Phase transitions in a system of long rods on two-dimensional lattices by means of information theory

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The orientational phase transitions that occur in the deposition of longitudinal polymers of length k (in terms of lattice units) are characterized by information theory techniques. We calculate the absolute value of an order parameter δ, which weights the relative orientations of the deposited rods, which varies between 0.0 (random orientation) and 1.0 (fully oriented in either of the two equivalent directions in an $L \times L$ square lattice). A Monte Carlo (MC) algorithm is implemented to induce a dynamics allowing for accommodation of the rods for any given density or coverage θ (ratio of the occupied sites over all the sites in the lattice). The files storing $\delta(t)$ (with time t measured in MC steps) are then treated by data recognizer wlzip based on data compressor techniques yielding the information content measured by a parameter $\eta(\theta)$. This allows us to recognize two maxima separated by a well-defined minimum for $\eta(\theta)$ provided $k \geqslant 7$. The first maximum is associated with an isotropic-nematic (I-N) phase transition occurring at intermediate density, while the second maximum is associated with some kind of nematic-isotropic transition at high coverage. In the cases of $k < 7$, the curves for $\eta(\theta)$ are almost constant, presenting a very broad maximum which can hardly be associated with a phase transition. The study varies L and k, allowing for a basic scaling of the found critical densities towards the thermodynamic limit. These calculations confirm the tendency obtained by different methods in the case of the intermediate-density I-N phase transition, while this tendency is established here in the case of the high-density phase transition.

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I. INTRODUCTION

The study of systems of hard rodlike particles has been an attractive and important topic in statistical physics for a long time. A pioneering contribution to this subject was made by Onsager [1], who predicted that very long and thin rods interacting by means of excluded-volume interaction only can lead to long-range orientational (nematic) order. This nematic phase, characterized by a big domain of parallel molecules, is separated from an isotropic state by a phase transition occurring at a finite critical density.

The problem proposed by Onsager is a clear example of an entropy-driven phase transition. Despite the physical relevance of this type of system with purely steric interactions, rigorous results are still very limited. In this vein, Heilmann and Lieb [2] showed that, for dimers, the system is disordered at all densities. The existence of nematic order in a system of large rods was rigorously demonstrated by Disertori and Giuliani [3]. In Ref. [4] the problem of hard rods was solved exactly on a treelike lattice. The authors showed rigorously the existence of a phase transition on this lattice. Later, Kundu and Rajesh [5] solved exactly a model of monodisperse long rigid rods with repulsive interactions on the random, locally treelike layered lattice. In the limit of hard interactions, two phase transitions are recovered as for the two-dimensional (2D) lattice.

The behavior of long rods has also been studied by using approximate methods [6,7]. Based on the configuration-counting procedure of the Guggenheim approximation [8], DiMarzio [6] showed the existence of nematic order in a lattice model of straight rigid rods. Identical results were obtained in Ref. [7], by using density-functional theory.

For the continuum problem, there is general agreement that in the case of deposition of infinitely thin rods in three dimensions the system undergoes a first-order phase transition [1]. On the other hand, in two dimensions, the nature of the phase transition depends crucially on the particle interactions and a rich variety of behaviors is observed [9–11].

In the case of lattice models, which is the topic of this paper, a system of straight rigid rods of length k on a square lattice, with two allowed orientations, was studied by Ghosh and Dhar [12]. Using Monte Carlo (MC) simulations and analytical arguments, the authors found strong numerical evidence showing that the system reaches nematic order at intermediate densities for $k \geqslant 7$ and provided a qualitative description of a second phase transition (from a nematic order to a non-nematic state) occurring at a density close to 1.

To illustrate this point, Fig. 1 shows the typical curve for density θ as a function of the chemical potential μ for a system of k-mers on a square lattice of side L. The adlayer undergoes an isotropic-nematic (I-N) phase transition from a low-density disordered phase to a nematic phase as θ is increased from 0 at $\theta = \theta_1$. As the density is increased above θ_1, a phase transition associated with the loss of the nematic order appears at $\theta = \theta_2 < 1$. The phase above θ_2 is not necessarily the same as the one present below θ_1, but the long-range order is lost as the order parameter defined below vanishes. A schematic representation of the plausible different phases occurring in the system are shown in the insets of Fig. 1: (i) the low-density disordered phase ($0 < \theta < \theta_1$), (ii) the intermediate-density nematic phase ($\theta_1 < \theta < \theta_2$), and (iii) the high-density non-nematic or differently ordered isotropic phase ($\theta_2 < \theta < 1$).

