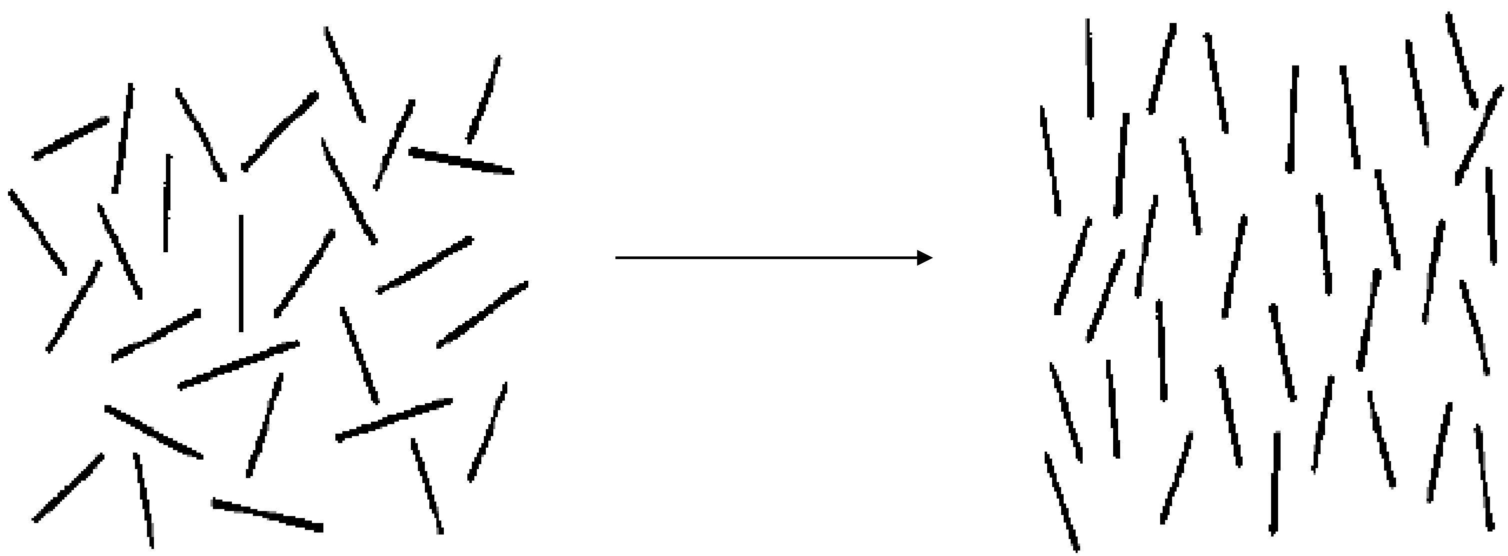
Elementary lattice models for the nematic phase transitions in liquid-crystalline systems

Silvio Salinas, IFUSP

SAIFR-IFT – II Condensed Matter Theory in the Metropolis

ICTP-SAIFR – 9-11, November 2022



isotropic

nematic (uniaxial)

1. The nematic phase transition

2. The Maier-Saupe-Zwanzig (MSZ) elementary model ....

3. MSZ model for mixtures of rods and discs

4. Mixtures of uniaxial and biaxial nematogenic elements

5. Elastomers: elastic MSZ model – biaxial structures

6. Field behavior – uniaxial and biaxial structures

7. Attempts to explain the cholesteric transition ….
……

Elementary lattice models for the nematic phase transitions …

The statistical mechanics of fluids is difficult …

The statistical mechanics of nematics is still worth ….

Even for the simplest models, no exact solution has been worked out …

De Gennes and Prost … famous 1993 book …

... so, we resort to quite elementary models ....

Elementary statistical models
(… at the mean-field level)

- simple way to investigate changes of parameters

- connections with phenomenological approaches (Landau-de Gennes expansions)

- unified approach to critical behavior

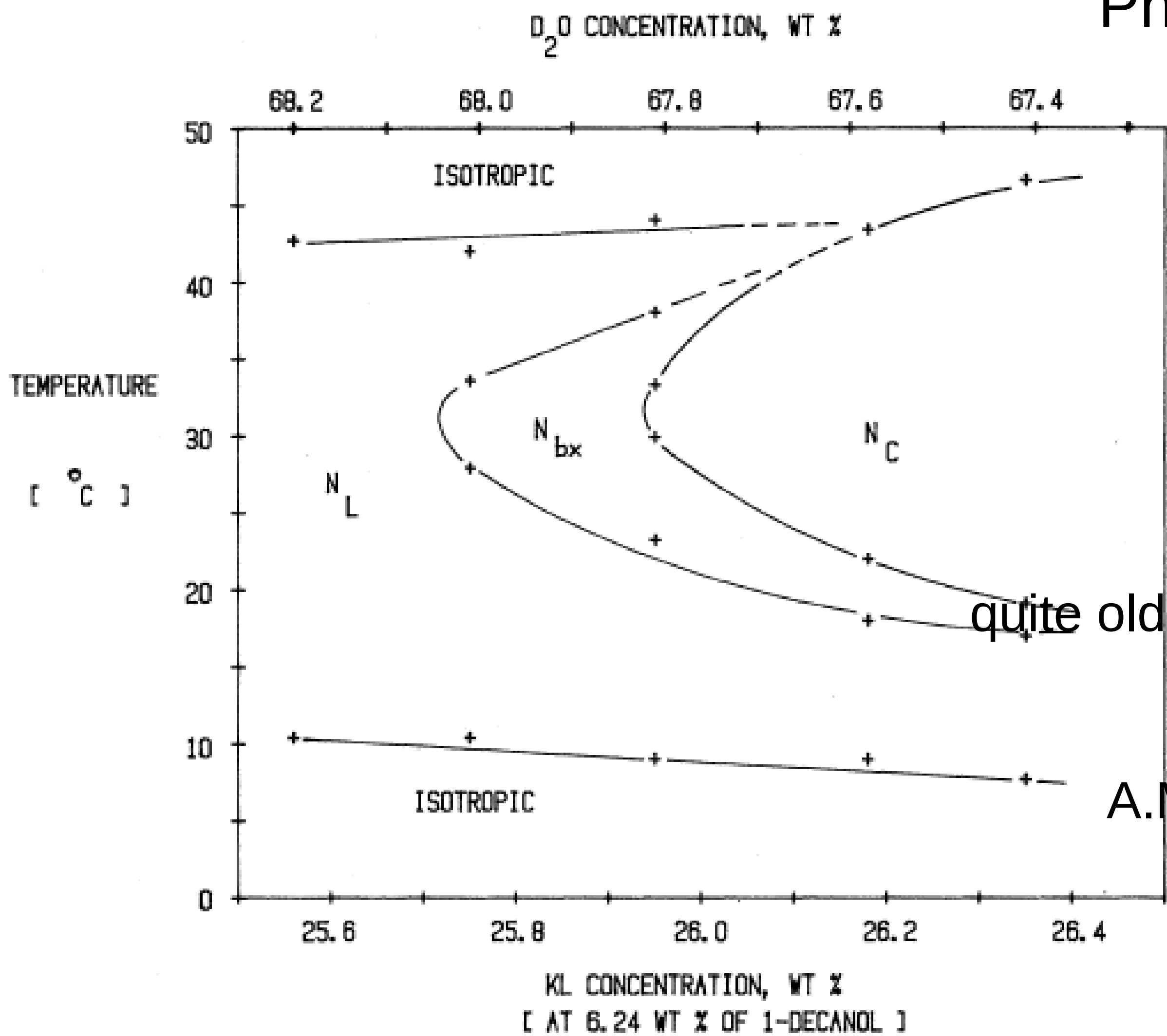
- interplay of theory, simulations, and experiments

