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Publisher: Taylor & Francis

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Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals

Publication details, including instructions for authors and subscription information:

<http://www.tandfonline.com/loi/gmcl19>

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Version of record first published: 04 Oct 2006

To cite this article: Peng-Ye Wang (1997): Transient Statistics of the Freedericksz Transition in Nematic Liquid Crystals, Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals, 302:1, 397-402

To link to this article: <http://dx.doi.org/10.1080/10587259708041854>

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TRANSIENT STATISTICS OF THE FREDERICKSZ TRANSITION IN NEMATIC LIQUID CRYSTALS

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Abstract: The transient statistical feature of the Fredericksz transition in nematic liquid crystals is investigated. The explicit first-passage-time distribution function is derived with the approximation of neglecting the noise in the path of the transient process. Monte Carlo results of numerical simulations show good agreement with the theoretical analysis when the initial field is close or above the critical value of the Fredericksz transition indicating that the effect of noise in the path is negligible in this case.

It is well known that the orientation of the director of nematic liquid crystals (NLC) can be changed with external fields and the effect of stochastic fluctuations on the director of the liquid crystal molecule is not avoidable¹⁻³. Therefore, the dynamics of the Fredericksz transition in NLC is a typical decay process of unstable equilibrium state affected by noise. The transient behavior of similar unstable equilibrium states has been investigated in various systems, such as lasers⁴⁻⁸, super-radiance⁹⁻¹⁰, chemical reaction¹¹⁻¹², spinodal decomposition¹³⁻¹⁴, etc. In the case of a random magnetic field, the transient dynamics of the Fredericksz transition have been studied theoretically by Sagúe et. al.¹⁵ where an asymptotic approximation¹⁶ to the first-passage-time (FPT) distribution was used.

Based on the nonlinear stochastic Langevin equation of the angle of the director, we derived the explicit analytical solutions of the distribution function of the angle of the director of the NLC and the distribution function of the FPT of the director orientation to a prescribed threshold with the approximation of neglecting the effect of noise in the path of the transient process. Monte Carlo results of numerical simulations show good agreement with the theoretical analysis when the initial field is close or above the critical value of the Fredericksz transition indicating that the effect of noise in the path is negligible in this case.

With the deterministic considerations, the dynamics of the Fredericksz transition of the NLC can be described with the equation of motion of the director¹:

$$\gamma \frac{\partial \theta}{\partial t} = k \frac{\partial^2 \theta}{\partial z^2} + \chi_a H^2 \sin \theta \cos \theta, \quad (1)$$

where k is the elastic constant, χ_a is the anisotropy of the susceptibility, γ is the coefficient of the viscosity, H is the magnetic field.

Following the usual approximation¹⁻³, we assume that the maximum external field does not greatly exceed the critical field $H_c = \pi/d \sqrt{k/\chi_a}$, where d is thickness of the NLC sample. In this case the angle of deformation of the director is small and $\sin\theta\cos\theta$ can be expanded in powers of θ we have, therefore

$$\gamma \frac{\partial \theta}{\partial t} = k \frac{\partial^2 \theta}{\partial z^2} + \chi_a H^2 \left(\theta - \frac{2}{3} \theta^3 \right). \quad (2)$$

With rigid boundary condition, i.e. $\theta = 0$ at the surfaces of NLC, to a good approximation, the solution of Eq. (2) can be taken as

$$\theta = \theta_m(t) \cos \frac{\pi z}{d}. \quad (3)$$

Substitution of Eq.(3) in Eq.(2) and multiplying Eq(2) by $\cos \frac{\pi z}{d}$ and performing the integration over z , one obtains the equation for $\theta_m(t)$

$$\gamma \frac{d\theta_m}{dt} = \left(\frac{H^2}{H_c^2} - 1 \right) \theta_m - \frac{1}{2} \frac{H^2}{H_c^2} \theta_m^3, \quad (4)$$

or, dropping the subscript m of $\theta_m(t)$ for clarity

$$\frac{d\theta}{dt} = A\theta - B\theta^3, \quad (5)$$

where $A = h^2 - 1$, $B = h^2/2$, $h^2 = H^2/H_c^2$, and the time t is normalized to γ^{-1} .