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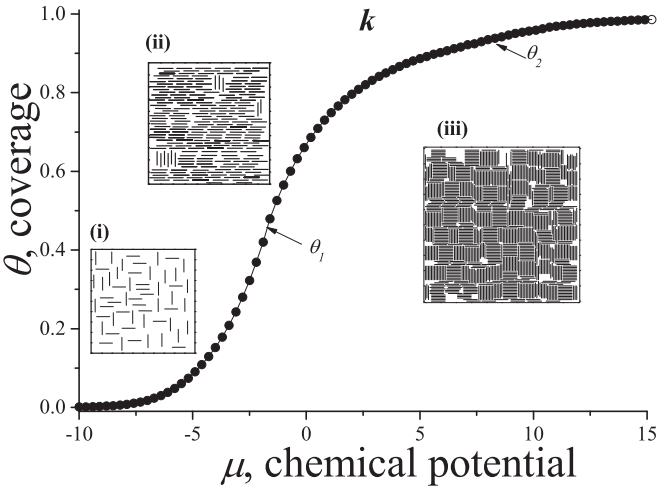

FIG. 1. Surface coverage θ as a function of the chemical potential μ for k-mers on square lattices of side L; although the actual curves vary with the ratio $L/k = f$, the general shape is preserved. Insets illustrate plausible orientational patterns: (i) the low-density disordered phase ($0 \leqslant \theta \leqslant \theta_1$), (ii) the intermediate-density long-range ordered phase ($\theta_1 \leqslant \theta \leqslant \theta_2$), and (iii) the high-density partly disordered phase ($\theta_2 \leqslant \theta \leqslant 1$).

Based on the seminal work of Ghosh and Dhar [12], a series of papers was devoted to the detailed study of the I-N transition occurring at intermediate density values in a system of long straight rigid rods on 2D lattices with discrete allowed orientations [13–19]. In these articles, it was shown that (1) the I-N phase transition from the low-density disordered phase to the intermediate-density ordered phase belongs to the 2D Ising universality class for square lattices and the three-state Potts universality class for honeycomb and triangular lattices [13,14], (2) the minimum value of k which allows the formation of a nematic phase is $k = 7$ for triangular lattices [15] and $k = 11$ for honeycomb lattices [14], and (3) the critical density characterizing the I-N transition θ_1 follows a power law as $\theta_1(k) \propto k^{-1}$ [15]. The corresponding proportionality constant was obtained in Refs. [18,19]. It was also shown that (4) the orientational order survives in a wide range of lateral interactions between the adsorbed k-mers [16,17] and (5) an Ising behavior is found for a 2D Zwanzig fluid of hard line segments which may orient either horizontally or vertically [18].

On the other hand, as it was mentioned in Ref. [12], the relaxation time increases very quickly as the density increases. Consequently, MC simulations at high density are very time consuming and may produce artifacts related to inaccurate equilibrium states. For these reasons, there have been few studies related to the second transition at θ_2 from the nematic to the high-density phase [20–22]. In Ref. [20], the authors provided numerical evidence for the existence of an N-$I2$ phase transition at high coverage ($I2$ to distinguish this isotropic phase from the low-density one as they are not necessarily the same) and they estimated that θ_2 varies between 0.87 and 0.93 for $k = 7$ and square lattices.

Kundu *et al.* [21,22] studied the problem of hard rigid rods on 2D square and triangular lattices by using an efficient MC scheme. The authors confirmed previous results [20] showing that $\theta_2 = 0.917(15)$ for square lattices and $k = 7$. In the case of triangular lattices, a value of $\theta_2 = 0.905(10)$ was obtained for $k = 7$. In addition, an exhaustive study of finite-size scaling showed that (a) for square lattices ($k = 7$), the values obtained for the critical exponents for the N-$I2$ transition are different from those of the Ising universality class, and (b) for triangular lattices ($k = 7$), the estimated exponents for the second transition are consistent with those of the 2D three-state Potts universality class.

Despite the number of recent contributions to the problem of straight rigid rods on discrete lattices [12–22], there are many aspects which are not yet completely solved, and the use of theoretical and computational tools to identify and characterize this sort of phase transitions is welcome. In this direction, an alternative numerical method to treat phase transitions has been presented [23]. The approach is based on the use of information theory using data compressor methods for the recognition of thermodynamic phases.

