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Corresponding states in nematic elasticity

M. Simões* and D. S. Simeão
Departamento de Física, Universidade Estadual de Londrina, Campus Universitário, 86051-990 Londrina, Parana, Brazil

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A comparative study of the temperature dependence of the elastic constants of the nematic liquid crystals known as PAA (*p*-azoxyanisole), MBBA 4′-methoxybenzylidene-4-*n*-butylaniline, and 5CB (4-*n*-pentyl-4′-cyanobiphenyl) will be made in this work. After a regularization of their values, and with use of a unique temperature scale, the experimental data of each of these parameters will be displayed along the lines of corresponding states that are not restricted to the neighborhoods of the nematic-isotropic phase transition point, as it would be the case in a usual corresponding states law, but encompass the entire nematic phase.

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I. INTRODUCTION

The study of the elastic constants of the nematic liquid crystals (NLC) is an old-standing problem [1–3] for which experimental [4–9], computational [10], and analytical methods [11–20] have been applied and, for each of these approaches, new sets of results have been found. Nevertheless, despite such developments, the understanding of the nematic elasticity is not yet complete. Along the development of the NLC physics a large set of experimental data on the values of the elastic constants has been accumulated. However, save for occasional references [4,15], a comparative and systematic study of the relations among data points of different compounds are scarce. In fact, as far as we know, for only a few compounds the complete behavior of all bulk elastic constants along the entire nematic phase has been measured [4,5,7–9]. The aim of this work is to introduce a systematic procedure to compare the elastic constants values along the entire nematic phase. A comparative study of the experimental data of the splay, twist and bend elastic constants [21], K_{11}, K_{22}, and K_{33}, respectively, for the compounds, PAA (*p*-azoxyanisole) [4], MBBA (4′-methoxybenzylidene-4-*n*-butylaniline) [4], and 5CB (4-*n*-pentyl-4′-cyanobiphenyl) [5,6], along the entire range of the nematic phase, will be performed.

In order to do it a new temperature scale will be introduced, the nematic scale. The advantage of such a procedure is that our comparison of the physical quantities will not be restricted to the neighborhoods of a critical point [22], but it will be extended along the entire nematic phase. With this procedure, it will be shown that the bulk elastic constants follow corresponding states laws; when the absolute values of each elastic constant and temperature interval are rescaled, the experimental points of each elastic constant coalesce to common curves, indicating the existence of universalities. Our results will be compared with the previous results of Berreman and Meiboom [15] that have made a study of the dependence of the elastic constants on the order parameter. It will be shown that their results can explain the differences of the profiles that we have found on the elastic constants profiles, but not its universality.

II. RESCALING EXPERIMENTAL DATA

Figure 1 exhibits the measured values of the elastic constants K_{11}, K_{22}, and K_{33} as a function of the temperature for different compounds. Each compound presents specific and individual values of elastic constants and temperature intervals. This work deals with the characterization of common properties that can be extracted from these experimental data and with the possibility of putting each of them along corresponding states curves. So, let us rescale all elastic constants values by the maximum value attained by each of them. The corresponding regularized elastic constant will receive a hat. So, $\hat{K}_{11}=K_{11}/k_1$, $\hat{K}_{22}=K_{22}/k_2$, and $\hat{K}_{33}=K_{33}/k_3$, where k_1, k_2, and k_3 are the maximum values attained by K_{22}, K_{22}, and K_{33}, respectively. Once this has been done for all data points, a graph with the points $\hat{K}_{22}\times\hat{K}_{11}$ and $\hat{K}_{33}\times\hat{K}_{11}$ has been produced. These results are shown in Fig. 2. The distribution of data points allows us to affirm that the individuality of the curves shown in Fig. 1 has disappeared and for both sets of points the experimental data become distributed along com-

