Phase Transitions in a System of Hard Rectangles on the Square Lattice

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(Dated: March 5, 2014)

The phase diagram of a system of monodisperse hard rectangles of size $m \times mk$ on a square lattice is numerically determined for $m = 2, 3$ and aspect ratio $k = 1, 2, \ldots, 7$. We show the existence of a disordered phase, a nematic phase with orientational order, a columnar phase with orientational and partial translational order, and a crystalline sublattice phase. The asymptotic behavior of the phase boundaries for large $k$ are determined using a combination of entropic arguments and a Bethe approximation. This allows us to generalize the phase diagram to larger $m$ and $k$, showing that for $k \geq 7$, the system undergoes three entropy driven phase transitions with increasing density. The nature of the different phase transitions are established and the critical exponents for the continuous transitions are determined using finite size scaling.

PACS numbers: 64.60.De, 64.60.Cn, 05.50.+q

I. INTRODUCTION

The study of entropy-driven phase transitions in a system of long hard rods has a long history dating back to Onsager’s demonstration [1] that the three dimensional system undergoes a transition from an isotropic phase to an orientationally ordered nematic phase as the density of the rods is increased [15]. Further increase in density may result in a smectic phase that partially breaks translational symmetry, and a solid phase [2, 3]. In two dimensional continuum space, the continuous rotational symmetry remains unbroken but the system undergoes a Kosterlitz-Thouless type transition from a low-density phase with exponential decay of orientational correlations to a high-density phase having quasi long range order [8, 14]. Experimental realizations include tobacco mosaic virus [15], liquid crystals [3], carbon nanotube gels [16], and brownian squares [17]. The phenomenology is, however, much less clear when the orientations are discrete, and the positions are either on a lattice or in the continuum, when even the existence of the nematic phase has been demonstrated only recently [18, 19].

Consider hard rectangles of size $m \times mk$ on a two-dimensional square lattice where each rectangle occupies $m$ ($mk$) lattice sites along the short (long) axis. The limiting cases when either the aspect ratio $k = 1$ or $m = 1$ are better studied. When $m = 1$ and $k \geq 7$, there are, remarkably, two entropy-driven transitions: from a low-density isotropic phase to an intermediate density nematic phase, and from the nematic phase to a high-density disordered phase [18, 20]. While the first transition is in the Ising universality class [21, 22], the second transition could be non-Ising [21], making it unclear whether the high density phase is a re-entrant low density phase or a new phase [20, 23]. When $k = 1$ (hard squares), the system undergoes a transition into a high density columnar phase. The transition is continuous for $m = 2$ [24, 25], and first order for $m = 3$ [23]. When $m \rightarrow \infty$, keeping $k$ fixed, the lattice model is equivalent to the model of oriented rectangles in two dimensional continuum, also known as the Zwanzig model [26]. For oriented lines in the continuum ($m, k \rightarrow \infty$), a nematic phase exists at high density [22]. The only theoretical results that exist are when $m = 1$ and $k = 2$ (dimers), for which no nematic phase exists [30, 33], $k \gg 1$, when the existence of the nematic phase may be proved rigorously [19], and an exact solution for arbitrary $k$ on a tree like lattice [2, 23].

Less is known for other values of $m$ and $k$. Simulations of rectangles of size $2 \times 5$ did not detect any phase transition with increasing density [34], while those of parallelepipeds on cubic lattice show layered and columnar phases, but no nematic phase [35]. In general, numerical studies of large rectangles are constrained by the fact that it is difficult to equilibrate the system at high densities using Monte Carlo algorithms with local moves, as the system gets trapped in long-lived metastable states.

