Numerical solutions of the Fokker Planck equation in the case of randomly oriented field acting on magnetic nanoparticles

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The resolution of the Fokker-Planck equation (PFE) for the probability density of an assembly of fine particles, based on previous calculations, is extended to the case where the direction of the applied field has a random orientation. Using the PFE, Coffey et al. [6] have proposed a method of calculating the relaxation time τ, assuming H directed at an arbitrary angle ψ to the easy axis ($H = H(\psi, \phi=0)$). In this report we will extend these calculations to the case where $H = H(\psi, \phi)$.

Keywords: Ferromagnetic relaxation; Ultrafine particles; Fokker Planck equation.

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I-INTRODUCTION

Magnetic ultrafine particles have received much attention since several decades due to the wide possibilities of technological applications, and to fundamental questions on the basic of some observed phenomena [1, 2]. The magnetic properties of such particles are usually studied by magnetization, susceptibilities and Mössbauer experiments. They have yield a picture of ferromagnetic particles relaxing between the directions of their anisotropy axis and interacting by dipolar forces. The superparamagnetic picture is widely used which usually neglects effects among them. In such case the magnetization curve of an assembly of such particles can be well described by a Langevin function with the two assumptions that each particle constitutes a single domain, and that the anisotropy energy is small enough to be neglected [3**]. The direction of the magnetic moment, m, of a single-domain particle fluctuates because of thermal agitation. This magnetic moment can cross over an energy barrier E_B with a relaxation time τ. Using the theory of stochastic processes, by considering a Brownian motion, Brown [4] derived a Fokker-Planck equation (PFE) for the probability density of the magnetic moment orientation, the eigenvalues of which are directly related to the relaxation times. Moreover, the effect of an external constant magnetic field H on the relaxation behaviour of an assembly of non-interacting single domain ferromagnetic particles with uniaxial anisotropy characterized by an anisotropy constant K was first studied by Brown [4] and Aharoni [5] under the two assumptions: (a) H is directed along the easy axis of magnetization and (b) that the relaxation of magnetization is dominated by a single relaxation mode, namely that associated with the time τ of reversal of the magnetization over the energy barrier between two stable orientational states. However, the first assumption is in general not valid as not traducing the real situation where H may have a random spatial orientation (Fig. 1). Using the PFE, Coffey et al. [6] have proposed a method of calculating the relaxation time τ, assuming H directed at an arbitrary angle ψ to the easy axis ($H = H(\psi, \phi=0)$**)**. In this report we will extend these calculations to the case where $H = H(\psi,\phi)$ (Fig. 1). A preliminary and brief discussion of the results obtained will be given.

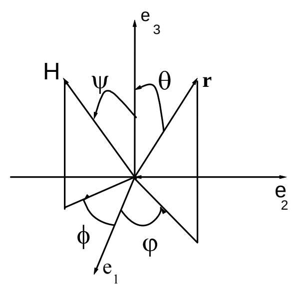

FIG. 1: The field and magnetization orientations in terms of spherical polar coordinates

II-THE FOKKER-PLANCK EQUATION

Consider an assembly of fine ferromagnetic particles, each of volume ν, in the presence of a magnetic potential νV arising from the internal anisotropy and the external applied magnetic field. The probability density distribution, W(r, t), of magnetic momentum direction r, satisfies the PFE, and is given, in spherical coordinates, by [4]:

$$\dot{W} = L_{FP} W \tag{1}$$

where

$$\begin{aligned} L_{FP}W &= \beta^{-1} b \Delta W + bW\Delta V \\ &+ b\left(\frac{\partial V}{\partial \theta}\frac{\partial W}{\partial \theta} + \frac{1}{\sin^2\theta}\frac{\partial V}{\partial \varphi}\frac{\partial W}{\partial \varphi} \right) \\ &+ \frac{b}{a\sin\theta}\left(\frac{\partial V}{\partial \theta}\frac{\partial W}{\partial \varphi} - \frac{\partial V}{\partial \varphi}\frac{\partial W}{\partial \theta} \right) \end{aligned} \tag{2}$$

In this equation Δ is the Laplacian in spherical coordinates, $\beta = \frac{v}{kT}$ where kT is the thermal energy, $b = \frac{a\gamma}{\left(1+a^2\right)M_S^2}$., γ is the gyromagnetic ratio, $a = \eta\gamma M_S$ in which η is the phenomenological damping constant from Gilbert's equation [7] with units such that a is a dimensionless damping parameter, and Ms is denoting the saturation magnetization.