- suggestions of occurrence of new experimental phenomena

Observation of a Biaxial Nematic Phase in Potassium Laurate–1-Decanol–Water Mixtures

L. J. Yu and A. Saupe
Liquid Crystal Institute, Kent State University, Kent, Ohio 44242
(Received 9 June 1980)

Phys. Rev. Lett 1980



quite old problem in São Paulo ...

L.Q. Amaral ...
A.M. Figueiredo Neto
....

FIG. 1. Phase diagram of the potassium laurate (KL)–1-decanol–D_2O system.

Observation of a Biaxial Nematic Phase in Potassium Laurate-1-Decanol-Water Mixtures

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VOLUME 45, NUMBER 12 PHYSICAL REVIEW LETTERS 22 SEPTEMBER 1980

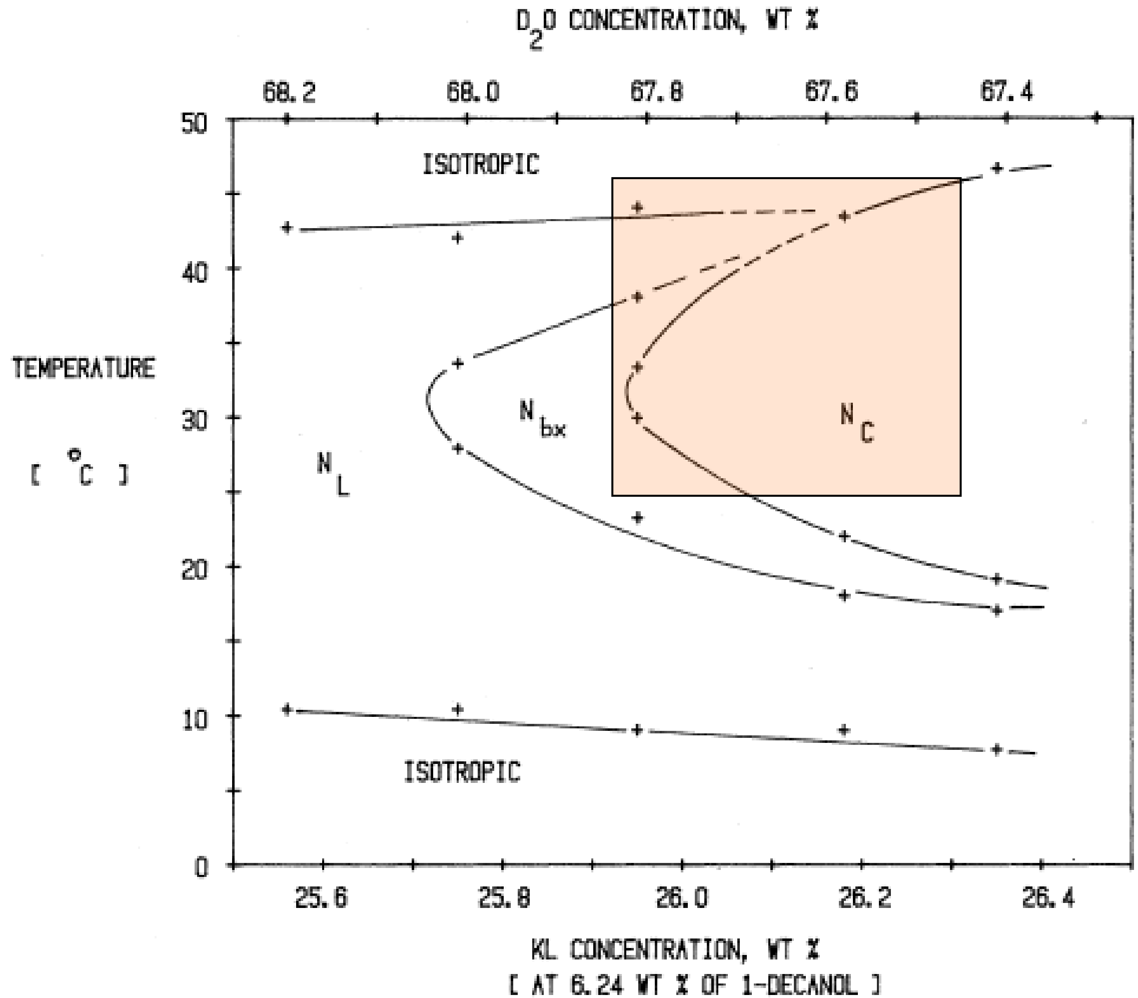


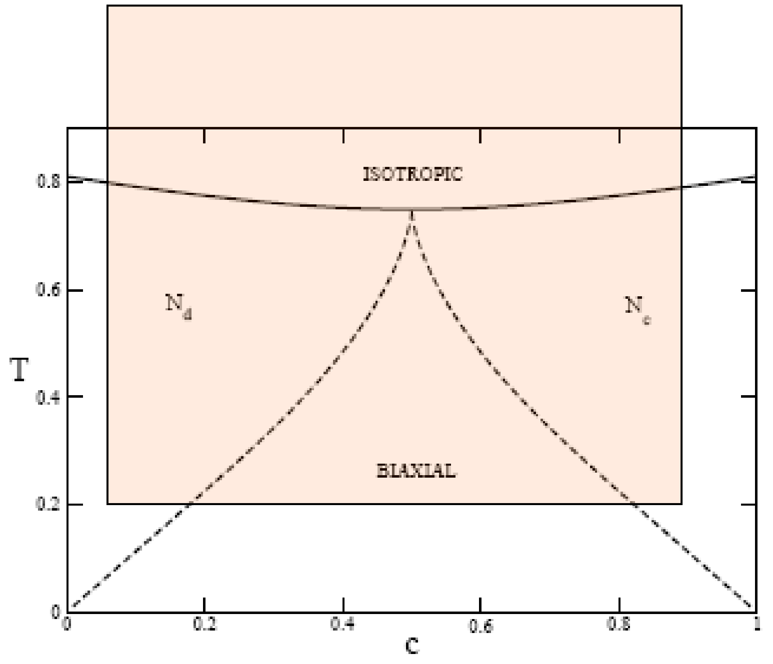
FIG. 1. Phase diagram of the potassium laurate (KL)−1-decanol−D_2O system.

11. Lyotropic systems, Antonio M. Figueiredo-Neto and Yves Galerne

Biaxial Nematic Liquid Crystals: Theory, Simulation, and Experiment, First Edition.
Edited by Geoffrey R. Luckhurst and Timothy J. Sluckin.

Table 11.1 *Lyotropic mixtures showing the biaxial nematic phase.*

Mixture components	Ref.
Potassium laurate (KL)–decanol (DeOH)–water	[4, 11]
Sodium decyl sulfate (SdS)–DeOH–water	[14]
Rubidium laurate (RbL)–DeOH–water	[15]
KL–decylammonium chloride (DaCl)–water	[16]
SdS–DeOH–water–Na_2SO_4	[17]
Sodium dodecyl sulfate (SDS)–DeOH–water	[18]
Sodium lauryl sulfate (SLS)–1-hexadecanol (HeOH)–water	[19]
Tetradecyltrimethylammonium bromide (TTAB)–DeOH–water	[20]



Statistical models of mixtures with a biaxial nematic phase
(Maier-Saupe mixture of rods and discs)

