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Calculation of the nematic entropy using digital images

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In this work we will use digital images to compute the entropy dependence on temperature of a nematic lyotropic sample. The set of images comprehend the entire temperature range between a reentrant nematic isotropic phase transition, at a low temperature, and a usual nematic isotropic phase transition at a higher temperature. We will show that, inside the nematic phase, the image entropy profile agrees accurately with the entropy given by the Maier-Saupe model. As far as we know, this is the first time that the entropy of a lyotropic nematic phase is evaluated by this method, which introduces a way to measure their macroscopic variables. Namely, being that the entropy is a thermodynamical potential, this result implies that digital images can be used to compute mean values of nematic random variables.

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Nowadays, digital image files have completely prevailed over the old plate photographic storage processes. A reason for this digital revolution is that today an image is stored as a succession of digits representing an ordered sequence of pixels, which are decomposed in three spectral colors, usually red, green, and blue (RGB). Each of these colors has its intensity quantified by numbers, normally $2^8 = 256$ binary digits [1]. While, in liquid crystals (LCs) physics, images created with LCs devices are at the center of instrumental applications [2,3], the use of these numerical files as a source of quantitative scientific knowledge is relatively recent. As far as we know, just in 1998 a proposal to study LCs phase transitions using image processing was made [4–9], and in 2006 a LCs textures study using digital images was proposed [10,11]. Since then, this kind of LCs approach has been increasingly used to measure LCs parameters and, surely, it comes to stay [12–22].

In this paper we will show that even fundamental thermodynamic LCs properties can be measured throughout image processing. We will present a method that uses it to evaluate the temperature dependence of the orientational entropy of a lyotropic LC sample. To do that, we will use two facts: first, a digital image can have its entropy directly measured [1]. Second, as the homogeneity of the nematic ordering can be recognized by its light transmission properties, the produced image must be a function of the director degree of alignment and, consequently, the entropy of both systems must be correlated. Namely, to interpret the image entropy in terms of the nematic concepts, it will be compared with the entropy given by the Maier-Saupe model [23], and we will found that they are proportional. And, to further examine the similarities between them, we will study a particular nematic phenomenon for which the entropy dependence on temperature is very characteristic; the entropy behavior of a lyotropic mixture of laurate of potassium at the phase space region where it presents two nematic isotropic phase-transitions: the usual one at a high temperature and a reentrant one at a low temperature [7,24,25]. The reason for this choice is clear, when only the nematic orientational properties are considered we would observe that, in the neighborhoods of NI reentrant region, the entropy would increase as the temperature is reduced. This apparently nonphysical phenomenon is so characteristic of a reentrant phase that it would be very interesting to observe how the entropy of images describe it. As we will see, the agreement between the entropy of images and the Maier-Saupe result persists even at the region of the reentrant phase transition: the image entropy corresponds entirely to the Maier-Saupe entropy.

To compute the image entropy of our photos we will use the approach presented in Ref. [1], which we now synthesize. We will take a digital image as ordered distribution pixels: a discrete set of colors locations, and respective intensities, completely covering a planar sheet. Each pixel is composed of three colors and along our calculations we will consider $\Omega_c(i)$ as the normalized distribution of intensities of a given color in the set of all pixels of a given image, i, runs over all the 256 values of the intensities of the corresponding color, c (R for red, G for Green, B for blue). When this is done, throughout the expression

$$\Sigma_c = -\sum_{i=0}^{255} \Omega_c(i) \ln[\Omega_c(i)], \qquad (1)$$

we can be compute the entropy Σ_c of the color c in the respective image [1]. The digital image has been taken by a CCD camera connected to a polarized light microscope (see Fig. 1). They were directly stored in a file driven by a computer and present a resolution of 1280 × 1024 pixels; the MatLab program was utilized to analyze them according to the above equation. Our samples were placed in a hot stage (MK200) device with temperature stability of up to 0.01 K, where the minimum temperature of the hot stage was controlled by a Heto circulating temperature bath also stable at 0.01 K. The optical measurements were performed only when the temperature of the sample was stabilized to better than 0.01 K. A heating rate of 8 mKs^{-1} was used during the acquisition of the experimental image frames.

