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Journal of Magnetism and Magnetic Materials 203 (1999) 265–267

Journal of magnetism and magnetic materials

www.elsevier.com/locate/jmmm

A single integral expression for the magnetisation of a textured superparamagnetic system

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Abstract

A superparamagnetic system consists of many single domain particles with relaxation times smaller than the time of measurement ($t = 100$ s), with the result that thermal agitation leads to zero magnetisation in zero field, $M(H = 0) = 0$, for $t > 100$ s. For particles in a fluid, an external field will result in a magnetisation given by the Langevin function as in paramagnetism. However, particles fixed into position in the presence of a field, obtain an orientational texture. We still find $M(H = 0) = 0$, but the magnetisation is not given by the Langevin function. The model of Chantrell et al. can yield an expression for M capable of including texture. This requires the calculation of the partition function of the system which is a double integral in the coordinate system used. Here we reduce this double integral to a single integral.

Keywords: Superparamagnetic particles

1. Introduction

In 1985 Chantrell et al. [1] presented a theory describing the relaxational behaviour of a system of superparamagnetic (relaxation time < 100 s) particles embedded in a solid nonmagnetic environment. They calculated the initial magnetic susceptibility of this type of system. The magnetic susceptibility is obtained from the slope of the magnetisation curve. In a solid environment, the magnetisation of the system depends largely on the anisotropy of the particles and also on the orientation of the particles' easy axes, or orientational texture. This was shown to be the case by Raikher [2]. The orientational texture can be varied by cooling to a solid in varying field strengths and field orientations. An expression for the magnetisation describing the dependencies on anisotropy and texture is desired. From Ref. [1] an expression for the magnetisation of a system of particles with easy axes fixed at an angle from the field is available. This involves two integrals where the first is the partition function of the system Z, and the second is calculable from the partition function. Therefore, we require a solution of the partition function. The partition function can be expressed as a double integral in the two angles of the coordinate system used. The paper of Chantrell et al. considered the case of a low field where this double integral was expanded and truncated. In this paper we show how the double integral can be reduced to a single integral. This is achieved by noting the null contribution of the odd field terms in the integral. This allows the replacement of exponential terms by hyperbolic terms. Noting the symmetry of the integrands allows the halving of the limits of integration. One of the integrals then reduces to a modified Bessel function of order zero, resulting in a single integral expression for the partition function. This should be useful where exact calculations are to be performed for all field strengths. Following Ref. [2] it is then possible to consider distributions of angles between easy axes and field.

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0304-8853/99/$ - see front matter
PII: S0304-8853(99)00269-3

2. The expression for the magnetisation curve

In a fluid environment the magnetisation M can be calculated from the equilibrium distribution [3]

$$M(\beta) = M_s L(\beta) = M_s\left[\coth(\beta) - \frac{1}{\beta}\right], \tag{1}$$

where $\beta = H\,M_s\,V/kT$, with V the particle volume, H the applied field, M_s the saturation magnetisation, kT the thermal energy and $L(\beta)$ is the well-known Langevin function of paramagnetism.

In the solid state the easy axes of the particles are frozen in position. If frozen in position, the Langevin function is only appropriate for the physically unlikely case of particles with zero anisotropy, where the easy axis has no meaning. If particles possessing anisotropy are frozen in position the Langevin function is not valid (except as a low field approximation for a random texture). In general, the magnetisation should be calculated from the expected value of $\cos\omega$, $\langle\cos\omega\rangle$ where from Fig. 1, ω is the angle between the moment of each particle $\mu(\mu = VM_s)$ and the field $\boldsymbol{H}$. The magnetisation can be written

$$M(\beta,\alpha,\psi) = M_s\langle\cos\omega\rangle = M_s\frac{\partial Z/\partial\beta}{Z}, \tag{2}$$

where $\alpha = KV/kT$ with K being the anisotropy constant and Z is the partition function given in Section 3. The problem reduces to calculating these two integrals Z and $\partial Z/\partial\beta$. These calculations are simplified by the reduction of the partition function Z which follows.

3. The reduction of the partition function

The partition function Z is given by

$$Z = \frac{1}{4\pi}\int_0^{2\pi}\int_0^{\pi}\exp(-\alpha\sin^2\vartheta + \beta\cos\omega)\sin\vartheta\,\mathrm{d}\vartheta\,\mathrm{d}\xi, \tag{3}$$

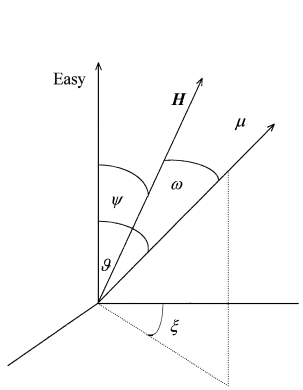

Fig. 1. The coordinate system of Chantrell et al. with particle easy axis, field $\boldsymbol{H}$ and moment $\boldsymbol{\mu}$.