Because the NLC molecules are subjected to complicated random forces, termed noise, we introduce a stochastic term in Eq.(5) accounting for the internal fluctuation of the system. This leads to a nonlinear Langevin equation:

$$\frac{d\theta}{dt} = A\theta - B\theta^3 + af(t), \quad (6)$$

where $f(t)$ is a Langevin force assumed to be a Gaussian random variable with zero mean and δ correlation function. The constant a describes the noise strength. We choose the following normalization:

$$\langle f(t) \rangle = 0; \quad \langle f(t)f(t') \rangle = 2\delta(t - t'). \quad (7)$$

The analytical solution of the stochastic differential equation (6) can not be obtained. We can setup a Fokker-Planck equation¹⁷ by which the probability density $W(\theta)$ of the stochastic variable θ can be calculated. Because the Langevin force is assumed to be δ -correlated and Gaussian distributed, we get the stationary Fokker-Planck equation:

$$a^2 \frac{dW(\theta)}{d\theta} = (A\theta - B\theta^3)W(\theta) \quad (8)$$

Integrating Eq.(8) gives the distribution function:

$$W(\theta) = Ce^{\left(\frac{1}{2}A\theta^2 - \frac{1}{4}B\theta^4\right)/a^2} \quad (9)$$

where C is a integrating constant which can be determined by the normalization condition:

$$\int_{-\infty}^{+\infty} W(\theta) d\theta = 1 \quad (10)$$

Having obtained the explicit expression of the stationary distribution function $W(\theta)$ we are now in the position of evaluating the FPT distribution function for a prescribed threshold which will give a statistical description of the transient (or turn-on) time of NLC. If a step external field (with final value of $h = H/H_c$) is applied to the NLC the director will develop from an initial angle having a distribution function $W(\theta)|_{h=h_0}$ where $h_0 = H_0/H_c$ and H_0 is the initial value of the step field (the asymptotic result of the FPT distribution in Ref.15 is limited to the case of $h_0 = 0$).

We neglect the effect of the noise in the transition duration (i.e. in the path). Based on this approximation, we derive the time dependence of the angle $\theta(t)$ by integrating Eq.(6) omitting the Langevin force and with a stochastic initial value. We get

$$\theta^2(t) = \frac{\theta^2(\infty)}{1 + \left(\frac{\theta^2(\infty)}{\theta^2(0)} - 1\right)e^{-2At}} \quad (11)$$

where $\theta(\infty) = \sqrt{A/B}$ is the final steady-state value of $\theta(t)$, and $\theta(0)$ is the stochastic initial steady-state angle having the distribution function $W(\theta(0))$ with the initial field h_0 . From Eq. (9) we have

$$W(\theta(0)) = C e^{\left(\frac{1}{2}A_0\theta^2(0) - \frac{1}{4}B_0\theta^4(0)\right)/a^2} \quad (12)$$

where $A_0 = h_0^2 - 1$ and $B_0 = h_0^2/2$.

As mentioned above, the FPT in the NLC system is defined as the time interval between the moment when the step external field is applied and the moment when the angle $\theta(t)$ reaches a prescribed threshold value θ_{th} for the first time. Let the threshold angle

$$\theta_{th} = b\theta(\infty), \quad (13)$$

where $0 < b < 1$ because $0 < \theta_{th} < \theta(\infty)$. Substitution of Eq.(13) in Eq.(11) gives

$$\theta^2(0) = \frac{A/B}{1 + \left(\frac{1}{b^2} - 1\right)e^{2At_1}}, \quad (14)$$

where t_1 is the FPT.