In the case of uniaxial symmetry, the anisotropy energy may be written as

$$\beta V = \alpha\left[1 - \left(re_3\right)^2\right] - \xi\left(re_H\right) \tag{5}$$

where $\alpha = \frac{Kv}{kT}$ represents the anisotropy parameter, $\xi = \frac{HM_S v}{kT}$ is the external field parameter, and

$$e_H = \frac{H}{\|H\|} = \sin\psi\cos\phi e_1 - \sin\psi\sin\phi e_2 + \cos\psi e_3$$

Then Eq. (5) becomes:

$$\begin{aligned} \beta V &= \alpha\sin^2\theta - \xi\cos\theta\cos\psi \\ &- \xi\sin\theta\cos\varphi\sin\psi\cos\phi \\ &+ \xi\sin\theta\sin\varphi\sin\psi\sin\phi \end{aligned} \tag{6}$$

The potential of Eq. (6) is no-axially symmetric unless ψ = 0, so the gyroscopic terms expressed in a^{-1}in Eq. (2) will not vanish since a is of the order 0.2 to 1.We will ignore these terms in a first approximation [6].

Eq. (1) takes then the following form

$$\begin{aligned} 2\tau_N \frac{dW}{dt} &= \Delta W + W\Delta(\beta V) \\ &+ \left(\frac{\partial(\beta V)}{\partial\theta}\frac{\partial W}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial(\beta V)}{\partial\varphi}\frac{\partial W}{\partial\varphi} \right) \end{aligned} \tag{7}$$

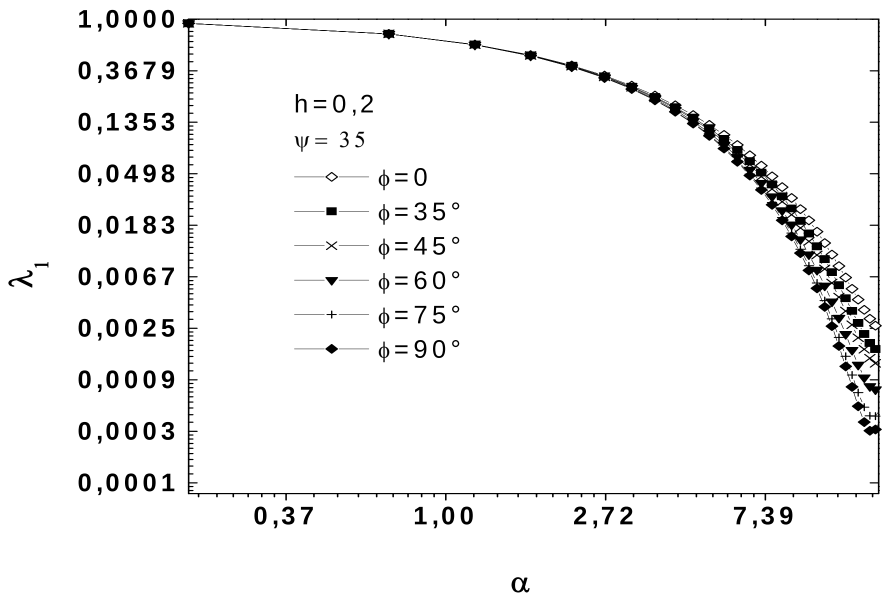

FIG.. 2: Variation of λ_1 as a function of α for different values of ϕ and h=0.2 and for ψ=35°

where $\tau_N = \dfrac{\beta}{2b}$ denotes the diffusional relaxation time.

The relaxation time τ is assumed to obey the relation $\tau = \tau_N/\lambda_1$, where $\lambda_1$is the smallest non-vanishing eigenvalue of the PFE.