In several works [23–25] these data compressor techniques were improved showing that they can be a very useful tool for the research of magnetic systems: the 2D Edwards-Anderson model near the ferromagnetic limit [23], the 2D and 3D Ising ferromagnetic models [24], and the 3D Edwards-Anderson model covering the full range of mixture between ferromagnetic and antiferromagnetic interactions [25]. In the present paper, the scheme introduced in Refs. [23–25] is applied to study orientational phase transitions in systems of adsorbed molecules. For this purpose, a system of straight rigid rods deposited on a square lattice is simulated by MC algorithms and order parameter sequences are generated and their corresponding indicators are later calculated by data compressor techniques. The first transition is revisited, confirming previous results in the literature [15]. The application of the information theory method to the N-$I2$ phase transition occurring at higher densities yields estimated values for θ_2 in the range $7 \leqslant k \leqslant 10$.

Summarizing, the detection of phase transitions by means of information theory is applied to this problem, confirming all the known results at low densities, while our results are reported at high densities; in this way our method is now available for use to attain a better understanding of nematic transitions in general. This paper is organized as follows. The model and the simulation scheme are described in Sec. II. In Sec. III, the method of data compression to obtain the critical densities is presented. Section IV is devoted to the main results of the application of our technique and the comparison with previous results. A summary and general conclusions are given in Sec. V.

II. MODEL AND SIMULATION SCHEME

In this paper, the adsorption of straight rigid particles containing k identical units (k-mers) on square lattices is considered. The distance between k-mer units is assumed to be equal to the lattice constant; hence exactly k sites are occupied by a k-mer when adsorbed. The only interaction between different rods is hard-core exclusion: No site can be occupied by more than one k-mer unit at the same time. The substrate is represented as an array of $M = L \times L$ adsorptive sites on a square lattice arrangement, where L denotes the

linear size of the array. In addition, conventional periodic boundary conditions are considered.

The problem has been studied by grand canonical MC simulations using a typical adsorption-desorption algorithm [26,27]. The procedure is as follows. Once the value of the chemical potential μ is set, a linear k-uple of nearest-neighbor sites is chosen at random. Then, if the k sites are empty, an attempt is made to deposit a rod with probability $W = \min\{1, \exp(\mu/k_BT)\}$, where k_B is the Boltzmann constant and T is the temperature; if the k sites are occupied by units belonging to the same k-mer, an attempt is made to desorb this k-mer with probability $W = \min\{1, \exp(-\mu/k_BT)\}$; otherwise, the attempt is rejected. In addition, diffusive relaxation of adparticles to nearest-neighbor positions, by either jumps along the k-mer axis in any direction or reorientation by rotation around any of the k-mer ends, must be allowed in order to reach equilibrium in a reasonable time [28]. A MC step (MCS) is achieved when M k-uples of sites have been tested to change its occupancy state.

In order to follow the formation of the nematic phase from the isotropic phase, we use the standard order parameter for square lattices [12,13,29]

$$\delta = \frac{|n_1 - n_2|}{(n_1 + n_2)}, \tag{1}$$

where n_1 (n_2) is the number of k-mers aligned along the horizontal (vertical) direction.

In our MC simulations, we varied the chemical potential and monitored both the density $\theta = kN/M$ (where N is the number of k-mers present in the lattice at that instant) and the order parameter δ. All calculations were carried out using the supercomputing infrastructure of the NLHPC (ECM-02) at Centro de Excelencia en Modelación y Computación Científica at Universidad de La Frontera CEMCC-UFRO, Chile.

III. INFORMATION RECOGNIZER

A data analysis method based on information recognition has yielded useful results on magnetic phase transitions [23–25], agitation in stock markets [30], variations in capitalization towards pensions [31], blood pressure [32], wind energy [33], and seismic activity [34]. In principle, this method recognizes the information content in any sequence such as a time series. In the present paper, we apply this powerful technique to the recognition of information content in the MC time series depicted in the preceding section.

The data recognizer wlzip was created to find repeated meaningful information in any sequence of data. It is freely available upon request [30]. Algorithms are similar to those of data compressors which recognize any repeated information regardless of its meaning. However, "word length zipper" (wlzip) recognizes only exact matches within a given sequence recognizing the positions of the digits in the numeric information. Thus, compressions done by wlzip represent specific properties of the system. Actually, wlzip compacts less than other compressors like rar or bzip2, but its data recognition is meaningful [24].