In addition to being the lattice version of the hard rods problem, the study of lattice models of hard rectangles is useful in understanding the phase transitions in adsorbed monolayers on crystal surfaces. The (100) and (110) planes of fcc crystals have square and rectangular symmetry and may be treated with lattice statistics if the adsorbate-adsorbate interaction is negligible with respect to the periodic variation of the corrugation potential of the underlying substrate [36]. For example, the critical behavior of a monolayer of chlorine (Cl) on Ag(100) is well reproduced by the hard square model ($k = 1$) and the high density $c(2 \times 2)$ structure of the Cl-adlayer may be mapped to the high density phase of the hard square problem [37]. Structures such as $p(2 \times 2)$, $c(2 \times 1)$ and $(2 \times 1)$ are ordered structures. Lattice gas model with repulsive interaction up to forth nearest neighbor has been used to study the phase behavior of selenium adsorbed on Ni(100) [38]. The results in this paper show that different phases with orientational and positional order may be obtained by only hard core exclusion.

At a more qualitative level, discrete models of hard
rods have been used to obtain realistic phase diagram for polydisperse systems \cite{39,40}, to describe orientational wetting of rods \cite{41}, to model and understand self-assembly of nano particles on monolayers \cite{42} and thermodynamics of linear adsorbates \cite{43,44}.

Lattice models of hard rectangles also falls in the general class of hard core lattice gas models of differently shaped particles. The study of these models also have been of continued interest in Statistical Physics as minimal models for the melting transitions. The different shapes studied include squares \cite{45,47}, hexagons on triangular \cite{48,49} and square lattices \cite{50}, triangles \cite{51}, and tetrominoes \cite{52}.

In this paper, we adapt and implement an efficient Monte Carlo algorithm with cluster moves that was very effective in studying the hard rod (m = 1) problem on lattices \cite{21,52}. The hard rectangle model and the algorithm are described in detail in Sec. II. We observe four distinct phases at different densities: isotropic, nematic, columnar, and sublattice phases. These phases, suitable order parameters to characterize them, and other thermodynamic quantities are defined in Sec. III. From extensive large scale simulations, we determine the rich phase diagram for m = 2, 3, and k = 1, . . . , 7. The phase diagram for m = 2 is discussed in Sec. IV. We find that all transitions except the isotropic-columnar transition for k = 6 are continuous. The critical exponents and universalities classes of the continuous transitions are determined. Section V contains the details about the phase diagram and the nature of the phase transitions for m = 3. In Sec. VI, we use a Bethe approximation and estimates of entropies for the different phases to determine the phase boundaries for large k, allowing us to generalize the phase diagram to arbitrary m and k. In particular, it allows us to take the continuum limit m → ∞, thus obtaining predictions for a system of oriented rectangles in the continuum. Sec. VII contains a summary and a discussion of possible extensions of the problem.

II. THE MODEL AND MONTE CARLO ALGORITHM

We define the model on a square lattice of size L × L with periodic boundary conditions. Consider a monodisperse system of rectangles of size m × mk such that the aspect ratio is k. A rectangle can be either horizontal or vertical. A horizontal (vertical) rectangle occupies mk sites along the x (y)-axis and m sites along the y (x)-axis. No two rectangles may overlap. An activity z = eμ is associated with each rectangle, where μ is the chemical potential.

We study this system using constant μ grand canonical Monte Carlo simulations. The algorithm that we implement is an adaptation of the algorithm with cluster moves that was introduced in Refs. \cite{21,52} to study the problem of hard rods (n = 1). We describe the algorithm below. Given a valid configuration of rectangles, in a single move, a row or a column is chosen at random. If a row is chosen, then all horizontal rectangles whose heads (bottom, left corner) lie in that row are removed, leaving the rectangles with heads in other rows untouched. The emptied row now consists of two kinds of sites: forbidden sites that cannot be occupied with horizontal rectangles due to the presence of vertical rectangles in the same row or due to rectangles with heads in the neighboring (m − 1) rows, and sites that may be occupied by horizontal rectangles in a valid configuration. An example illustrating the forbidden sites is shown in Fig. I(a). It is clear that the sites that may be occupied are divided into intervals of contiguous empty sites. The problem of occupation of the emptied row with a new configuration now reduces to the problem of occupying the empty intervals. However, the empty intervals may be occupied independent of each other, as the occupation of one is not affected by the configuration of rectangles in the remaining ones. Thus, the re-occupation of the emptied row reduces to a problem of occupying a one dimensional interval with rods. This problem is easily solvable and the equilibrium probabilities of each new configuration may be easily calculated. We refer to Refs. \cite{20,52} for the calculation of these probabilities. If a column is chosen instead of a row, then a