In Fig. 2 we see the profile that we have found for Σ_R (R, red color) as a function of temperature, for a lyotropic mixture (concentration in weight percent) of potassium laurate (KL: 27.06), decanol (DeOH: 6.17), and deuterium oxide

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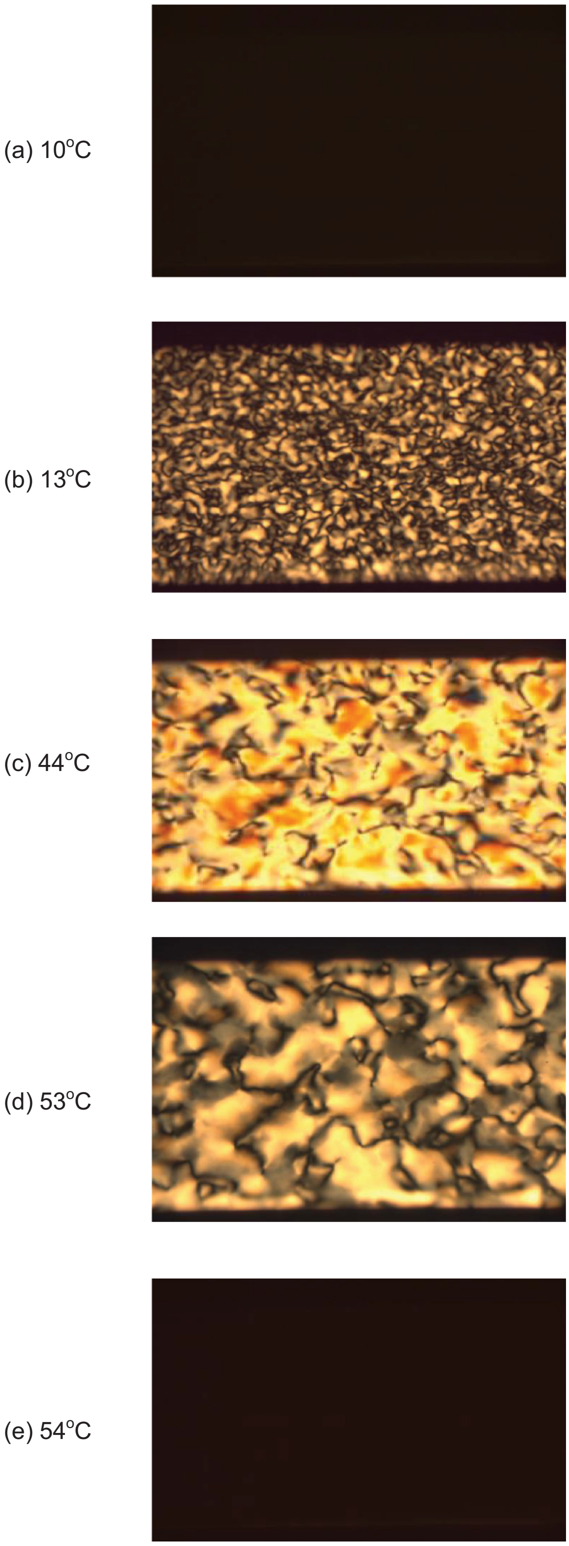

FIG. 1. (Color online) Lyotropic nematic textures: (a) I_{RE}, (b) N_C near the I_{RE}, (c) N_C, (d) N_C near the I, and (e) I. I_{RE}, N_C, and I are the reentrant isotropic, calamitic nematic, and isotropic phases, respectively.

