the strongly interacting regime ($\lambda = 5$, right column), the effect of elongation becomes significant. A marked enhancement of the loss power is observed at low frequencies for larger X_0 , whereas at higher frequencies the normalized loss power is basically shape independent.

Increasing anisotropy σ (from the top to the bottom rows) generally suppresses the magnitude of these variations and shifts the crossover between the enhancement and the shape-independent range of parameters. For large σ , the curves tend to flatten, particularly at high frequencies, suggesting that strong anisotropy limits the ability of intercore interactions to enhance heating efficiency.

Overall, the figure demonstrates that particle elongation, through its effect on intercore interactions, significantly alters the frequency dependence of the heating efficiency. The impact is negligible for weak interactions but becomes substantial in the moderate-to-strong interaction regimes, where elongation enhances low-frequency losses by more than one order of magnitude at no expense to high-frequency performance.

The enhancement of losses at low frequencies is particularly relevant for magnetic hyperthermia applications, where operational constraints limit the accessible frequency range.

In this context, elongation-induced interactions effectively shift the dissipation spectrum towards experimentally viable frequencies, thereby improving heating efficiency under realistic conditions, albeit at the expense of reduced performance at higher frequencies.

IV. CONCLUSIONS

In this work, we have investigated the dynamic magnetic response of ellipsoidal multicore nanoparticles, focusing on the combined effects of particle elongation, intercore dipolar interactions, and magnetic anisotropy. By employing Brownian dynamics simulations with explicit modeling of both Néel and Brownian relaxation mechanisms, we have systematically analyzed how these factors shape the magnetic susceptibility spectra and heating performance. A key methodological element of this study is the use of a spectral reconstruction technique based on non-negative least-squares fitting of autocorrelation functions, which enables a stable and physically consistent identification of multiple relaxation modes across a wide range of timescales.

To complement the simulations, we have developed a theoretical description of the static susceptibility of multicore ellipsoids that incorporates demagnetization effects within a modified mean-field framework. This model captures the essential role of particle shape in modulating internal fields and provides a useful baseline for interpreting deviations arising from strong intercore correlations.

We have shown that particle elongation plays a fundamentally different role depending on the strength of intercore interactions. In the limit of weak coupling, elongation primarily modifies the Brownian rotational timescale, leading to a predictable shift of the susceptibility peak without qualitative changes to the spectral shape. However, as dipolar interactions increase, elongation significantly enhances internal magnetic correlations, which results in a pronounced slowing down of the magnetic dynamics. This manifests as a broadening of the susceptibility spectra, the emergence of multiple relaxation modes, and a shift of dominant dissipation processes towards lower frequencies.

A key finding of this study is that elongation amplifies dipolar correlations within the multicore structure by reducing

demagnetization effects along the major axis. This promotes partial alignment of core magnetic moments, as confirmed by the analysis of orientational distributions, and leads to an increase in the static susceptibility with particle elongation—in contrast to the behavior of single-core ellipsoids. At the same time, deviations from mean-field predictions highlight the importance of spatial correlations in strongly interacting systems.

These microscopic changes in magnetic structure have direct consequences for energy dissipation. We demonstrate that elongation induces a redistribution of the specific loss power, enhancing heating efficiency at low frequencies. At high frequencies, instead, the SLP is basically shape independent. This effect becomes particularly pronounced in systems with strong dipolar interactions and moderate anisotropy. Importantly, such a shift of dissipation towards lower frequencies is advantageous for applications such as magnetic hyperthermia, where operational constraints limit the accessible frequency range.

Overall, our results establish a clear link between particle geometry, internal magnetic correlations, and dynamic response in multicore systems. They show that particle elongation is not merely a geometric parameter but a powerful tool for tuning magnetic relaxation and energy dissipation. These findings provide a framework for the rational design of multicore magnetic nanoparticles with tailored dynamic properties, opening new possibilities for optimizing their performance in technological and biomedical applications.

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DATA AVAILABILITY

There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

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