FIG. 1. (Color online) An illustration of the Monte Carlo algorithm. (a) Configurations before and after the evaporation of horizontal rectangles with head on a particular row (denoted by an arrow). Sites denoted by cross symbols cannot be occupied by horizontal rectangles in the new configuration. (b) An example of the flip move for rectangles of size 2 × 6. A rotatable or flippable plaquette of size 6 × 6, consisting of three aligned rectangles, is shown by the dashed line. After the flip move, the horizontal rectangles become vertical.
similar operation is performed for the vertical rectangles whose heads lie in that column.

In addition to the above evaporation-deposition move, we find that the autocorrelation time is reduced considerably by introducing a flip move. In this move, a site \((i, j)\) is picked at random. If it is occupied by the head of a horizontal rectangle, then we check whether \((i, j + m), (i, j + 2m), \ldots, (i, j + m - 1)k\) sites are occupied by the heads of horizontal rectangles. If that is the case, we call this set of aligned rectangles a rotatable plaquette. In the flip move, each rectangle in the rotatable plaquette is rotated by \(\pi/2\) so that the rectangles become vertical. An example of the flip move is shown in Fig. 1(b). If \((i, j)\) is occupied by the head of a vertical rectangle and a rotatable plaquette of vertical rectangles is present, then the rectangles are rotated to horizontal. A Monte Carlo move corresponds to \(2L\) evaporation–deposition moves and \(L^2\) flip moves. It is easy to check that the algorithm is ergodic and obeys detailed balance.

We implement a parallelized version of the above algorithm. In the evaporation-deposition move, we simultaneously update all rows that are separated by \(m\). Once all rows are updated in this manner, the columns are updated. We also parallelize the flip move. The lattice is divided into \(L^2/(m^2k^2)\) blocks of size \(mk \times mk\). The flipping of each of these blocks is independent of the other and may therefore be flipped simultaneously. We flip a rotatable plaquette with probability \(1/2\). The parallelization and efficiency of the algorithm allows us to simulate large systems (up to \(L = 810\)) at high densities (up to 0.99).

We check for equilibration by starting the simulations with two different initial configurations and making sure that the final equilibrium state is independent of the initial condition. One configuration is a fully nematic state, where all rectangles are either horizontal or vertical and the other is a random configuration where rectangles of both vertical and horizontal orientations are deposited at random.

III. THE DIFFERENT PHASES

Snapshots of the different phases that we observe in simulations are shown in Fig. 2. First is the low density isotropic (I) phase in which the rectangles have neither orientational nor translational order [see Fig. 2(a)]. Second is the nematic (N) phase in which the rectangles have orientational order but no translational order [see Fig. 2(c)]. In this phase, the mean number of horizontal rectangles is different from that of vertical rectangles. The third phase is the columnar (C) phase, having orientational order and partial translational order [see Fig. 2(e)]. In this phase, if majority of rectangles are horizontal (vertical), then their heads, or bottom left corners, preferably lie in rows (columns) that are separated by \(m\). Thus, it breaks the translational symmetry in the direction perpendicular to the orientation but not parallel to the orientation. Clearly, there are \(2m\) symmetric C phases. The fourth phase is the crystalline sublattice (S) phase with no orientational order [see Fig. 2(f)]. We divide the square lattice into \(m^2\) sublattices by assigning to a site \((i, j)\) a label \((i \mod m) + m \times (j \mod m)\). The sublattice labeling for the case \(m = 2\) is shown in Fig. 2(a). In the S phase, the heads of the rectangles preferably occupy one sublattice, breaking translational symmetry in both the directions.