A high degree of compression recognized by wlzip means that specific repetitive information has been detected along the data chain; this is characteristic of a monotonic behavior,

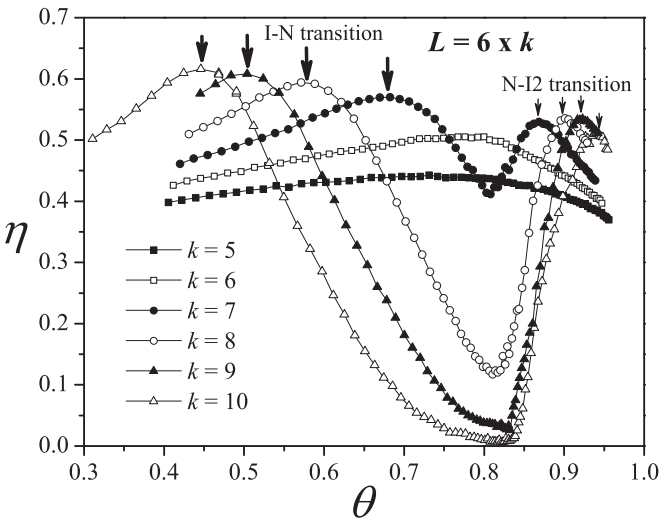

FIG. 2. Information recognizer indicator η for the compressed files of the absolute value of the orientational parameter δ as a function of the density θ. The curves correspond to $k = 5$ and $L = 30$ (closed squares), $k = 6$ and $L = 36$ (open squares), $k = 7$ and $L = 42$ (closed circles), $k = 8$ and $L = 48$ (open circles), $k = 9$ and $L = 54$ (closed triangles), and $k = 10$ and $L = 60$ (open triangles).

suggesting that the system does not alter its properties within the data window under consideration. On the other hand, low degrees of compression mean that most of the information is not repeated in the data chain, namely, a system that changes constantly its properties along the data chain, as in phase transitions or chaotic regimes.

The measure of information content is called mutability and will be denoted by the symbol η; it will be defined as a relative indicator. A sequence of σ entries is compressed by wlzip and the size or weight of the compressed file is found to be $w^*(\sigma)$; the weight of the original file was $W(\sigma)$. Then the relative mutability $\eta(\sigma)$ is simply given by the ratio

$$\eta(\sigma) = \frac{w^*(\sigma)}{W(\sigma)}. \tag{2}$$

In the present work we will consider $\sigma = 15\,000$ MCSs in the equilibrated time series for the order parameter δ defined in Eq. (1). In previous studies [24], it was shown that the method is very robust in recognizing the maxima for mutability even when the time series is decreased to a few thousand MCSs. Actually, this is one of the main advantages of this method based on information theory in comparison to other methods where a large time series is needed to recognize the critical points. Just to be on the safe side, we did the analysis for the cases of $k = 7$, 8, 9, and 10 for different lattices sizes using 30 000 MCSs without finding significant differences with respect to those reported below, namely, the maxima remain at their values. Eventually σ could be optimized to attain a better numeric precision, but for the present purposes of recognizing the two maxima for $\eta(\sigma)$ and appreciating the way they depend on k it is enough to consider mutability over $\sigma = 15\,000$ instants in the sequence.

We also investigated the dependence on the initial state (or random seed) at the beginning of the series without finding differences in the positions of the maxima or minima of Fig. 2.

This is also an advantage of the information theory method where the accent is on the variation of the information content along the data chain and not on the actual values of the data chain.

IV. RESULTS AND DISCUSSION

Simulations have been conducted for different values of k-mer length ($5 \leqslant k \leqslant 10$) and lattice sizes ($L/k = 5,6,7,8$). The coverage θ is varied, giving rise to a sequence $\delta(k,L,\theta)$ after equilibration.

A time window of 15 000 MCSs is defined over which wlzip is let to act to calculate $\eta(k,L,\theta)$ in the way defined by Eq. (2). In Fig. 2, we plot this function with respect to θ as a free variable for some typical cases: $k = 5$ and $L = 30$ (closed squares), $k = 6$ and $L = 36$ (open squares), $k = 7$ and $L = 42$ (closed circles), $k = 8$ and $L = 48$ (open circles), $k = 9$ and $L = 54$ (closed triangles), and $k = 10$ and $L = 60$ (open triangles).