(D_2O: 66.77) [24,25] at a nematic calamitic (N_C) phase. Each point of the figure gives the entropy Σ_{R} of a different photo and, for each photo, the calculations given by Eq. (1) have been performed. The resulting picture has the form of the letter u, where the picks at each of its borders point to the N_C-reentrant isotropic (I_{RE}) and the usual N_C-isotropic (I) phase transitions, respectively, and, at the same time, also distinguishing two regions. The first corresponds to the entropy behavior at low temperatures, where the entropy decreases with increasing temperature. The other, at higher temperatures, presents the reverse behavior; the entropy increases with temperature. The

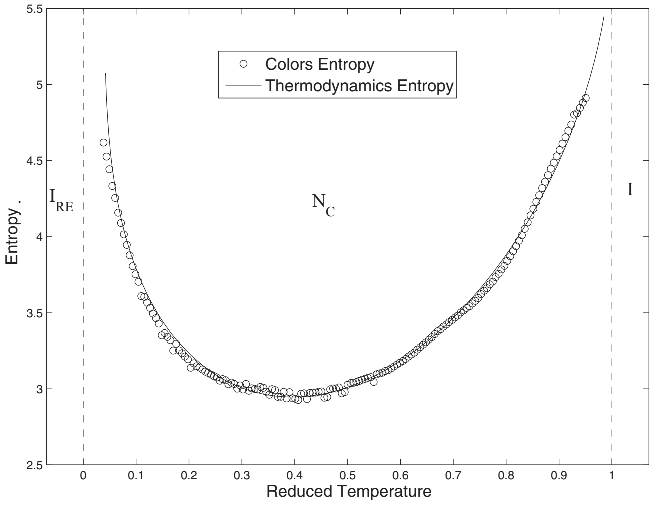

FIG. 2. Entropy versus temperature of a lyotropic sample, as described in the text. The dotted lines correspond to the image entropy, each point corresponding to a different photo for which the statistical approach described at Eq. (1) has been applied. The continuous line corresponds to the entropy of a nematic sample as predicted by the Maier-Saupe model. The excellent adjustment of these two curves, including the neighborhoods of the nematic reentrant phase transition, reveals that the image entropy corresponds to the nematic entropy obtained throughout the Maier-Saupe approach.

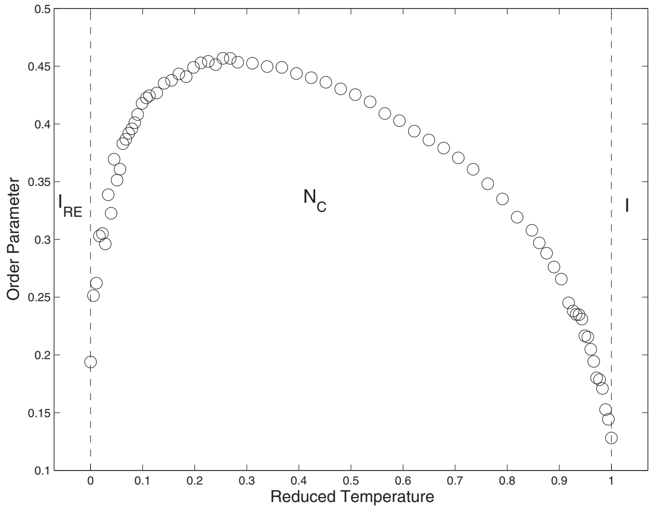

FIG. 3. Order parameter profile of a nematic sample, as described in the text, presenting a reentrant nematic isotropic phase transition at low temperatures and the usual nematic isotropic phase transition at high temperatures. This profile of S has been used to compute the Maier-Saupe entropy described in the legend of Fig. 2.

apparently nonphysical behavior at low temperatures can be understood if we remember that the images that we see in a lyotropic LC sample result from micellar alignment and, in a lyotropic material, we must also consider micellar changes with temperature. As long as the physics of this behavior has no direct consequences in the image, the image entropy is only part of the total entropy. The exact temperature values of these transitions are: $I_{\mathrm{RE}} - N_{\mathrm{C}}$ (10.15°C) and $N_{\mathrm{C}} - I$ (53.80°C) [25], respectively. A heating rate of $\sim$8 mKs^{-1} was used during the image acquisition. The nematic samples, not aligned, were sealed in planar glass cells with width of 0.5 mm along the light path and placed in a hot stage with an accuracy of 0.01 K. The image frames of nematic textures were obtained by the CCD camera, with a resolution of 1280 × 1024 pixels, connected to a polarized light microscope [4,6]. In our nematic textures the red color was predominant.