From the symmetry of the system we would expect up to 7 phases. The orientational symmetry could be present...
or broken while the translational symmetry could be unbroken, partially broken or fully broken. If the orientational symmetry is broken, then the translational symmetry could be broken either parallel or perpendicular to the preferred orientations. Out of the 7 possibilities, we do not observe (i) a phase with no orientational order but partial translational order, (ii) a phase with orientational order and complete translational order (iii) a smectic like phase in which orientational order is present and translational symmetry parallel to the orientation is broken.

To distinguish among the four different phases we define the following order parameters:

\[ Q_1 = (N_h - N_v)/(N_v + N_h), \]  
\[ Q_2 = \left( \prod_{j=0}^{m^2-1} n_j e^{2\pi ij/m^2} \right) / \rho, \]  
\[ Q_3 = \left( \prod_{j=0}^{m-1} r_j e^{2\pi ij/m} - \prod_{j=0}^{m-1} c_j e^{2\pi ij/m} \right) / \rho, \]  
\[ Q_4 = (n_0 - n_1 - n_2 + n_3), \]

where \( N_h \) and \( N_v \) are the total number of horizontal and vertical rectangles respectively, \( n_i \) is the number of rectangles whose heads are in sublattice \( i \), \( r_j \) are the number of rectangles whose heads are in row \( j \) (mod \( m \)), and \( c_j \) are the number of rectangles whose heads are in column \( j \) (mod \( m \)). All four order parameters are zero in the I phase. \( Q_1 \) is non-zero in the N and C phases, \( Q_2 \) is non-zero in the C and S phases, \( Q_3 \) is non-zero only in the C phase, and \( Q_4 \) is non-zero only in the S phase. \( Q_4 \) in Eq. (1d) has been defined for \( m = 2 \). Its generalization to \( m \geq 3 \) is straightforward.

We now define the thermodynamic quantities that are useful to characterize the transitions between the different phases. \( Q_i \)'s second moment \( \chi_i \), compressibility \( \kappa \) and the Binder cumulant \( U_i \) are defined as

\[ \chi_i = \langle Q_i^2 \rangle L^2, \]  
\[ \kappa = \left( \langle \rho^2 \rangle - \langle \rho \rangle^2 \right) L^2, \]  
\[ U_i = 1 - \frac{\langle Q_i^4 \rangle}{3 \langle Q_i^2 \rangle^2}. \]

The transitions are accompanied by the singular behavior of the above thermodynamic quantities at the corresponding critical densities. Let \( \epsilon = (\mu - \mu_c) / \mu_c \), where \( \mu_c \) is the critical chemical potential. The singular behavior is characterized by the critical exponents \( \alpha, \beta, \gamma, \nu \) defined by \( Q \sim (1 - \epsilon)\beta, \epsilon < 0, \chi \sim |\epsilon|^{-\gamma}, \kappa \sim |\epsilon|^{-\alpha}, \) and \( \xi \sim |\epsilon|^{-\nu}, \) where \( \xi \) is the correlation length, \( |\epsilon| \to 0, \) and \( Q \) represents any of the order parameters. Only two exponents are independent, others being related to them through scaling relations.

The critical exponents \( \alpha, \beta, \gamma \) and \( \nu \) are obtained by finite size scaling of the different quantities near the critical point:

\[ U \simeq f_u (\epsilon L^{1/\nu}), \]  
\[ Q \simeq L^{-\beta/\nu} f_q (\epsilon L^{1/\nu}), \]  
\[ \chi \simeq L^{\gamma/\nu} f_\chi (\epsilon L^{1/\nu}), \]  
\[ \kappa \simeq L^\nu f_\kappa (\epsilon L^{1/\nu}), \]

where \( f_u, f_q, f_\chi, \) and \( f_\kappa \) are scaling functions.