From an inspection of Fig. 2, it is observed that there are two different behaviors: (a) For $k = 5$ and $k = 6$, the curves for η are almost constant, presenting a very broad maximum which can hardly be associated with a phase transition, and (b) for $k \geqslant 7$, this behavior changes notoriously and the corresponding curves show two well-marked maxima (the second one sharper than the first one) with a minimum in between; the first maximum is in the range of intermediate densities and the second one in the range of high densities; the minimum in between sharpens as k grows, while the maxima tend to separate, moving in opposite directions along the θ axis.

As described in a previous work [24], the lack of recognition of meaningful repetitions is not the same under different circumstances. Near a critical point, where a chaotic succession of data should occur, repetitions of values for δ will be seldom and wlzip will compress very little, giving higher values for η. Thus, what wlzip should give is high contrast between monotonic regimes as compared to chaotic regimes. Consequently, each maximum in the data of Fig. 2 should be indicative of the existence of a critical point: The first maximum can be associated with θ_1, while the second maximum can be associated with θ_2. Reinforcing these arguments, note that the positions on the θ axes of the first (second) maximum shift to the left (right) upon increasing the k-mer size. These observations are a clear indication that the critical density characterizing the first (second) transition decreases (increases) upon increasing k. This behavior has already been reported for the I-N transition [15] and it is expected for the N-$I2$ transition [12], which is confirmed here by Fig. 2. The analysis of Fig. 2 shows that data compressor techniques supply an alternative way of identifying and characterizing orientational phase transitions in systems of adsorbed molecules. Hereafter, curves of $\eta(k,L,\theta)$, supplemented by finite-size scaling analysis, will be used to obtain θ_1 and θ_2 for square lattices and k ranging between 7 and 10.

One of the important points here is the evolution in the high-coverage regime. In spite of this being slow, the relaxation mechanism used in the simulations helps to unblock the dynamics. This is illustrated in Fig. 3, where instants for six different θ values are captured for a system of $k = 10$ and $L = 80$. The corresponding $\langle\delta(\theta)\rangle$ (closed squares, left vertical axis) and $\eta(\theta)$ (open triangles, right vertical axis) curves are included to appreciate the way the second transition appears and is detected by both a descent in $\langle\delta(\theta)\rangle$ and a sharp maximum in the mutability $\eta(\theta)$ of the order parameter. The snapshots on top clearly show how the long-range ordered phase is lost breaking into growing patches of the perpendicular orientation. The second maximum in the figure is to be attributed then to the loss of the long-range order phase.

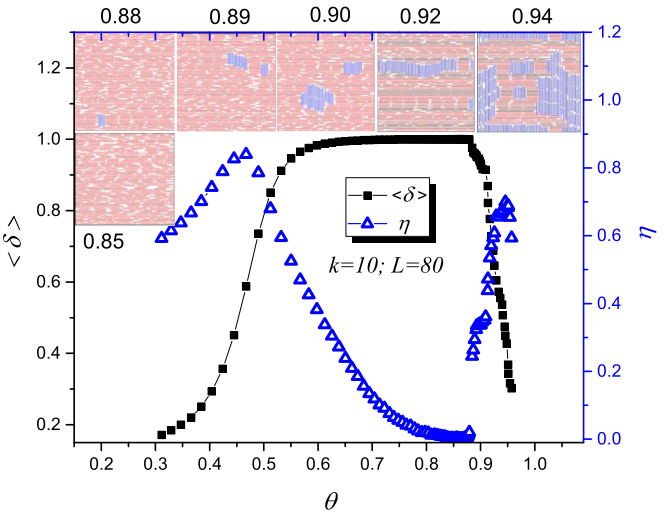

FIG. 3. Orientational order parameter δ (squares, left vertical axis) and information recognizer indicator η (triangles, right vertical axis) as functions of the density θ for $k = 10$ and $L = 80$. The evolution of the ordering as the coverage grows is captured by means of snapshots given at the top. The corresponding θ values are indicated over each image with the exemption of the first one, which is given underneath.