1. E. do Carmo, D.B. Liarte and SRS – PRE 2010 – elementary indeed

2. E.F. Henriques and SRS – EPJE 2012 – a bit less elementary

"Maier- Saupe theory"
(of the uniaxial nematic transition)

$$\mathcal{H} = -A \sum_{i,j} \sum_{\mu,\nu=1,2,3} S_i^{\mu\nu} S_j^{\mu\nu} \implies -A \sum_{i=1}^{N} \sum_{\mu,\nu=1,2,3} S_i^{\mu\nu} \left\langle S_j^{\mu\nu} \right\rangle$$

$$S_i^{\mu\nu} = \frac{1}{2}\left(3 n_i^{\mu} n_i^{\nu} - \delta_{\mu\nu}\right), \qquad |\vec{n}_i| = 1, \quad i = 1, 2, ..., N$$

$$\left\langle S_j^{\mu\nu} \right\rangle = Q_{\mu\nu} \qquad \mathrm{Tr}\ \mathbf{Q} = 0$$

$$\mathbf{Q} = \begin{pmatrix} -\frac{1}{2}S & 0 & 0 \\ 0 & -\frac{1}{2}S & 0 \\ 0 & 0 & S \end{pmatrix}$$

“Maier-Saupe (MS) model”
(for the uniaxial nematic transition)
(analogous to the Curie-Weiss model of ferromagnetism)

$$\mathcal{H} = -\frac{A}{N} \sum_{1 \le i < j \le N} \sum_{\mu,\nu=1,2,3} S_i^{\mu\nu} S_j^{\mu\nu}$$

$$Z = \sum_{\{\vec{n}_i\}} \exp\left[\frac{\beta A}{N} \sum_{1 \le i < j \le N} \sum_{\mu,\nu=1,2,3} S_i^{\mu\nu} S_j^{\mu\nu}\right]$$

Discrete version of the Maier-Saupe model

Maier-Saupe-Zwanzig (MSZ) model

$$Z = \sum_{\{\vec{n}_i\}} \exp\left[\frac{\beta A}{N} \sum_{1 \le i < j \le N} \sum_{\mu,\nu=1,2,3} S_i^{\mu\nu} S_j^{\mu\nu}\right]$$

$$\vec{n}_i = \begin{cases} (\pm 1, 0, 0) \\ (0, \pm 1, 0) \\ (0, 0, \pm 1) \end{cases}$$

three-state (Potts) model

$$S_i^{\mu\nu} \Longrightarrow \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix}, \quad \begin{pmatrix} -1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad \begin{pmatrix} 2 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