Since the distribution function of $\theta(0)$ is known, we can derive the distribution function of t_1 with the transformation relation:

$$W(t_1) = W(\theta(0)) \frac{d\theta(0)}{dt_1} \quad (15)$$

Combination of Eqs.(12), (14) and (15) gives the distribution function of the FPT:

$$W(t_1) = 2C \sqrt{\frac{A^3}{B} \left(\frac{1}{b^2} - 1\right)} \left(1 + \left(\frac{1}{b^2} - 1\right)e^{2At_1}\right)^{-3/2} \exp \left(2At_1 + \frac{A_0}{2a^2} \frac{A/B}{1 + \left(\frac{1}{b^2} - 1\right)e^{2At_1}} - \frac{B_0}{4a^2} \left(\frac{A/B}{1 + \left(\frac{1}{b^2} - 1\right)e^{2At_1}} \right)^2 \right) \quad (16)$$

In the case that the initial field is equal to the critical value, i.e. $A_0 = 0$ Eq.(20) reduces to

$$W(t_1) = \frac{4}{\Gamma(1/4)} \left(\frac{B_0}{4a^2}\right)^{1/4} \sqrt{\frac{A^3}{B} \left(\frac{1}{b^2} - 1\right)} \left(1 + \left(\frac{1}{b^2} - 1\right)e^{2At_1}\right)^{-2/3} e^{\left(2At_1 - \frac{B_0}{4a^2} \left(\frac{A/B}{1 + \left(\frac{1}{b^2} - 1\right)e^{2At_1}} \right)^2 \right)}, \quad (17)$$

where $\Gamma(1/4)$ is a gamma function¹⁸.

In order to see the degree of approximation of Eq.(16), in Fig. 1 we plot both the analytical result of Eq. (16) and the Monte Carlo data of the numerical simulation with

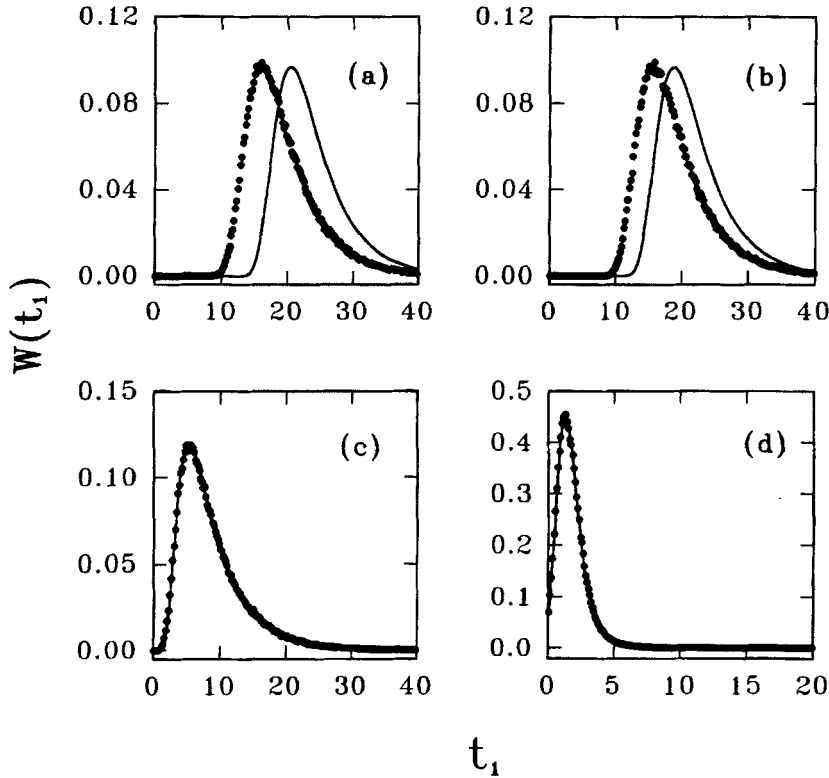


Fig.1. Plot of Eq. (16) (solid curves) and Monte Carlo data (dots) for $h^2 = 1.2$, $a^2 = 10^{-5}$, $b^2 = 0.1$ and $h_0^2 =$ (a) 0, (b) 0.5, (c) 1.0 and (d) 1.01.

Eq.(6). It can be seen that when the initial field is very close or above the critical value (i.e. $h_0 \approx 1$ or $h_0 > 1$), Eq. (16) agrees well with the Monte Carlo result, while for the case that the initial field is below the critical value (usually $h_0 = 0$) deviation is apparent, which indicate that the effect of noise in the path is negligible in cases that the initial field is very close or above the critical value.

This research was supported by the National Natural Science Foundation of China.

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