In Fig. 4, $\eta(k,L,\theta)$ is plotted for intermediate densities ($0.45 \leqslant \theta \leqslant 0.6$), $k = 9$, and different values of L/k as indicated. The maxima in the curves are clear evidence of

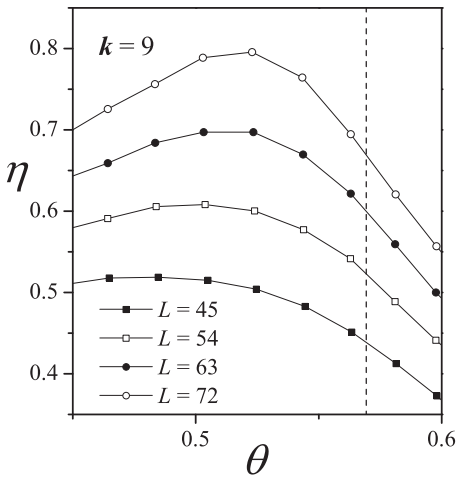

FIG. 4. Information recognizer indicator η for the compressed files for the absolute value of the parameter δ as a function of density θ ($0.45 \leqslant \theta \leqslant 0.6$). The curves were obtained for $k = 9$ and different lattice sizes as indicated. A clear tendency for an I-N transition density to approach the value 0.569 (vertical dotted line) is observed. See the discussion in the text.

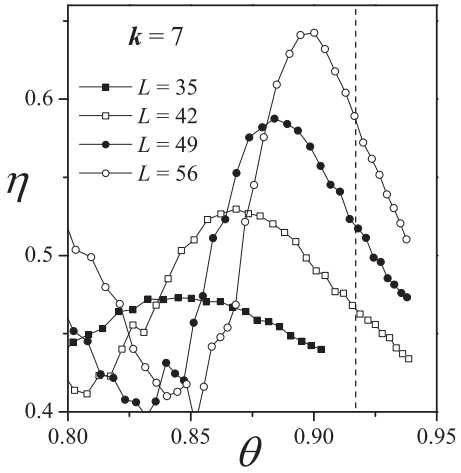

FIG. 5. Same as Fig. 4 but for $k = 7$ in the high-density range ($0.8 \leqslant \theta \leqslant 0.95$). The vertical dotted line indicates the value of the corresponding N-$I2$ transition density 0.917 (see the discussion in the text).

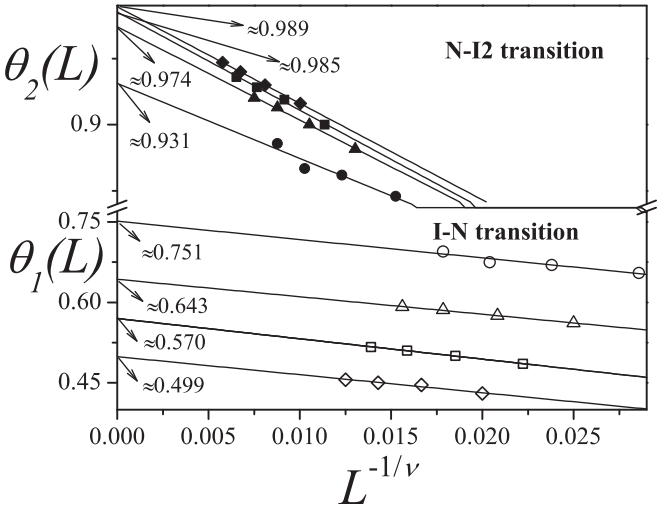

FIG. 6. Extrapolation of $\theta_1(L)$ (open symbols) and $\theta_2(L)$ (closed symbols) towards the thermodynamic limit according to Eq. (4) for $k = 7$ (circles), $k = 8$ (triangles), $k = 9$ (squares), and $k = 10$ (diamonds).

the existence of the I-N phase transition. The vertical line denotes the value of the critical density in the thermodynamic limit, $\theta_1(k = 9) \approx 0.569$. This value was obtained in Ref. [15]. A similar study, conducted for $k = 7$ in the high-density range ($0.8 \leqslant \theta \leqslant 0.95$), is presented in Fig. 5. This time, the maxima reveal the presence of the N-$I2$ phase transition in the system and the vertical line indicates the critical density obtained in Ref. [22], $\theta_2(k = 7) \approx 0.917$.

In order to express $\eta(k,L,\theta)$ as a function of continuous values of θ, it is convenient to fit $\eta(k,L,\theta)$ with some approximating function through the least-squares method. Around each maximum, the fitting curve is expected to behave like the Gaussian function[1]

$$\eta(k,L,\theta) = \frac{1}{\sqrt{2\pi}\,\Delta_L} \exp\left\{-\frac{1}{2}\left[\frac{\theta - \theta_{1\,[2]}(L)}{\Delta_L}\right]^2\right\}, \qquad (3)$$

where $\theta_{1\,[2]}(L)$ is the concentration at which the first (second) maximum in $\eta(k,L,\theta)$ occurs and Δ_L is the standard deviation from $\theta_{1\,[2]}(L)$.