In order to give an interpretation to image entropy, we will assume that, when we consider the entire nematic sample, the homogeneity of the light transmitted throughout the sample is proportional to the average distribution of the director alignment. So, we follow Maier-Saupe [26] and assume that the probability of finding a nematic micellar axis deviating by an angle θ from the director orientation is given by [23],

$$P(\theta)d\theta = \frac{d[\mathrm{Cos}(\theta)]e^{k[\cos^2(\theta)-\frac{1}{3}]}}{Z}, \tag{2}$$

where $k = 3\,SV/2\,K_BT$, S is the scalar order parameter, V is the aligning potential between the nematic molecules/micelles, K_B is the Boltzmann constant, T the temperature, and $Z = 2\int_0^\pi d[\mathrm{Cos}(\theta)]\exp[k(\cos^2(\theta) - \frac{1}{3})]$ is the angular partition function. Having the probability of a given angular distribution $P(\theta)$, the corresponding entropy can be calculated with the use of the expression

$$\Sigma = -K_B \int_0^\pi d[\mathrm{Cos}(\theta)]P(\theta)\ln[P(\theta)], \tag{3}$$

which will be named Maier-Saupe entropy. A straightforward calculation shows that the exact solution for Σ is given by

$$\Sigma = \frac{1}{4}\left\{1 + 2k - \frac{2e^{k\sqrt{k}}}{\sqrt{\pi}\,\mathrm{erf}\,i(\sqrt{k})} - 2\ln\left[\frac{e^{k\sqrt{k}}}{\sqrt{\pi}\mathrm{erf}\,i(\sqrt{k})}\right]\right\}, \tag{4}$$

where $\mathrm{erf}\,i\,(x)$ is the imaginary error function, with argument x.

As consequence of our homogeneity hypotheses, we assume that Eqs. (1) and (4) are proportional. To compare these equations we must know the temperature T dependence of the parameters appearing at $k = 3\,SV/2\,K_BT$. The dependence of S on T has been measured previously [27], and we will use that result here, exhibited in Fig. 3. We see that the order parameter has a maximum around $T \approx 0.3$ and it diminishes for low and high temperatures, where we found, respectively, the reentrant and the usual NI phase transitions. k also depends on T throughout interacting potential V (remember, we are studying a lyotropic system). Using the experimental data for S given above, and assuming that the dependence of V on T is small, i.e., $V \approx V_0(1 + a_1T + a_2T^2 + \cdots)$, where $a_1, a_2 \ldots$ are small, we have found for Σ the profile represented by the thin continuous line of Fig. 2.

The main result of this paper arises from the fine agreement between the two curves shown in Fig. 2, they concord not only at the region of the normal NI phase transition, but also at the region of the reentrant NI phase transition. The apparent unexpected behavior of reentrant isotropic phase, materialized in Fig. 3 throughout the order parameter increasing as the temperature increases, is also revealed in Fig. 2 by the entropy decreases with the increasing temperature. Of course, the description of these results by the Maier-Saupe approach does not constitute a surprise, the real novelty is that these results are also perfectly matched by the direct measurement of the digital image entropy.

The fact that digital image entropy of nematic LCs describes the Maier-Saupe entropy is the novelty introduced by this paper. An immediate consequence is that with this method we can compute experimental values of nematic statistical parameters. For example, with the derivative of the data displayed in Fig. 2, we can straightforwardly obtain the specific heat of the nematic orientational order. As a generalization, if we measure the image entropy as a function of a given external parameter, from the corresponding derivative we would obtain the associated random variable.

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