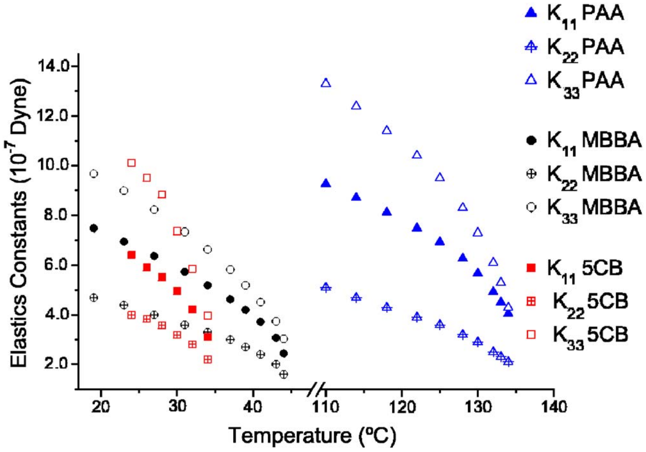

FIG. 1. (Color online) Experimental data of the bulk elastics constants of the liquid crystals: PAA [4], MBBA [4], and 5CB [5].

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*Electronic address: simoes@uel.br

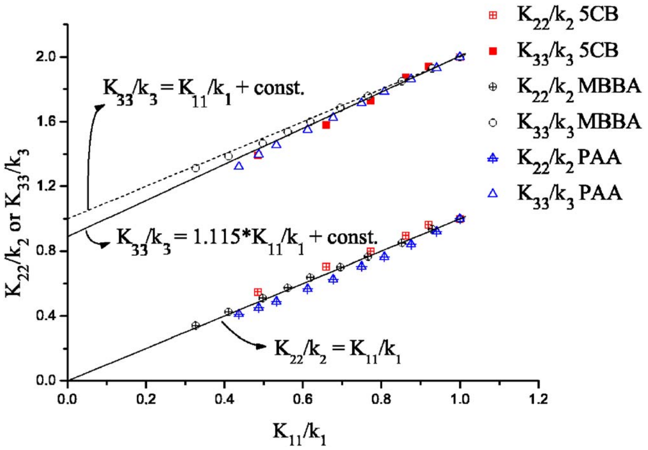

FIG. 2. (Color online) Normalized experimental data of the elastics constants. The lower set of points give the data of $\hat{K}_{22}\times\hat{K}_{11}$, the upper set display the points of $\hat{K}_{33}\times\hat{K}_{11}$. The experimental data of the elastic constant K_{ii}, $i=1,2,3$, was normalized with relation to the maximum value reached by each elastic constant. The profiles of these experimental data points suggest that, normalized in this way, these two sets are connected by a linear relation. We have taken advantage of the fact that the absolute values of the data points have no physical meaning, to give to these two sets positions that stress their different angular coefficients. The straight line plotted over the data of $\hat{K}_{22}\times\hat{K}_{11}$ has coefficient angular exactly one; the statistical treatment (least square) has furnished the value 0.997 ± 0.032. The data of $\hat{K}_{33}\times\hat{K}_{11}$ also seem to be distributed according to a straight line. The statistical treatment furnished the value 1.115 ± 0.028. The errors of the data points corresponding to $\hat{K}_{22}$ and $\hat{K}_{11}$ are about 14% along the $\vec{e}_y$ axis, and 6% along the $\vec{e}_x$ axis. Likewise, the errors corresponding to the data points of $\hat{K}_{33}$ are about 6% on both directions.

mon curves, suggesting the existence of relations between the elastic constants that do not depend on the material. The profile assumed by the experimental data suggests that, along the entire nematic phase, such relations would have a linear nature. These data also reveal that the inclination of the straight line plotted over the data corresponding to $\hat{K}_{22}\times\hat{K}_{11}$ is 1. (In fact $A=0.997\pm0.032$). Otherwise, when the experimental data of the curve $\hat{K}_{33}\times\hat{K}_{11}$ is considered, the best adjustment is obtained with the coefficient angular $A=1.115\pm0.028$. In the next section we will see that this result has a direct consequence; as a function of the temperature, the curves of $\hat{K}_{11}$ and $\hat{K}_{22}$ have the same slope. These results resemble a similar one previously found by Berreman and Meiboom [15]. By comparing their theoretical results with the experimental data, they found that the K_{33} presents an order parameter dependence expressively different from the one observed for K_{11} and K_{22}. While for K_{11} and K_{22} the dominant order parameter term is S^2, for K_{33} there is an additional contribution of S^3 that is not negligible. So, according to these results, the value that we have found for the angular coefficient of $\hat{K}_{22}\times\hat{K}_{11}$, results from the fact that K_{11} and K_{22} have the same dependence on S. Otherwise, the different value found for the angular coefficient of $\hat{K}_{33}\times\hat{K}_{11}$, is a consequence of the above mentioned non-negligible contribution of the S^3 term.