With the previous results for $\theta_1(L)$ and $\theta_2(L)$, a scaling analysis can be done. Thus, it is expected that

$$\theta_{1\,[2]}(L) = \theta_{1\,[2]}(\infty) + A_{1\,[2]} L^{-1/\nu_{1\,[2]}}, \qquad (4)$$

where $A_{1\,[2]}$ is a nonuniversal constant and $\nu_{1\,[2]}$ is the critical exponent of the correlation length. The I-N phase transition belongs to the 2D Ising universality class for square lattices and, consequently, $\nu_1 = 1$ [13]. In the case of the N-$I2$ phase transition, ν_2 will be taken as 0.90 ± 0.05 [22].

Figure 6 shows the plots towards the thermodynamic limit of $\theta_1(L)$ and $\theta_2(L)$ according to Eq. (4) for the data in Figs. 4 and 5 (and similar data obtained for $k = 7$, 8, and 10). From extrapolations, it is possible to obtain $\theta_1 \equiv \theta_1(L \to \infty)$ and $\theta_2 \equiv \theta_2(L \to \infty)$. In the case of the first transition, $\theta_1 \approx 0.751$ for $k = 7$, $\theta_1 \approx 0.643$ for $k = 8$, $\theta_1 \approx 0.570$ for $k = 9$, and $\theta_1 \approx 0.499$ for $k = 10$. In all cases, the simulation error was of the order of 1%. For the second transition, the obtained values of the critical density were $\theta_2 \approx 0.931$ for $k = 7$, $\theta_2 \approx 0.974$ for $k = 8$, $\theta_2 \approx 0.985$ for $k = 9$, and $\theta_2 \approx 0.989$ for $k = 10$. In this case, the simulation error was of the order of 3%. The values of θ_1 and θ_2 are collected in Table I. The table also includes the values of θ_1 and θ_2 previously reported in the literature [15,22].

Finally, the values compiled in Table I are shown in Fig. 7. In the case of the I-N phase transition, it is well known that the critical density follows a power law as $\theta_1(k) = Ak^B$, with $A = 4.80 \pm 0.05$ [19] and $B = -1$ [12,15,18,19]. This expression was derived for large values of the k-mer size ($k \to \infty$) [12]. In the present study, due to the small size of the studied particles ($7 \leqslant k \leqslant 10$), some deviations were observed with respect to the value of A reported in Ref. [19], where the simulations were performed for rods of length up to $k = 32$. However, the values calculated using data compressor techniques (closed symbols) coincide (within statistical errors) with previous results in the literature (open symbols) [15].

On the other hand, for the N-$I2$ phase transition, Ghosh and Dhar found that $\theta_2(k) \approx 1 - Ck^{-2}$ for large k, where C

TABLE I. Critical densities θ_1 and θ_2 (as indicated in the text) for straight rigid rods on a square lattice and k ranging from 7 to 10. The values in the second and fourth columns correspond to previous calculations in Refs. [15] and [22], respectively. The errors in columns 3 and 5 are of the order of 1% and 3%, respectively.

k	θ_1 [15]	θ_1 (this work)	θ_2 [22]	θ_2 (this work)
7	0.729(4)	0.751	0.917(15)	0.931
8	0.647(3)	0.643		0.974
9	0.569(2)	0.570		0.985
10	0.502(1)	0.499		0.989

[1]Even though the behavior of $\eta(k,L,\theta)$ is known not to be Gaussian in the whole range of θ, this quantity is approximately Gaussian near each peak and Eq. (3) is a good approximation for the purpose of locating its maximum.

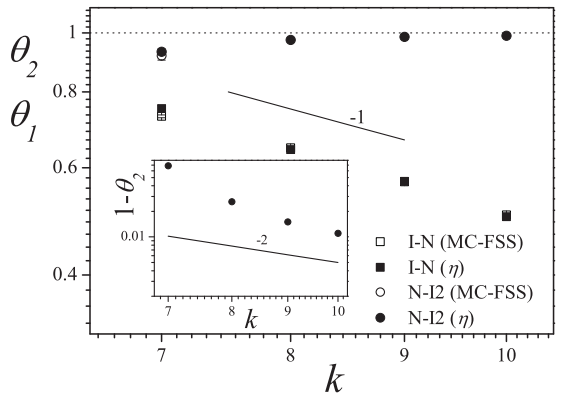

FIG. 7. Critical densities θ_1 and θ_2 as a function of k (on a log-log scale). The symbols are defined in the legend. The inset shows $1-\theta_2$ as a function of k.