**IV. PHASE DIAGRAM AND CRITICAL BEHAVIOR FOR m = 2**

In this section, we discuss the phase diagram for the case \( m = 2 \) and aspect ratio \( k = 1, 2, \ldots, 7 \). The critical exponents characterizing the different continuous transitions are determined numerically.

**A. Phase Diagram**

The phase diagram obtained from simulations for \( m = 2 \) and integer \( k \) are shown in Fig. 3. The low density phase is an I phase for all \( k \). The case \( k = 1 \) is different from other \( k \). In this case, the problem reduces to a hard square problem and orientational order is not possible as there is no distinction between horizontal and vertical rectangles. The hard square system undergoes only one transition with increasing density, it being a continuous transition from the I phase to a C phase [24, 15, 47]. This transition belongs to the Ashkin Teller universality class (see Refs. [24, 28] for recent numerical studies). For \( k = 2, 3 \), we find that the system undergoes one continuous transition directly from the I phase to a crystalline S phase. On the other hand, the system with \( k = 4, 5, 6 \) may exist in I, C, or S phases. With increasing density, the system undergoes two phase transitions: first from the I to a C phase which could be continuous or first order, and second, from the C to a S phase which is continuous. For \( k = 7 \), we observe three continuous transitions with increasing density: first from the I to the N phase, second into the C phase and third into the S phase. By confirming the existence of the N and C phases for \( k = 8 \), we expect the phase behavior for \( k \geq 8 \) to be similar to that for \( k = 7 \).

The system undergoes more than one transition only for \( k \geq k_{min} = 4 \). We now present some supporting evidence for this claim. In Fig. 4 (a) we show the probability distribution of the nematic order parameter \( Q_1 \), when \( k = 4 \), for different values of \( \mu \) and fixed \( L \), close to the I-C and the C-S transitions. For lower values of \( \mu \), the distribution is peaked around zero corresponding to the I phase. With increasing \( \mu \), the distribution becomes flat and two symmetric maxima appear at \( Q_1 \neq 0 \) (\( Q_3 \) also becomes nonzero simultaneously), corresponding to the S phase. On increasing \( \mu \) further, the two maxima continuously merge into a single peak at \( Q_1 = 0 \), corresponding to the S phase (\( Q_3 \) also becomes zero and \( Q_4 \)
the above, we conclude that the C phase exists for \( k \in (0, 1) \) and \( k \in (1, 2) \). The data points are from simulation, while the continuous lines and shaded regions are guides to the eye. The shaded portion denotes regions of phase coexistence.

The N phase exists only for \( k = 6 \). To see this, notice that the I-C transition \( k = 2 \) is first order (see Fig. 3). If a nematic phase is crossed, the order parameter becomes nonzero). Fig. 4 (b) shows the distribution of \( Q_1 \) for three different system sizes at a fixed value of \( \mu \) for which \( P(Q_1) \) has two symmetric maxima at \( Q_1 \neq 0 \). The two peaks become sharper and narrower with increasing \( L \). We find the similar behavior for \( P(Q_3) \) also. From the above, we conclude that the C phase exists for \( k = 4 \) albeit for a very narrow range of \( \mu \). For \( k = 2 \) and \( k = 3 \) we do not observe the existence of a columnar phase and find that the probability distributions of \( Q_1 \) and \( Q_3 \) are peaked around zero for all \( \mu \). It is quite possible that the C phase exists for \( k = 2, 3 \) in a narrow range of \( \mu \), but within the system sizes that we have simulated, we observe only one transition. Hence, we conclude that \( k_{\text{min}} = 4 \).

The N phase exists only for \( k \geq 7 \). This is also true for \( m = 1 \) [18]. To see this, notice that the I-C transition for \( k = 6 \) is first order (see Fig. 3). If a nematic phase exists for \( k = 6 \), then the first transition would have been continuous and in the Ising universality class [21].