III. CORRESPONDING STATES OF ELASTIC CONSTANTS

Besides the values assumed by the rheological parameters, there is another important physical aspect that distinguishes the macroscopic behavior of some NLCs; the nematic-isotropic (NI) and the nematic-crystalline (NC) phase transitions give to each compound a typical nematic temperature interval [22]. If for all compounds a unique temperature could be attributed to a similar critical point, at least around it part of the effects attributed to the diversity found on the strength of the interaction could be attenuated. Usually, this procedure is implemented with a temperature rescaling, in such a way that the temperature of a fixed critical point is made the same for all compounds. Nevertheless, for some liquid crystals not only one fixed point is found, but two; the NI and the NC phase-transition points. So, for these compounds we can go beyond a simple shift in the temperature value; the existences of two critical points permit the collective establishment of two fixed temperatures and, as a consequence, the definition of a new temperature scale; the nematic scale [23,24].

Following these assumptions, all compounds studied here have had the temperature linearity rescaled in such a way that for the NC it was attributed the temperature $t=0$, while for the NI it was attributed the temperature $t=1$. That is, if T_{NI} is the Kelvin temperature of the NI phase transition point and T_{NC} is the Kelvin temperature of the NC transition point, then the nematic temperature t is related with the Kelvin temperature T by the linear relation,

$$t=\frac{T-T_{\mathrm{NC}}}{T_{\mathrm{NI}}-T_{\mathrm{NC}}}. \tag{1}$$

Figure 3 results from the application of the above temperature re-scaling to the data of the three elastic constants. After a normalization of the values of each set of the elastic constants, and the use of the nematic temperature scale, the three sets of elastic constants data coalesce in three different sets of points in a typical and apparently universal curve.

At Figure 4 the profile of the elastic constants exhibited at Fig. 3 has been superposed in such a way that the relative temperature development of the three elastic constants data points can be directly compared. As have been found in Fig. 2, the data curves for the $\hat{K}_{11}$ and $\hat{K}_{22}$ lie along the same curve. Nevertheless, this does not happen with $\hat{K}_{33}$, which presents a distinct nematic temperature dependence.

IV. FINAL REMARKS AND CONCLUSION

Figures 3 and 4 contain the main results of this work. These plots of normalized elastic constants values as a function of the nematic temperature scale have revealed that the three bulk elastic constants K_{11}, K_{22}, and K_{33} follow the corresponding states curves. Nevertheless, the superposition of the data points is not restricted to the neighborhoods of the

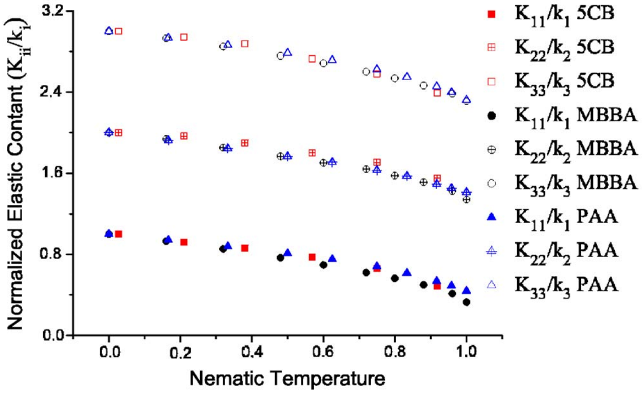

FIG. 3. (Color online) The normalized experimental data of $\hat{K}_{11}$, $\hat{K}_{22}$, and $\hat{K}_{33}$, as a function of the nematic temperature scale. The experimental data of the PAA, MBBA, and 5CB are represented by a triangle, a circle, and a square, respectively, as in Fig. 1. Each kind of elastic constant coalesce along a characteristic curve, showing that each of them behave according to the same fundamental law. Due to the normalization, the absolute values of the elastic constants are irrelevant in this figure, they have been plotted in three different positions for visual facilities.