is some constant [12]. As mentioned above, the range of k studied in this paper does not allow a quantitative comparison of our results with the theoretical expression derived by Ghosh and Dhar [12]. This situation is clearly reflected in the inset of Fig. 7, where $1-\theta_2$ is plotted as a function of k. As observed in the figure, the asymptotic regime $1-\theta_2 \propto k^{-2}$ is not reached yet for the values of k used in these simulations; however, it is barely appreciated that the larger curvature for the results is for the lower k values. Nevertheless, the results in Fig. 7 indicate that (1) $\theta_2(k=7)$ agrees (within statistical errors) with previous calculation [22] and (2) according to the prediction of Ref. [12], θ_2 tends to 1 as the k-mer size is increased. In addition, it is important to note that the values corresponding to $k \geqslant 8$ are reported.

The time needed for previous calculations increases enormously as the coverage θ increases. This means that the last points to the right in Figs. 2 and 5 were extremely difficult to obtain, especially so for the larger systems. Apparently, these difficulties prevented previous authors [12] from obtaining θ_2 values for a variety of sizes which we were able to estimate here using our method. Another difficulty that we found is that calculations initiated with different random seeds do not necessarily repeat the values of η producing a family of curves which, nevertheless, all maximize at the same value of θ. In other words, the maximum is always located at the same place, but each curve needs to be obtained in a continuous way. This is a practical limitation for larger systems at this moment.

V. CONCLUSION

In the present paper, we have addressed the critical properties of long straight rigid rods adsorbed on square lattices at intermediate and high densities. The results were obtained by combining MC simulations and information theory based on the use of data compressor methods.

The main general conclusion of this work is that information recognition in the time series generated by the induced MC dynamics in the systems described above leads to an alternative method to describe the orientational phase transitions at different deposition coverage values. To have at our disposal an additional method to characterize phases is always an advantage. Supporting this affirmation, the analysis in Fig. 2 presents the most general picture, where the low- and high-coverage transitions are shown for the deposition of the larger polymers considered here.

Our method succeeds in detecting the low- to intermediate-coverage maximum for k-mers larger that seven units, while similar behavior was not found for shorter k-mers deposited on square lattices. This is a known result but it is still surprising as it is not clear what geometrical or topological reasons are behind this discontinuity: Depositions of polymers shorter than seven square lattice units do not show a nematic transition, while deposition of polymers of length 7 or larger present a long-range order nematic transition at intermediate coverage θ_1.

For $k \geqslant 7$ a second transition is also present at larger coverage values maximized at θ_2. This finding suggests that the system is without any order for $\theta < \theta_1$ and then presents orientational order for $\theta_1 < \theta < \theta_2$ to finally rearrange in a different way (not necessarily absolute disorder) for $\theta > \theta_2$. This second transition is harder to characterize since the dynamics at high coverage is very slow, so equilibration is harder to reach. Eventually the system could get trapped in a long-lived metastable state, leading to errors in the estimation of θ_2. Actually, a more comprehensive treatment focusing on this second transition is needed, which is beyond the scope of the present paper.

The dependence of θ_1 with the lattice size was obtained (Fig. 4) and was later escalated to the thermodynamic limit (Fig. 6). The conclusion is very direct: For any $k \leqslant 7$ value an extrapolation for the first maximum towards the thermodynamic limit can be found. Taking advantage of this procedure, the critical density dependence on the particle size k has been reported for the first transition. As in previous work [15], we found that $\theta_1(k)$ follows a power law as $\theta_1(k) \propto k^{-1}$ (see the lower part of Fig. 7).

The scheme was repeated for the second phase transition (N-$I2$ transition) occurring in the system. In this case, the values of $\theta_2(L)$ were determined from the positions of the second maxima of the curves of η vs θ (Fig. 5). Extrapolating these data to the thermodynamic limit, the behavior of θ_2 as a function of the k-mer size was numerically obtained (see the upper part of Fig. 7). The results indicate that θ_2 tends to 1 as size k is increased, in agreement with the theoretical prediction of Ref. [12].

The information method itself is quite robust since it does not require long data chains to detect the general shape of the curve leading to the phase transitions. It is also independent of the initial conditions on which the calculations are launched. The measurement of the information content is what matters, which is a measure of variability. This opens the possibility of using this method for other nematic processes.

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