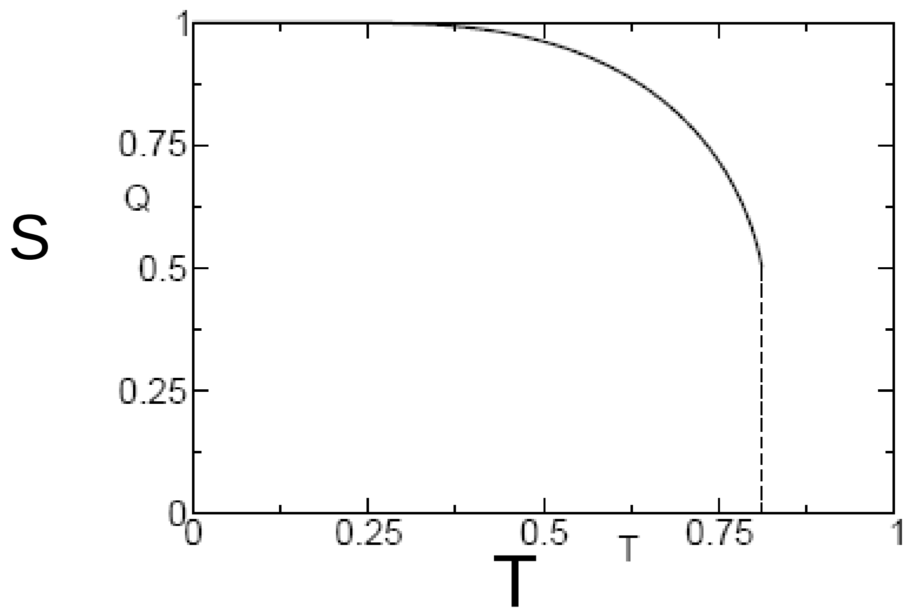
MSZ model (three-state model)

... connections with Landau–de Gennes expansion ...

... well-known first-order nematic-isotropic transition ...

$$f = f_0 + \frac{1}{2}\left(1 - \frac{3\beta A}{4}\right) I_2 - \frac{3\left(\beta A\right)^2}{16} I_3 + (\ldots) I_2^2 + (\ldots) I_2 I_3 + \ldots$$

$$I_2 = \mathbf{Tr}\,\mathbf{Q}^2, \qquad I_3 = \mathbf{Tr}\,\mathbf{Q}^3$$



... calculations on the Bethe lattice

E Carmo, AP Vieira, SRS, PRE 2011

Six-state (Freiser-Zwanzig) model
(for intrinsically biaxial nematic aggregates)

$$Q\,(1) = \begin{pmatrix} 1+\Delta & 0 & 0 \\ 0 & 1-\Delta & 0 \\ 0 & 0 & -2 \end{pmatrix},\ Q\,(2) = \begin{pmatrix} 1-\Delta & 0 & 0 \\ 0 & 1+\Delta & 0 \\ 0 & 0 & -2 \end{pmatrix},$$

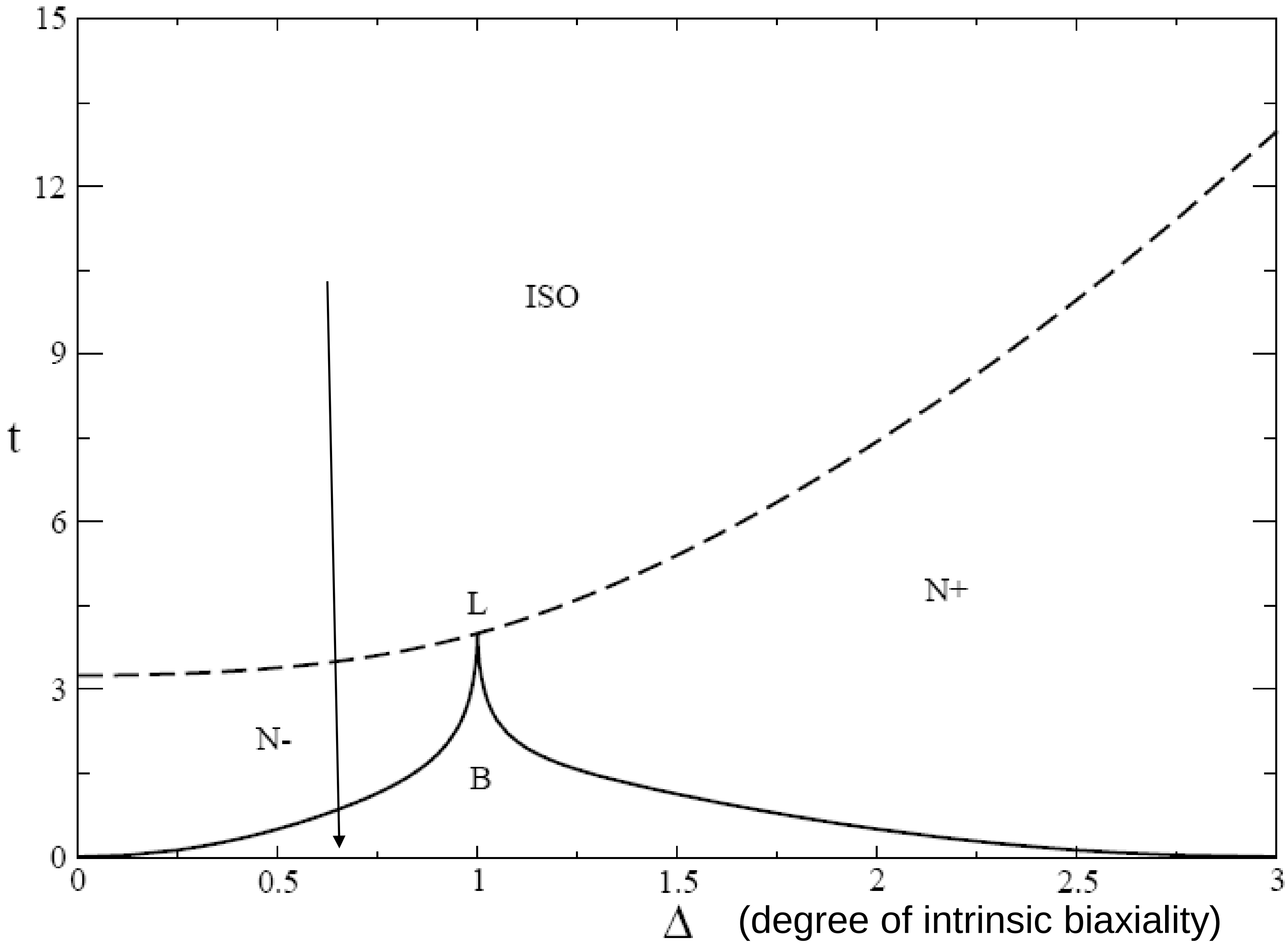
$$Q\,(3) = \begin{pmatrix} 1+\Delta & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & 1-\Delta \end{pmatrix},\ Q\,(4) = \begin{pmatrix} 1-\Delta & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & 1+\Delta \end{pmatrix},$$

