TIME CONSTANTS OF SUPERPARAMAGNETIC PARTICLES

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Time constants of uniaxial single-domain particles have previously been calculated from a convergent series for small energy barriers and from a single-term asymptotic expression for very large. The present paper develops a more complete asymptotic expansion for large values and a numerical-quadrature method for the intermediate range.

The nonequilibrium behavior of a thermally agitated single-domain particle is determined by a Fokker–Planck equation [1]. For a uniaxial particle in zero field, the transient solutions are of the form $\Phi(x)\exp(\frac{1}{2}\kappa x^2 - t/\tau)$, where Φ satisfies the differential equation

$$(1-x^2)\Phi''(x) + [\kappa x(1-x^2) - 2x]\Phi'(x) + \lambda\Phi = 0 \tag{1}$$

and the boundary condition: finiteness at $x = \pm 1$. Here $\kappa = 2K_1 v/kT$, where K_1 is the anisotropy constant, v the particle volume, k Boltzmann's constant, and T the Kelvin temperature; x is the cosine of the angle between the magnetization and the particle axis; and $\lambda = v/kTh'\tau$, where h' is a material constant. The quantity of interest is the longest finite τ, hence the smallest nonzero eigenvalue of λ; the corresponding eigenfunction is odd in x.

Asymptotically for very large κ, λ is approximately [1]

$$\lambda_0 = (2\kappa^3/\pi)^{\frac{1}{2}}\exp(-\kappa/2); \tag{2}$$

but the accuracy of the approximation has not been investigated. For $\kappa = 0$, (1) becomes Legendre's equation, and $\lambda = 2$. For small and moderate κ, λ has been calculated [2] by a numerical method from a truncated convergent series solution for Φ. As κ increases, this method requires more and more terms and more and more and more figures in each term, and rapidly becomes impractical. With a 10-digit calculator (Hewlett–Packard HP-45), the seventh decimal place of λ begins to behave erratically at $\kappa = 11$, where λ_0 (= 0.1189623) still deviates from λ (= 0.0959544) by 24%. With a 12-digit calculator (Texas Instruments SR-52), the seventh decimal place begins to be erratic at $\kappa = 18$, where λ_0 (= 0.0075197) deviates from λ (= 0.0065876) by 14%. It therefore seems desirable to develop an alternate method of calculation for moderately large κ; in particular, to replace the single-term approximation (2) by a more complete asymptotic expansion.

A method that at first seems inviting is the phase-integral (Liouville–Green, Horn–Jeffreys, WKB, etc.) [3] method. This gives two linearly independent solutions of eq. (1) in each of the ranges $\epsilon_1 < x < 1 - \epsilon_2$ and $-1 + \epsilon_2 < x < -\epsilon_1$, where ϵ_1 and $\epsilon_2 > 0$; each solution contains an asymptotic series in $1/\kappa$. The problem of relating these solutions to solutions valid near 0 and ± 1 is complicated by the Stokes phenomenon. In the zeroth order in $1/\kappa$, this method leads again to formula (2). The first-order calculation is very laborious but ultimately yields

$$\lambda = \lambda_0\{1 + (1/\kappa)[\lambda(2\gamma - \ln 2) + 2\lambda\ln\kappa - 2] + O(1/\kappa^2)\}, \tag{3}$$

where γ is Euler's constant. With neglect of the unknown $O(1/\kappa^2)$ terms, this gives a result that is still in error by 7.6% at $\kappa = 11$ and by 1.7% at $\kappa = 18$. Calculations to higher orders would be extremely laborious. Furthermore, this method takes no advantage of the fact that when κ is large, λ is exponentially small, so that the terms in (3) containing a factor $(1/\kappa)\lambda$ may become negligible while terms containing factors $1/\kappa^2$, $1/\kappa^3$, etc. are still significant.

This suggests basing the calculation on the smallness of λ rather than on the largeness of κ. Therefore let us assume a solution $\Phi = \sum_{n=0}^{\infty}\Phi_n\lambda^n$. Substitution of this in (1) leads to a chain of differential equations that are easily solved in terms of integrals. The boundary condition, $\lim_{x\to\pm 1}\Phi(x)$ finite, becomes, on division by Φ_0 and application of L'Hospital's rule, $1 + \sum_{n=1}^{\infty}\lambda^n F_n(1) = 0$, where $F_0(t) = 1$ and

$$F_n(t) = -\int_0^t \exp(\tfrac{1}{2}\kappa u^2)\,du \int_0^u (1-v^2)^{-1} \times \exp(-\tfrac{1}{2}\kappa v^2)F_{n-1}(v)\,dv. \tag{4}$$

Inversion of the order of integration reduces the double integration to a single integration in which the integrand contains Dawson's integral, a well tabulated function with convenient, overlapping convergent and asymptotic series.

Numerical integrations in the range $\kappa = 10$ to 18 established the following results: (1) At $\kappa = 10$, neglect of the F_4 term leads to an error of less than 0.001%, and neglect of the F_3 term to an error of only 0.024%. (2) Neglect of the F_2 term, i.e. use of the formula $\lambda = -1/F_1(1)$, gives an error of about 2% at $\kappa = 10$, about 0.2% at $\kappa = 16$, and less than 0.1% for $\kappa \geq 18$. Thus for 0.1% accuracy in the range 10 to 18, F_2 must be considered, but 5% accuracy in it is sufficient.

In the complete asymptotic expansion of $F_1(1)$, the dominant part is of the form $-\lambda_0^{-1} \Sigma_{n=0}^{\infty} d_n \kappa^{-n}$ ($d_0 = 1$). The recessive part is of the form $\Sigma_{s=0}^{\infty} (e_s + f_s \ln \kappa) \kappa^{-s-1}$. The asymptotic expansion, appropriately truncated, gives a value of F_1 correct to better than 1% for $\kappa \geq 10$, 0.1% for $\kappa \geq 13$, and 0.01% for $\kappa \geq 19$. The error in λ by omission of the recessive part of F_1 is comparable with the error by neglect of F_2. When F_2 is needed, the leading term in its asymptotic expansion is sufficient. At $\kappa = 18$, neglect of F_2 and of the recessive part of F_1 gives error -0.22%. Hence for accuracy 0.22% or better at $\kappa \geq 18$, $\lambda = \lambda_0[1 + d_1/\kappa + d_2/\kappa^2 + \cdots]^{-1}$; $d_1, d_2, \ldots, d_{10} = 2, 7, 36, 249, 2190, 23535, 299880, 4426065, 74294010, 1397669175$, respectively.

Further development of this method will be particularly important if it can be applied to cubic anisotropy, where the behavior at large κ is subject to some uncertainty [4, 5].

References

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