using the coordinate system of Chantrell et al. given in Fig. 1. The angle ω is determined by the relation

$$\cos\omega = \cos\vartheta\cos\psi + \sin\vartheta\sin\psi\cos\xi. \tag{4}$$

Z therefore is given by

$$Z = \frac{1}{4\pi}\int_0^{2\pi}\int_0^{\pi}\exp(-\alpha\sin^2\vartheta + \beta\cos\vartheta\cos\psi + \beta\, sin\,\vartheta\sin\psi\cos\xi)\sin\vartheta\,\mathrm{d}\vartheta\,\mathrm{d}\xi. \tag{5}$$

Expanding the exponentials in β, we find that the odd terms in β result in the integrals given below, (for $n = 0, 1, 2\ldots$)

$$\int_0^{\pi}\exp(-\alpha\sin^2\vartheta)(\beta\cos\vartheta)^{2n+1}\sin\vartheta\,\mathrm{d}\vartheta = 0, \tag{6}$$

$$\int_0^{2\pi}(\beta\cos\xi)^{2n+1}\,\mathrm{d}\xi = 0. \tag{7}$$

Due to symmetry they are zero and do not contribute to Z. With this knowledge we can reduce the β exponentials to the hyperbolic cosines (which contain only even terms), so that

$$Z = \frac{1}{4\pi}\int_0^{2\pi}\int_0^{\pi}\exp(-\alpha\sin^2\vartheta)\cosh(\beta\cos\vartheta\cos\psi) \times\cosh(\beta\sin\vartheta\sin\psi\cos\xi)\sin\vartheta\,\mathrm{d}\vartheta\,\mathrm{d}\xi. \tag{8}$$

Now, noting the symmetry of the integrands we can halve the intervals of integration to give

$$Z = \frac{1}{\pi}\int_0^{\pi}\int_0^{\pi/2}\exp(-\alpha\sin^2\vartheta)\cosh(\beta\cos\vartheta\cos\psi) \times\cosh(\beta\sin\vartheta\sin\psi\cos\xi)\sin\vartheta\,\mathrm{d}\vartheta\,\mathrm{d}\xi. \tag{9}$$

Changing the order of integration and separating the ξ component, we have

$$Z = \int_0^{\pi/2}\exp(-\alpha\sin^2\vartheta)\cosh(\beta\cos\vartheta\cos\psi) \times\int_0^{\pi}\frac{1}{\pi}\cosh(\beta\sin\vartheta\sin\psi\cos\xi)\,\mathrm{d}\xi\,\sin\vartheta\,\mathrm{d}\vartheta. \tag{10}$$

From Eq. 9.6.16 of Abramowitz and Stegun [4], which, in the variables of that text is

$$I_0(z) = \frac{1}{\pi}\int_0^{\pi}\cosh(z\cos\theta)\,\mathrm{d}\theta,$$

where I_0 is the modified Bessel function of order zero, we can write

$$Z = \int_0^{\pi/2}\exp(-\alpha\sin^2\vartheta)\cosh(\beta\cos\vartheta\cos\psi) \times I_0(\beta\sin\vartheta\sin\psi)\sin\vartheta\,\mathrm{d}\vartheta. \tag{11}$$

In order to calculate the magnetisation we also require $\partial Z/\partial \beta$, which is written

$$\frac{\partial Z}{\partial \beta} = \int_0^{\pi/2} \exp(-\alpha \sin^2 \vartheta) [\cosh(\beta \cos \vartheta \cos \psi) \times I_1(\beta \sin \vartheta \sin \psi) \sin \vartheta \sin \psi + \sinh(\beta \cos \vartheta \cos \psi) \times I_0(\beta \sin \vartheta \sin \psi) \cos \vartheta \cos \psi] \sin \vartheta \, d\vartheta, \quad (12)$$

where I_1 is the modified Bessel function of order one. The calculation of these single integrals is quicker and less prone to numerical difficulties.

4. Conclusion

This gives us an expression $M(\beta, \alpha, \psi)$ valid for a system of particles all with easy axes at an angle ψ to the field, which is a delta-like distribution corresponding to very high cooling fields. Furthermore the integrals presented here can, using infinite sum descriptions for the functions involved, be written as multiple summations, several of which have been obtained by the authors which they hope to present later.

Acknowledgements

This paper is based on the work performed under the Commission of European Communities DG XII Human Capital and Mobility contract no: ERBCHICT940165. PJC would like to thank the School of Enginneering, WIT for full funding of his attendance at MNP. The late Jean-Louis Dormann of the Université de Versailles is warmly remembered for his many helpful conversations.

References

[1] R.W. Chantrell, N.Y. Ayoub, J. Popplewell, J. Magn. Magn. Mater. 53 (1985) 199.

[2] Yu.L. Raikher, J. Magn. Magn. Mater. 39 (1983) 11.

[3] W.T. Coffey, P.J. Cregg, Yu.P. Kalmykov, On the Theory of Debye and Néel Relaxation of Single Domain Ferromagnetic Particles, Adv. Chem. Phys. 83 (1993) 263.

[4] M. Abramowitz, I.A. Stegun (Eds.), Handbook of Mathematical Functions, Dover, New York, 1965.