$$Q\,(5) = \begin{pmatrix} -2 & 0 & 0 \\ 0 & 1+\Delta & 0 \\ 0 & 0 & 1-\Delta \end{pmatrix},\ Q\,(6) = \begin{pmatrix} -2 & 0 & 0 \\ 0 & 1-\Delta & 0 \\ 0 & 0 & 1+\Delta \end{pmatrix}.$$

parameter Δ gauges the degree of (intrinsic) biaxiality

six-state MSZ-Freiser model

E. Nascimento, E.F. Henriques, A.P. Vieira & SRS, PRE, 2015



(degree of intrinsic biaxiality)

Binary mixtures of intrinsically uniaxial and intrinsically biaxial elements ...
system 1 – MSZ model (purely uniaxial – 3 states)
system 2 – MSZF model (6 states – Δ is a parameter of biaxiality)
- Connections with the "IBM model"

PHYSICAL REVIEW E **92**, 062503 (2015)

Maier-Saupe model for a mixture of uniaxial and biaxial molecules

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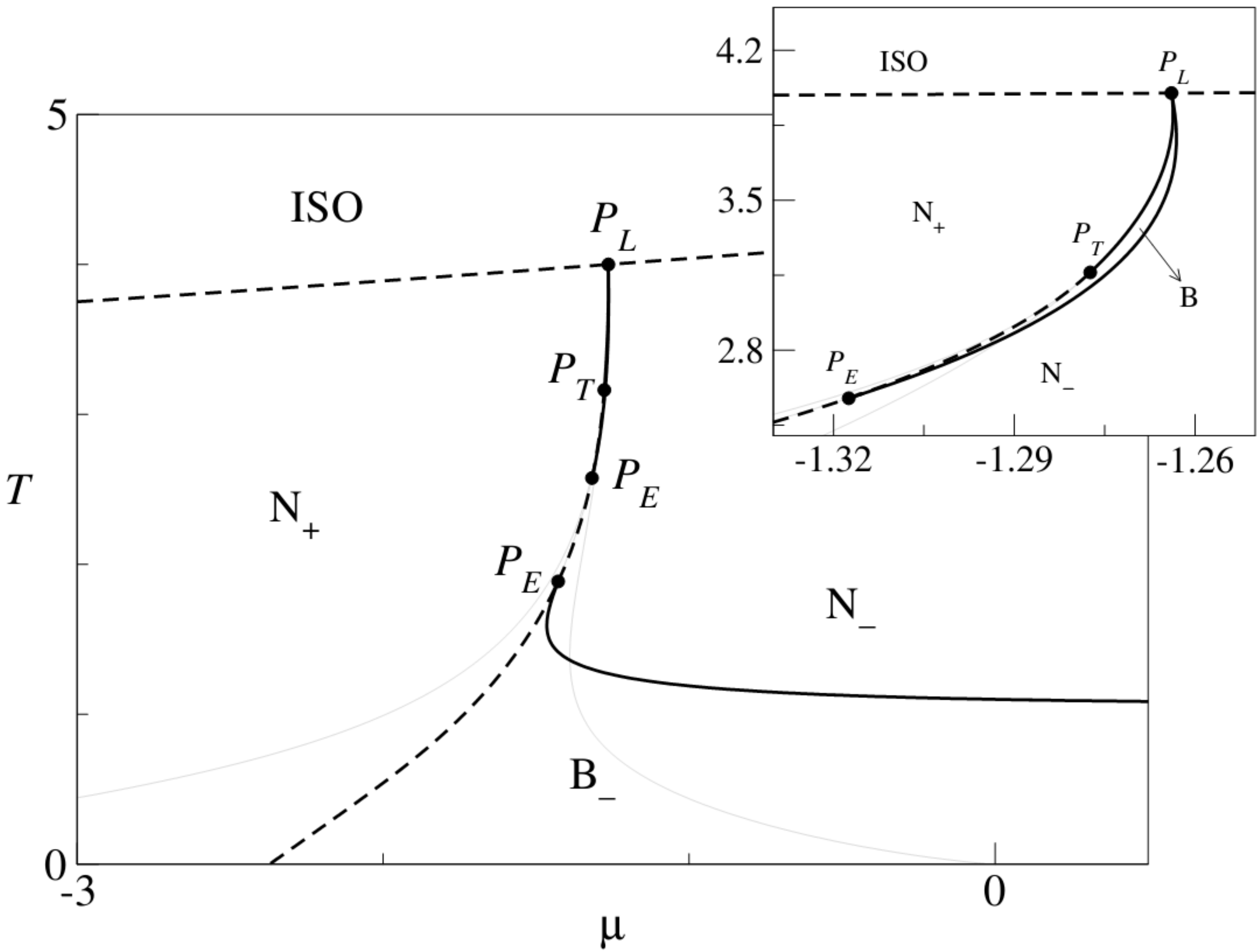
(Received 1 July 2015; published 1 December 2015)

We introduce shape variations in a liquid-crystalline system by considering an elementary Maier-Saupe lattice model for a mixture of uniaxial and biaxial molecules. Shape variables are treated in the annealed (thermalized) limit. We analyze the thermodynamic properties of this system in terms of temperature T, concentration c of intrinsically biaxial molecules, and a parameter Δ associated with the degree of biaxiality of the molecules. At the mean-field level, we use standard techniques of statistical mechanics to draw global phase diagrams, which are shown to display a rich structure, including uniaxial and biaxial nematic phases, a reentrant ordered region, and many distinct multicritical points. Also, we use the formalism to write an expansion of the free energy in order to make contact with the Landau–de Gennes theory of nematic phase transitions.

