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New approximate formulae for the retardation factors of nematic liquid crystals with simple uniaxial anisotropy

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Simple formulae which yield a close approximation to the exact analytic solution for the longitudinal and transverse relaxation times $T_{\parallel}$ and $T_{\perp}$ of the components of the dipole moment of a nematic liquid crystal with simple uniaxial anisotropy are presented. The new formula for $T_{\parallel}$ yields a substantial correction to the Meier–Saupe formula [1966, *Molec. Crystals*, **1**, 515]. It appears that both the longitudinal and transverse relaxation processes may be accurately described by a single Debye type relaxation mechanism with relaxation times $T_{\parallel}$ and $T_{\perp}$.

Meier and Saupe [1] have given a simple approximate formula, namely

$$\frac{T_{\parallel}}{\tau_D} = \frac{e^{\sigma} - 1}{\sigma}, \tag{1}$$

for the longest relaxation time $T_{\parallel}$ of the electric polarization in the direction parallel to the director axis for their extended Debye theory of relaxation model of a nematic liquid crystal having simple uniaxial anisotropy. The nematic potential is of the form

$$V(\vartheta) = q \sin^2 \vartheta. \tag{2}$$

In equation (2), q is the crystalline anisotropy and ϑ is the polar angle. Thus the nematic potential barrier parameter σ is

$$\sigma = \frac{q}{kT}. \tag{3}$$

$\tau_D = \zeta/2kT$ is the Debye relaxation time, where ζ is the viscous drag coefficient. We have recently shown [2] how the exact analytic solutions of the Meier–Saupe model for the components $\alpha_{\parallel}(\omega)$ and $\alpha_{\perp}(\omega)$ of the electric polarizability parallel (longitudinal) and perpendicular (transverse) to the director axis (ω denotes the angular frequency of the applied AC field) and the corresponding correlation times $T_{\parallel}$ and $T_{\perp}$ may be found for the simple uniaxial potential by adopting methods used in the study of magnetic relaxation [3]. We have also shown that both processes may be described by a *single* Debye type relaxation mechanism with relaxation times $T_{\parallel}$ and $T_{\perp}$. However, our exact solution for $T_{\parallel}$ differs significantly from the approximate formula of Meier and Saupe equation (1) for high barrier heights ($\sigma > 3$).

In this paper we report new simple approximate formulae for $T_{\parallel}$ and $T_{\perp}$ which give an accurate representation of the exact solutions for all barrier heights σ. The mathematical details of the calculations (which are rather lengthy) are given in [2, 3] for the interested reader, as the purpose of this short communication is simply to acquaint the liquid crystal community with the most important results of our investigation.

The exact solution for the longitudinal relaxation time $T_{\parallel}$ is [2, 3]

$$\frac{T_{\parallel}}{\tau_D} = M(1, 5/2, \sigma) + \frac{3/2}{M(3/2, 5/2, \sigma)} \times \sum_{n=1}^{\infty} \frac{(-\sigma^2)^n (n + 3/4)\Gamma(n + 3/2)\Gamma(n + 1/2)}{(n + 1)[\Gamma(2n + 5/2)]^2} \times M(n + 3/2, 2n + 5/2, \sigma) M(n + 1, 2n + 5/2, \sigma) \tag{4}$$

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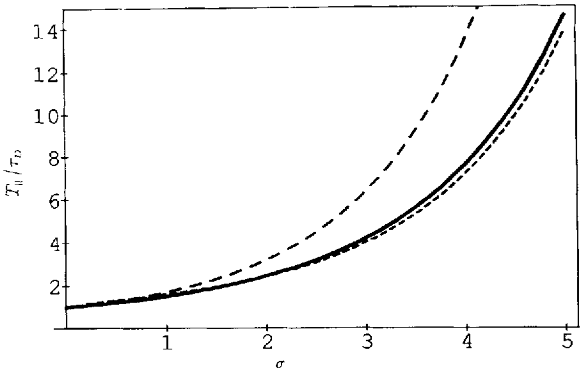

Figure 1. Longitudinal correlation time $T_\parallel/\tau_D$.

Table 1. Longitudinal correlation time $T_\parallel/\tau_D$.

σ	Equation (4)	Equation (5)	Equation (1)
0·5	1·2286	1·3334	1·2974
1	1·528	1·6146	1·7183
2	2·4603	2·4314	3·1945
3	4·1982	3·9991	6·3618
4	7·6061	7·1736	13·4
5	14·589	13·817	29·483
6	29·43	28·125	67·071
7	61·935	59·739	156·52
8	134·89	131·12	372·49
9	301·97	295·3	900·23
10	691·02	678·78	2202·5
20	5·0679 × 10^{6}	5·0475 × 10^{6}	2·4258 × 10^{7}
30	5·9662 × 10^{10}	5·9558 × 10^{10}	3·5622 × 10^{11}
40	8·4602 × 10^{14}	8·452 × 10^{14}	5·8846 × 10^{15}
50	1·3264 × 10^{19}	1·3256 × 10^{19}	1·0369 × 10^{20}
60	2·2149 × 10^{23}	2·2139 × 10^{23}	1·9033 × 10^{24}

where $M(a,b,z)$ is Kummer's function [4]. Our new approximate formula, first derived in the context of the theory of magnetic relaxation [5, 6] is

$$\frac{T_\parallel}{\tau_D}=\frac{e^{\sigma}-1}{\sigma}\left(\frac{2}{1+1/\sigma}(\sigma/\pi)^{1/2}+2^{-\sigma}\right)^{-1}, \qquad (5)$$

which is equation (1) with a correction term. The behaviour of this function in comparison to equation (1) and the exact solution, equation (4) is shown in figure 1 and table 1. In figure 1, equation (5) relates to the small dashes, equation (1) to the large dashes and equation (4) to the solid line. The inclusion of the correction term given by equation (5) in equation (1) ensures the correct asymptotic behaviour [7]

$$g_\parallel \simeq \frac{\pi^{1/2}}{2}\sigma^{-3/2}e^{\sigma}. \qquad (6)$$

It is apparent that the uncorrected equation (1) considerably overestimates $g_\parallel$ for $\sigma > 1$.