### B. Critical behavior for the isotropic-sublattice (I-S) phase transition

The system of rectangles with \( m = 2 \) undergoes a direct I-S transition for \( k = 2, 3 \). We study this transition using the order parameter \( Q_2 \) [see Eq. (1b)]. \( Q_2 \) is nonzero in the S phase and zero in the I phase. The data collapse of \( U_2, Q_2, \) and \( \chi_2 \) for different values of \( L \) near the I-S transition are shown in Fig. 5 for \( k = 2 \) and in Fig. 6 for \( k = 3 \). From the crossing of the Binder cumulant data for different \( L \), we estimate the critical chemical potential \( \mu_c \approx 5.32 (\rho_c \approx 0.93) \) for \( k = 2 \) and \( \mu_c \approx 6.01 (\rho_c \approx 0.925) \) for \( k = 3 \). The order parameter increases continuously with \( \mu \) from zero as \( \mu_c \) is crossed, making the transition continuous. Since the S phase has a four fold symmetry, we expect the transition to be in the Ashkin-Teller universality class. Indeed, we find a good collapse with \( \beta/\nu = 1/8 \) and \( \gamma/\nu = 7/4 \) numerically.

- **Fig. 3.** (Color online) Phase diagram for rectangles of size \( 2 \times 2k \). I, N, C and HD denote isotropic, nematic, columnar and high density phases respectively. The HD phase is a C phase for \( k = 1 \) and a S phase for \( k > 1 \). The data points are from simulation, while the continuous lines and shaded portions are guides to the eye. The shaded portion denotes regions of phase coexistence.

- **Fig. 4.** (Color online) (a) The probability distribution of \( Q_1 \) for \( k = 4 \) at different \( \mu \) values, when \( L = 416 \). (b) The same for different system sizes when \( \mu = 6.55 \).

- **Fig. 5.** (Color online) Data collapse for different \( L \) near the I-S transition for rectangles of size \( 2 \times 4 \) (\( m = 2, k = 2 \)). We find \( \mu_c \approx 5.32 (\rho_c \approx 0.93) \). The exponents are \( \beta/\nu = 1/8 \), \( \gamma/\nu = 7/4 \) and \( \nu \approx 1.15 \).
C. Critical behavior of the isotropic-columnar phase (I-C) transition

The I-C transition is seen for $k = 4, 5, 6$. When for $k = 4$, $\mu_c$ for the I-C and the C-S transitions are close to each other, making $k = 4$ unsuitable for studying the critical behavior. We, therefore, study the I-C transition for $k = 5$ ($2 \times 10$ rectangles) and $k = 6$ ($2 \times 12$ rectangles).

The critical behavior is best studied using the order parameter $Q_3$ [see Eq. (1c)]. $Q_3$ is non-zero only in the C phase. First, we present the critical behavior for $k = 5$. The simulation data for different system sizes are shown in Fig. 6. From the crossing of the Binder cumulant curves, we obtain $\mu_c \approx 4.98$ ($\rho_c \approx 0.876$). The transition is found to be continuous. There are four possible columnar states: majority of heads are either in even or odd rows (when horizontal orientation is preferred), or in even or odd columns (when vertical orientation is preferred). Due to this four fold symmetry, we expect the I-C transition to be in the Ashkin-Teller universality class. The data for different $L$ collapse with $\beta/\nu = 1/8$, $\gamma/\nu = 7/4$, and $\nu = 0.80$. We find $\mu_c \approx 4.98$ ($\rho_c \approx 0.876$). Data are for rectangles of size $2 \times 10$.