DOI: 10.1103/PhysRevE.92.062503 PACS number(s): 61.30.Cz

...depending on parameters, there is a huge variety of phase diagrams ....
... there are chances of contacts with more recent experiments ...



.... recent overviw of our work ......

crystals

MDPI

Article

Magnetic Field and Dilution Effects on the Phase Diagrams of Simple Statistical Models for Nematic Biaxial Systems

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check for updates

Abstract: We use a simple statistical model to investigate the effects of an applied magnetic field and of the dilution of site elements on the phase diagrams of biaxial nematic systems, with an emphasis on the stability of the Landau multicritical point. The statistical lattice model consists of intrinsically biaxial nematogenic units, which interact via a Maier–Saupe potential, and which are characterized by a discrete choice of orientations of the microscopic nematic directors. According to previous calculations

Real-space renormalization-group treatment of the Maier-Saupe-Zwanzig model for biaxial nematic structures

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The Maier-Saupe-Zwanzig model for the nematic phase transitions in liquid crystals is investigated in a diamond hierarchical lattice. The model takes into account a parameter to describe the biaxiality of the microscopic units. Also, a suitably chosen external field is added to the Hamiltonian to allow the determination of critical parameters associated with the nematic phase transitions. Using the transfer-matrix technique, the free energy and its derivatives are obtained in terms of recursion relations between successive generations of the hierarchical lattice. In addition, a real-space renormalization-group approach is developed to obtain the critical parameters of the same model system. Results of both methods are in excellent agreement. There are indications of two continuous phase transitions. One of them corresponds to a uniaxial-isotropic transition, in the class of universality of the three-state Potts model on the diamond hierarchical lattice. The transition between the biaxial and the uniaxial phases is in the universality class of the Ising model on the same lattice.

PHYSICAL REVIEW E **105**, 044705 (2022)

Phase behavior of a lattice-gas model for biaxial nematics

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We employ a lattice-gas extension of the Maier-Saupe model with discrete orientation states to study the phase behavior of a statistical model for biaxial nematogenic units in mean-field theory. The phase behavior of the system is investigated in terms of the strength of isotropic interaction between anisotropic objects, as well as the degree of biaxiality and the concentration of those units. We obtain phase diagrams with isotropic phases and stable biaxial and uniaxial nematic structures, various phase coexistences, many types of critical and multicritical behaviors, such as ordinary vapor-liquid critical points, critical end points, and tricritical points, and distinct Landau-like multicritical points. Our results widen the possibilities of relating the phenomenological coefficients of the Landau–de Gennes expansion to microscopic parameters, allowing an improved interpretation of theoretical fittings to experimental data.

DOI: 10.1103/PhysRevE.105.044705

construction of generic Maier-Saupe models

general form of the interaction between pairs of nematogenic molecules

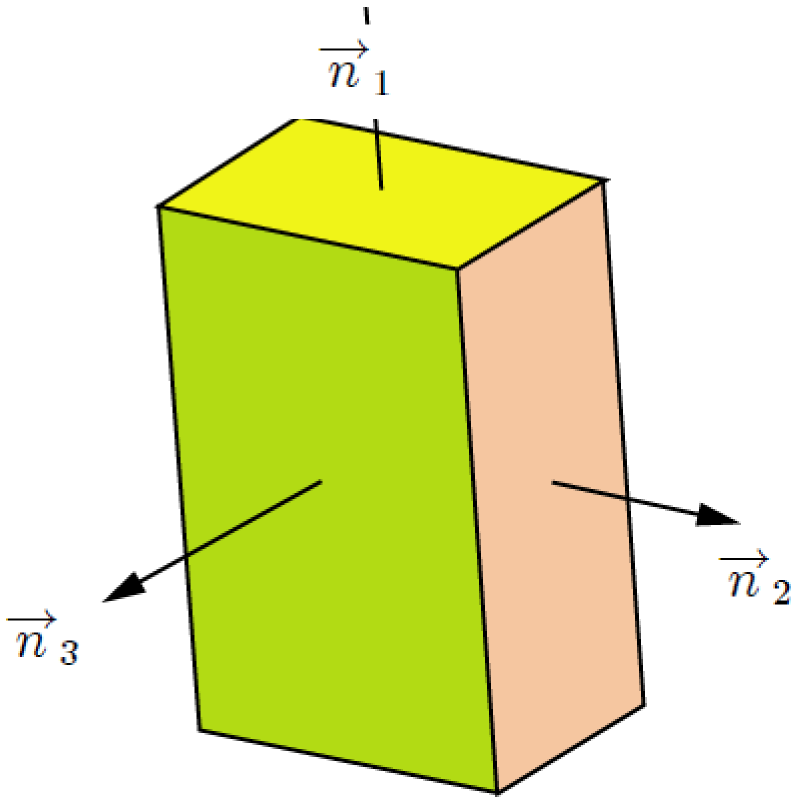
(in terms of the directors $\overrightarrow{n}_1$ and $\overrightarrow{n}'_1$ and the normal axes to these directors)

$$V = -A\left\{\mathbf{S}\cdot\mathbf{S}' + \gamma\left(\mathbf{S}\cdot\mathbf{B}' + \mathbf{B}\cdot\mathbf{S}'\right) + \lambda\,\mathbf{B}\cdot\mathbf{B}'\right\}$$

- proposal of AM Sonnet, EG Virga, GE Durand,
- Phys. Rev. E67, 061701 (2003)