Numerical resolution of this equation is based of the use of the normalized spherical harmonics [6] such as

$$W(\theta,\varphi,t) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} a_{l,m}(t)\, Y_{l,m}(\theta,\varphi) \qquad (8)$$

where $Y_{l,m}(\theta,\varphi) = N_{l,m}\, P_{l,m}(\cos\theta)\, e^{im\varphi}$

and $N_{l,m} = \left[\dfrac{(2l+1)(l-m)!}{4\pi(l+m!)}\right]^{\frac{1}{2}}$

and the following expression is obtained

$$\begin{aligned}
2\tau_N \frac{d}{dt} b_{l,m} + l(l+1) b_{l,m} = 2\alpha & \left[\begin{array}{l} \dfrac{(l+1)(l+m-1)(l+m)}{(2l-1)(2l+1)} b_{l-2,m} + \dfrac{l(l+1)-3m^2}{(2l-1)(2l+3)} b_{l,m} \\ - \dfrac{l(l-m+2)(l-m+1)}{(2l+1)(3l+3)} b_{l+2,m} \end{array}\right] \\
& + \frac{2\alpha h \cos\psi}{(2l+1)} \left[(l+1)(l+m) b_{l-1,m} - l(l-m+1) b_{l+1,m}\right] \\
& + \frac{\alpha h \sin\psi}{(2l+1)} \left[\begin{array}{l} (l+1)(l+m-1)(l+m)(\cos\phi + \sin\phi) b_{l-1,m-1} \\ + l(l-m+2)(l-m+1)(\cos\phi + \sin\phi) b_{l+1,m-1} \\ - (l+1)(\cos\phi - \sin\phi) b_{l-1,m+1} \\ - l(\cos\phi - \sin\phi) b_{l+1,m+1} \end{array}\right]
\end{aligned} \qquad (9)$$

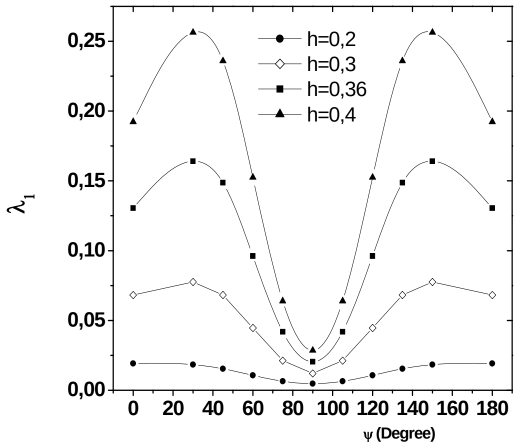

FIG. 3: Variation of λ_1 as a function of ψ for different values of the field h and for α=10 and $\phi = 0$

where $b_{l,m}$ are such as

$$b_{l,m}(t) = \left\langle P_l^m(\cos\theta)\cos m\varphi \right\rangle - \left\langle P_l^m(\cos\theta)\cos m\varphi \right\rangle_0 \qquad (10)$$

and where

$$\left\langle P_l^m(\cos\theta)\cos m\varphi \right\rangle = \frac{a_{l,m} + (-1)^m a_{l,-m}}{2a_{0,0}\, N_{l,m}} = \frac{\mathrm{Re}(a_{l,m})}{a_{0,0}\, N_{l,m}} \qquad (11)$$

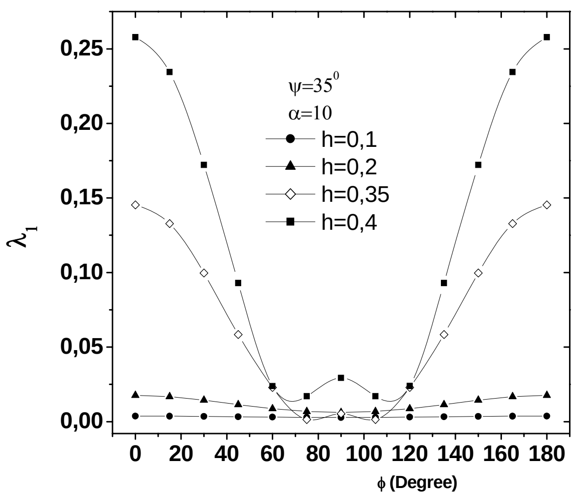

FIG. 4: Variation of λ_1 as a function of ϕ for different values of the field h and for α=10 and ψ=35°