For $k = 6$, the I-C transition is surprisingly first order. Fig. 7(a) shows the time profile of density near the I-C transition. $\rho$ alternates between two well defined densities, one corresponding to the I phase and the other to the C phase. This is also seen in the probability distribution for density [see Fig. 3(b)]. Near the I-C transition it shows two peaks corresponding to the I and the C phases. Thus, at $\mu = \mu_{IC}^c$, the density has a discontinuity, which is shown by the shaded region in the phase diagram (see Fig. 3). The probability distribution of the order parameter $Q_3$ shows similar behavior [see Fig. 3(c)]. Near $\mu = \mu_{IC}^c$ the distribution shows three peaks: one at $Q_3 = 0$ corresponding to the I phase and the other two at $Q_3 \neq 0$, corresponding to the C phase. At $\mu_{IC}^c$ the three peaks become of equal height and the order parameter $Q_3$ jumps from zero to a non-zero value. These peaks sharpen with increasing system size [see Fig. 3(d)]. These are typical signatures of a first order transition. Hence, we conclude that the I-C transition may be continuous or first order depending on $k$.

D. Critical behavior of the isotropic-nematic phase (I-N) transition

We find that the nematic phase exists only for $k \geq 7$. We study the I-N phase transition for $k = 7$ using the order parameter $Q_1$ [see Eq. (1a)]. $Q_1$ is non-zero in the N phase and zero in the I phase. In the nematic phase the rectangles may choose either horizontal or vertical orientation. Thus, we expect the transition to be in the Ising universality class. When $m = 1$, this has been verified.
using extensive Monte Carlo simulations [21]. Here, we confirm the same for $m = 2$. The data for $U_1$, $|Q_3|$ and $\chi_1$ for different $L$ collapse onto one curve when scaled with the two dimensional Ising exponents $\beta/\nu = 1/8$, $\gamma/\nu = 7/4$, and $\nu = 1$ (see Fig. 9). We find $\mu_c \approx 1.77$ ($\rho_c \approx 0.746$). We note that the value of $U_2$ at the point where the curves for different $L$ cross is slightly smaller than the Ising value 0.614. This suggests that larger system sizes are necessary for better collapse of the data.

**E. Critical behavior of the nematic-columnar phase (N-C) transition**

The N-C transition is also studied for $k = 7$, using the order parameter $Q_3$. $Q_3$ is zero in the nematic phase but nonzero in the columnar phase. At the I-N transition orientational symmetry gets broken. If the nematic phase consists of mostly horizontal (vertical) rectangles, then there is no preference over even and odd rows (columns). In the columnar phase the system chooses either even or odd rows (columns), once the orientational symmetry is broken. Due to the two broken symmetry phases we expect this transition to be in the Ising universality class. We indeed find good data collapse when $U_3$, $|Q_3|$ and $\chi_3$ for different system sizes are scaled with Ising exponents (see Fig. 10). The critical chemical potential or critical density is obtained from the crossing point of the binder cumulant $U_3$ for different $L$. We find $\mu_c \approx 1.92$ ($\rho_c \approx 0.766$) for this transition. We expect the critical behavior to be same for $k > 7$. 

**FIG. 8.** (Color online) Data for the density $\rho$ and the order parameter $Q_3$ for rectangles of size $2 \times 12$. (a) Equilibrium time profile of $\rho$ for $\mu = 3.02$ and $L = 720$. Probability distribution, near the I-C transition, of (b) $\rho$ for different values of $\mu$ when $L = 576$, (c) $Q_3$ for different values of $\mu$ when $L = 576$, and (d) $Q_3$ for $L = 240$ ($\mu = 2.99$) and $L = 576$ ($\mu = 3.02$).

**FIG. 9.** (Color online) The data for different $L$ near the I-N transition collapse when scaled with the Ising exponents $\beta/\nu = 1/8$, $\gamma/\nu = 7/4$, $\nu = 1$ and $\mu_c \approx 1.77$. The critical density $\rho_c \approx 0.746$. Data are for rectangles of size $2 \times 14$.