- on the basis of

- JP Strailey, Phys. Rev. A10, 1881 (1974)



construction of generic Maier-Saupe models

general form of the interaction between pairs of nematogenic molecules

(in terms of the directors $\overrightarrow{n}_1$ and $\overrightarrow{n}'_1$ and the normal axes to these directors)

$$V = -A\left\{\mathbf{S}\cdot\mathbf{S}' + \gamma\left(\mathbf{S}\cdot\mathbf{B}' + \mathbf{B}\cdot\mathbf{S}'\right) + \lambda\,\mathbf{B}\cdot\mathbf{B}'\right\}$$

$$S^{\mu\nu} = \left(n_{1\mu}n_{1\nu} - \frac{1}{3}\delta_{\mu\nu}\right).$$

or

$$\mathbf{S} = \begin{pmatrix} n_{1x}n_{1x} - \frac{1}{3} & n_{1x}n_{1y} & n_{1x}n_{1z} \\ n_{1y}n_{1x} & n_{1y}n_{1y} - \frac{1}{3} & n_{1y}n_{1z} \\ n_{1z}n_{1x} & n_{1z}n_{1y} & n_{1z}n_{1z} - \frac{1}{3} \end{pmatrix},$$

or

$$\mathbf{S} = \overrightarrow{n}_1 \otimes \overrightarrow{n}_1 - \frac{1}{3}\mathbf{I},$$

where $\mathbf{I}$ is a unit matrix, the symbol $\otimes$ indicates a tensor product, and unit vector $\overrightarrow{n}_1$ is the “main director” of the nematogenic molecule.

construction of generic Maier-Saupe models

general form of the interaction between pairs of nematogenic molecules

(in terms of the directors $\overrightarrow{n}_1$ and $\overrightarrow{n}'_1$ and the normal axes to these directors)

$$V = -A\left\{\mathbf{S}\cdot\mathbf{S}' + \gamma\left(\mathbf{S}\cdot\mathbf{B}' + \mathbf{B}\cdot\mathbf{S}'\right) + \lambda\,\mathbf{B}\cdot\mathbf{B}'\right\}$$

$$\boldsymbol{B} = \overrightarrow{n}_2 \otimes \overrightarrow{n}_2 - \overrightarrow{n}_3 \otimes \overrightarrow{n}_3, \qquad \text{or} \qquad B^{\mu\nu} = \left(n_{2\mu}n_{2\nu} - n_{3\mu}n_{3\nu}\right)$$

or

$$\mathbf{B} = \begin{pmatrix} n_{2x}n_{2x} - n_{3x}n_{3x} & n_{2x}n_{2y} - n_{3x}n_{3y} & n_{2x}n_{2z} - n_{3x}n_{3z} \\ n_{2y}n_{2x} - n_{3y}n_{3x} & n_{2y}n_{2y} - n_{3y}n_{3y} & n_{2y}n_{2z} - n_{3y}n_{3z} \\ n_{2z}n_{2x} - n_{3z}n_{3x} & n_{2z}n_{2y} - n_{3z}n_{3y} & n_{2z}n_{2z} - n_{3z}n_{3z} \end{pmatrix},$$

where $\overrightarrow{n}_2$ and $\overrightarrow{n}_3$ are unit vectors normal do the "main director" $\overrightarrow{n}_1$ of the nematogenic molecule (and normal to each other).

construction of generic Maier-Saupe models

general form of the interaction between pairs of nematogenic molecules

(in terms of the directors $\overrightarrow{n}_1$ and $\overrightarrow{n}'_1$ and the normal axes to these directors)

$$V = -A\left\{\mathbf{S}\cdot\mathbf{S}' + \gamma\left(\mathbf{S}\cdot\mathbf{B}' + \mathbf{B}\cdot\mathbf{S}'\right) + \lambda\,\mathbf{B}\cdot\mathbf{B}'\right\}$$

Special cases of physical interest

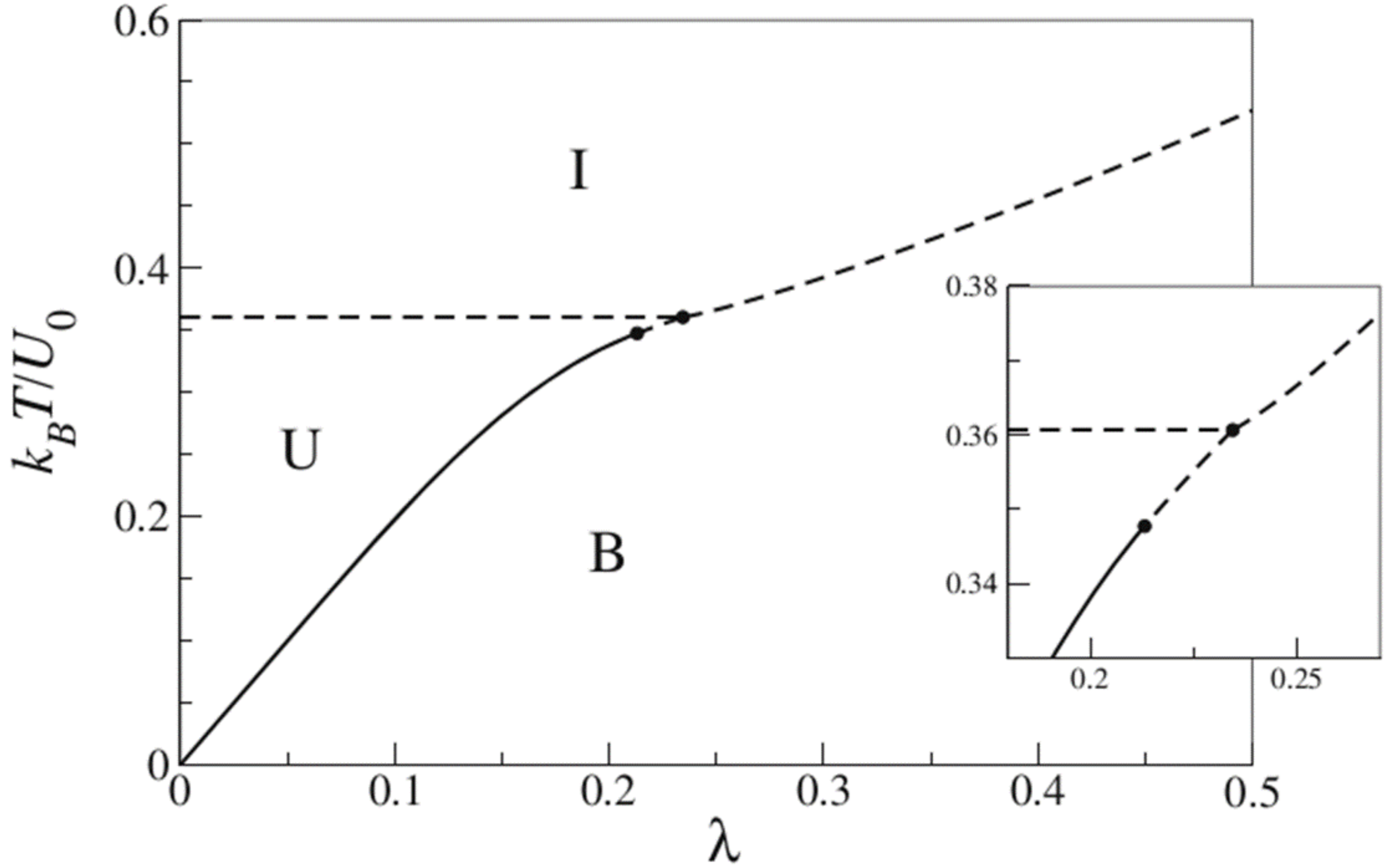
(i) $\gamma = \lambda = 0 \quad \Longrightarrow$ uniaxial system