The exact solution for $\alpha_\perp(\omega)$ shows [2] that for all σ the process is again accurately described by a single Debye type mechanism with the transverse relaxation time $T_\perp$. This arises because the first and second modes are near degenerate for large $\sigma \gtrsim 8$, while the third mode has negligible contribution. On the other hand for small $\sigma < 8$, the first mode makes the dominant contribution. This behaviour is also apparent in the two-dimensional version of the model [8]. The exact solution for the transverse correlation time $T_\perp$ was obtained in [2] in terms of continued fractions. In this case, $T_\perp$ may not easily be expressed in terms of hypergeometric functions [2]; however we have found [9], using the effective eigenvalue method [10], that $T_\perp$ is accurately represented for all σ by

$$g_\perp=\frac{T_\parallel}{\tau_D}=\frac{2(1-S)}{2+S}, \qquad (7)$$

where

$$S=\langle P_2(\cos\vartheta)\rangle_0 \qquad (8)$$

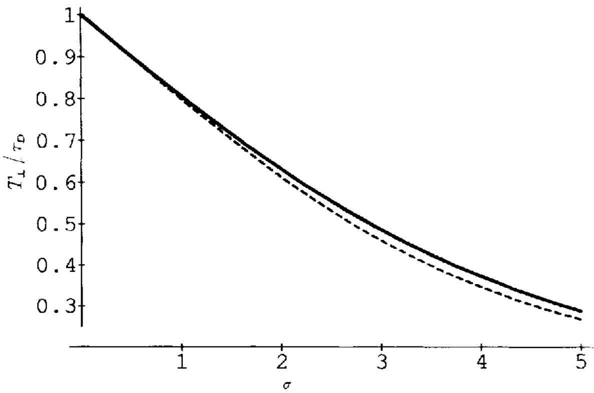

Figure 2. Transverse correlation time $T_\perp/\tau_D$.

Table 2. Transverse correlation time $T_\perp/\tau_D$.

σ	Exact solution	Equation (7)
0·2	0·960103	0·959805
0·4	0·920519	0·919362
0·6	0·881398	0·878885
0·8	0·84288	0·838594
1	0·805093	0·798708
2	0·630597	0·61222
3	0·485632	0·459744
4	0·372227	0·346555
5	0·287754	0·267232
6	0·227046	0·212746
7	0·184174	0·174997
8	0·153807	0·148148
9	0·131859	0·128395
10	0·115509	0·113352

is the equilibrium order parameter given by

$$S=\frac{2\sigma M(3/2,5/2,\sigma)}{15M(1/2,3/2,\sigma)}, \tag{9}$$

(the subscript 0 denoting the absence of a field) and equation (9) may be represented [11] in terms of the error functions of imaginary argument as

$$S=\frac{2[\mathrm{e}^{\sigma}-\frac{1}{2}(\pi/\sigma)^{1/2}\,\mathrm{erfi}\,(\sigma^{1/2})]}{5(\pi/\sigma)^{1/2}\,\mathrm{erfi}\,(\sigma^{1/2})}. \tag{10}$$

The behaviour of equation (7) in comparison with the exact solution is shown in figure 2 and table 2, showing that equation (7) yields a close approximation to $T_{\perp}$ for all σ. For large σ

$$g_{\perp}\sim\frac{1}{\sigma} \tag{11}$$

In conclusion, we have shown how exact expressions for the longitudinal and transverse correlation times $T_{\parallel}$, $T_{\perp}$ may be obtained for the extended Debye theory of dielectric relaxation of nematic liquid crystals due to Meier and Saupe [12], and that both transverse and longitudinal relaxation processes may be accurately described by a *single* Debye type relaxation mechanism with relaxation times $T_{\parallel}$ and $T_{\perp}$ given by eqns (5) and (7), respectively. The most significant result of our formula for $T_{\parallel}$ is that it predicts a value for $T_{\parallel}$ which is approximately 25 per cent less than that of the previously used formula of Meier and Saupe [1] equation (1). It is a matter of conjecture however if this is of experimental significance, because of the inherent assumptions of the Meier–Saupe model, namely that each molecule possesses a purely longitudinal dipole moment, that it experiences a potential proportional to $\sin^2\vartheta$, that it is otherwise unaffected by its neighbours and that its damping is described by a constant friction coefficient. The crude nature of these assumptions may in practice be such as to render insignificant the 25 per cent difference between the two formulae for $T_{\parallel}$. Regardless of these considerations, the Meier–Saupe model has the advantage, like the Debye model of an isotropic fluid, that it can be solved exactly, so providing a relatively easily understood qualitative description of experimental results.

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