III- RESULTS AND DISCUSSION

Figures 2 to 6 show the evolution of λ_1 as function of the variation of the parameter α, ϕ, ψ and h. These simulations are consistent with those obtained by Coffey et al. [6] and give a generalization of them. However plot of λ_1 as a function of Ψ shows (Fig.3) the appearance of a maximum of the eigenvalue at Ψ = 30° contrary to what has been reported in the case where H = H(ψ,ϕ=0) [6] in which this maximum appears at Ψ = 45°. Similarly, plot of λ_1 as a function of Φ (Fig. 4) shows a maximum of λ_1 at ϕ = 90°, together with those at ϕ = 180° and 0°, which brings a new solution compared to the case cited above. Moreover, the maximum of λ_1 at ϕ = 90° appears only for values of h superior to 0.3, pointing out the role played by the amplitude of the applied field. In all these simulations, the fundamental property of the non axially symmetric potential (Eq. (6)) consisting in λ_1 (π/2, Φ) < λ_1 (0, Φ) and λ_1 (Ψ,π/2) < λ_1 (Ψ,0), so that the Néel relaxation time for large h and α is a maximum for this orientation of the field while it is a minimum at the π/4 orientation is conserved. Slight different behaviour of λ_1 as a function of α is observed compared to the results of Coffey et al. [6]. Indeed, plots of λ_1 for one of the three parameters varying and the two others fixed, show that as Φ increases, for fixed values of h and ψ, λ_1 decreases (Fig. 2), and that the same behaviour of λ_1 is observed when varying ψ for fixed values of h and Φ, and also when varying h with fixed values of Φ and ψ (figs.5 and 6). In all these cases our simulations permitted an extension of the the interval of variation of α, compared to those of reference [6].

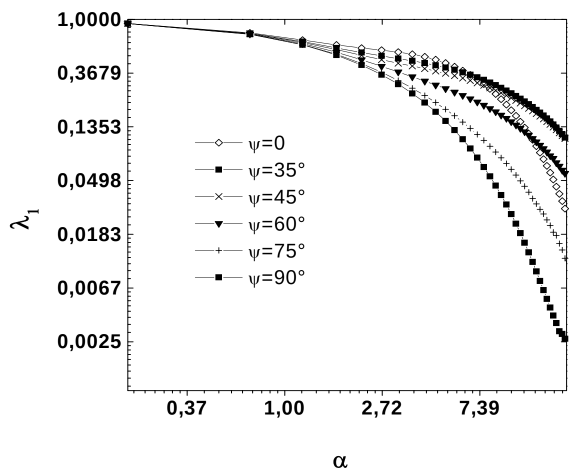

FIG.. 5: Variation of λ_1 as a function of α for different values of the angle ψ and for h=0.4

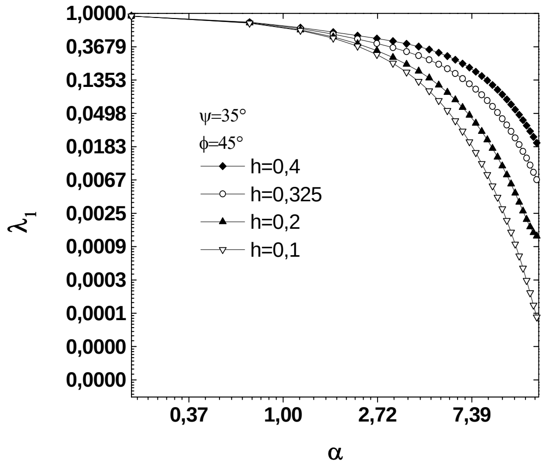

FIG.. 6: Variation of λ_1 as a function of α for different values of h and for ψ=35° and ϕ=45°

IV- CONCLUSION

Numerical solutions of the PFE are brought in the case of randomly oriented magnetic field acting on an assembly of magnetic ferromagnetic fine particles, which constitute zn extension of previous calculations by Coffey et al. [6]. The results obtained which brought modifications to previous ones, are briefly discussed. In particular, the randomly character of the angle Φ modified the behaviour of λ_1.

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