(ii) $\lambda = \gamma^2 \quad \Longrightarrow$ "most usual case" (geometric-mean approximation)

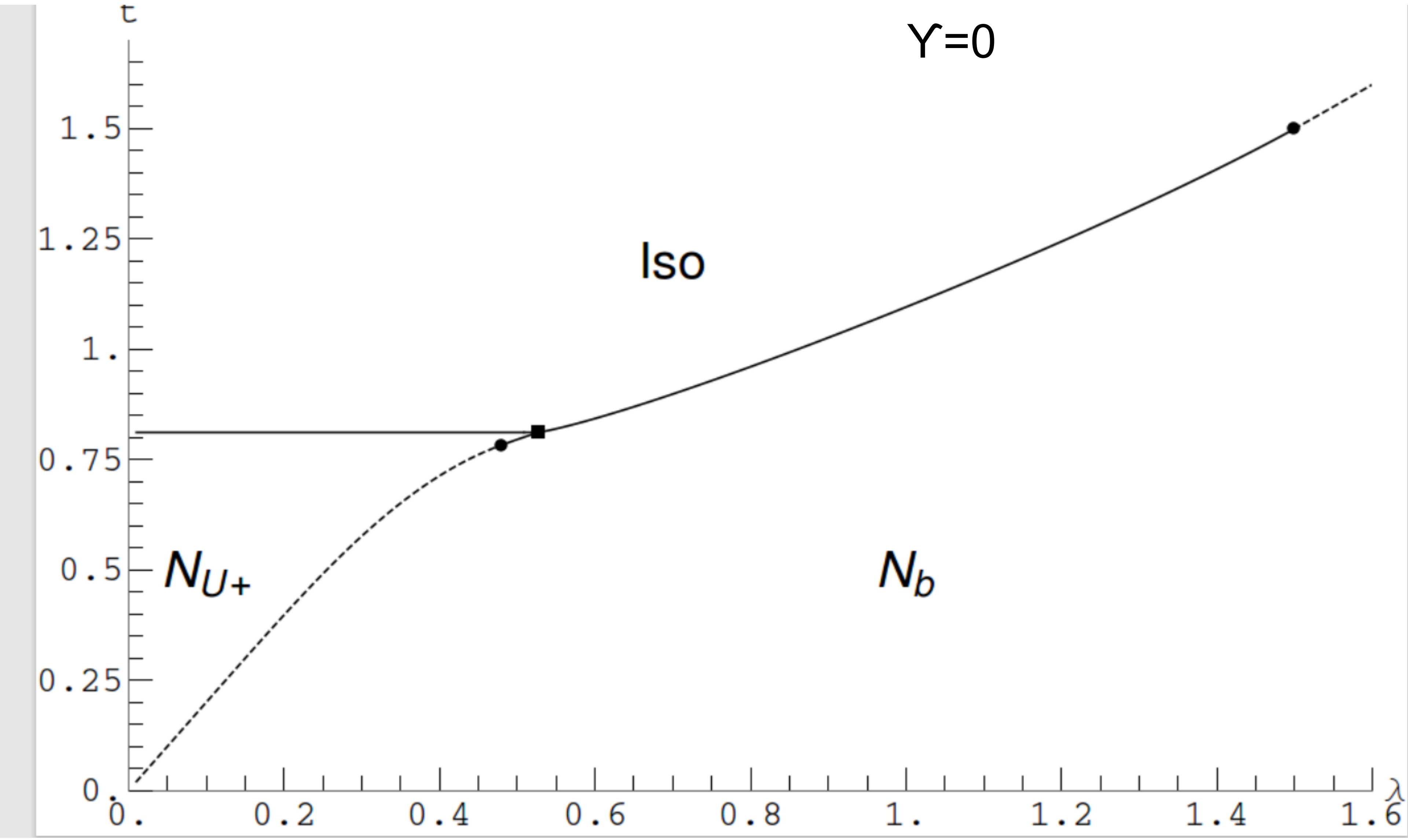
(iii) $\gamma = 0; \quad \lambda \neq 0 \quad \Longrightarrow$ quite interesting case (contact with new thermotropics)

E. Nascimento, A. Vieira, SRS, BJP, 2016 ....

ϒ=0



Nascimento, Vieira, SRS, BJP, 2016



F. Oliveira, 2022

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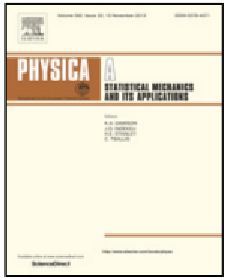

Modulated structures in a Lebwohl–Lasher model with chiral interactions

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HIGHLIGHTS

- We introduce a simple statistical lattice model to study chiral nematics.
- The system is investigated through a Bethe approximation.
- The phase diagram presents isotropic, nematic and modulated structures.
- The chiral phases exhibit a complex behavior as function of model parameters.

This work is a nematic extension of the magnetic Dzyaloshinkii-Moriya chiral mechanism. With O(2) symmetry, it is a nematic analogue of the chiral clock models ...

Thank you very much for your patience ....