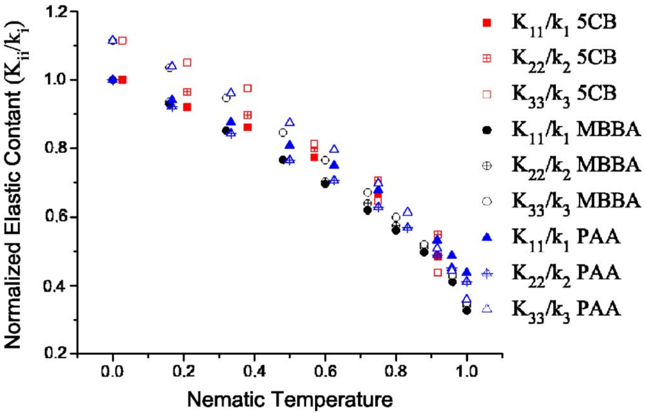

FIG. 4. (Color online) Normalized experimental data of $\hat{K}_{11}$, $\hat{K}_{22}$, and $\hat{K}_{33}$, as a function of the nematic temperature. According to what have been shown at Fig. 2, $\hat{K}_{22}$ and $\hat{K}_{11}$ have the same temperature behavior, while $\hat{K}_{33}$ possesses a different one. We have chosen to display data points in such a way that they agree at the nematic-isotropic phase transition and disagree at the nematic-crystalline phase transition point. Such a choice has a unique objective to stress the differences in the evolution of these curves.

nematic-isotropic phase transition region, as it would be expected from the theory of the critical phenomena [25], but it extends along the entire range of the nematic phase.

One known result about the liquid crystals physics says that, while the nematic-isotropic phase transition can be understood as a result of the Mayer-Saupe interaction between uniaxial nematic molecules, the diversity found in the elastic constants cannot [16]. That is, if it is assumed that the interaction between nematic molecules depends exclusively on the angle between their main axes [26], it would be found that the following set of relations between the bulk elastic constants:

$$K_{11} = K_{22} \neq K_{33}, \tag{2}$$

is valid. Of course, the experimental data contradict this relationship and, consequently, these results indicate that the physics of the nematic phase cannot be entirely determined by the Mayer-Saupe interacting term. Nevertheless, our results also indicate that K_{11} and K_{22} are much more related than could be initially suspected. The fact that K_{11}/k_1 and K_{22}/k_2 share the same temperature development can be interpreted as an indication that if the Mayer-Saupe interaction is not enough to take care of all phenomenology observed on the elastic constants it has, at least, a determinant contribution in its observed values. Furthermore, the results of Berreman and Meiboom [15] quoted above reveal that such common behavior of K_{11}/k_1 and K_{22}/k_2 would be dominated by a S^2 order parameter term, while the diverse behavior found on K_{33} would be due to the non-negligible presence of a S^3 term. If, by one side these results seem to reveal the essence of the profiles of the universalities found above, it must be stressed that our results present a significant difference from the one presented by Berreman and Meiboom [15]. They have made their analysis for each compound, and their results have led to a separate study of the behavior of each one. Our use of the nematic temperature scale has revealed the universality of the elastic constants profiles, that, by means of the linear scaling applied above, would be valid for the entire nematic phase. Consequently, our result reveals an improvement with relation to the work of Berreman and S. Meiboom, the universality of the temperature dependence of the elastic constants when expressed through the nematic temperature scale.

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