**FIG. 10.** (Color online) The data for different $L$ near the N-C transition collapse when scaled with the Ising exponents $\beta/\nu = 1/8$, $\gamma/\nu = 7/4$, $\nu = 1$ and $\mu_c \approx 1.92$. The critical density $\rho_c \approx 0.766$. Data are for rectangles of size $2 \times 14$. 

The C-S transition exists for \( k \geq 4 \). This transition is studied by choosing \( k = 5 \). We characterize the C-S transition using the order parameter \( Q_4 \) which is non-zero only in the S phase. In the C phase the system chooses one particular orientation and either even or odd rows or columns, depending on the orientation. This corresponds to two sublattices being chosen among four of them. In the C-S transition the translational symmetry gets broken completely by choosing a particular sublattice, but along with that the orientational symmetry gets restored. This transition is found to be continuous.

The data of \( U_4 \), \( |Q_4| \) and \( \chi_4 \) for different \( L \) near the C-S transition collapse well when scaled with the exponents \( \beta/\nu = 1/8 \), \( \gamma/\nu = 7/4 \), \( \nu = 0.87 \) and \( \mu_c \approx 9.65 \). The critical density \( \rho_c \approx 0.958 \). Data are for rectangles of size \( 2 \times 10 \).

\[ \text{FIG. 11.} \] (Color online) The data for different \( L \) near the C-S transition collapse when scaled with exponents \( \beta/\nu = 1/8 \), \( \gamma/\nu = 7/4 \), \( \nu = 0.87 \) and \( \mu_c \approx 9.65 \). The critical density \( \rho_c \approx 0.958 \). Data are for rectangles of size \( 2 \times 10 \).

\[ \text{FIG. 12.} \] (Color online) Phase diagram for rectangles of size \( 3 \times 3k \). HD denotes high density. The HD phase is a C phase for \( k = 1 \) and a S phase for \( k > 1 \). The data points are from simulation while the continuous line and shaded portions are a guide to the eye. The shaded portions denote regions of phase coexistence. Except the I-N transition, all the transitions are found to be first order.

\[ \text{V. PHASE DIAGRAM AND CRITICAL BEHAVIOR FOR} \ m = 3 \]

\[ \text{A. Phase diagram} \]

The phase diagram that we obtain for \( m = 3 \), is shown in Fig. 12. When \( k = 1 \), the corresponding hard square system has a single, first order transition from the I phase into the C phase. The shaded region between two points denotes a region of phase coexistence. For \( 2 \leq k \leq 6 \), the system undergoes two first order transitions with increasing density: first an I-C transition and second a C-S transition. This is unlike the case \( m = 2 \), where for \( k = 2 \) and 3 we find only one transition. For \( k = 7 \), we find three transitions as in the \( m = 2 \) case. The first transition from I to N phase is continuous while the second from N to C phase appears to be first order. Although we cannot obtain reliable data for the third transition into the S phase, we expect it to be first order. We note that the minimum value of \( k \) beyond which the nematic phase exists is \( 7 \) for both \( m = 2 \) and \( m = 3 \), and matches with that for \( m = 1 \).
B. The isotropic-columnar phase (I-C) transition

The I-C transition exists when $k \leq 6$. We study the this transition for $k = 6$, using the order parameter $Q_3$. Now there are six possible choices for the C phase: heads are predominantly in one of the rows 0, 1 or 2 (mod 3) with all the columns equally occupied (if horizontal orientation is preferred) or in one of the columns 0, 1 or 2 (mod 3) and all the rows are equally occupied (if vertical orientation is preferred). Making an analogy with the six state Potts model, we expect the I-C transition to be first order. The probability distribution of the density $\rho$ and the order parameter $|Q_3|$ for $k = 3$ near the I-C transition is shown in Fig. 13. The distributions are clearly double peaked at and near the transition point, one corresponding to the I phase and the other to the C phase. We find that these peaks become sharper with increasing system size. This is suggestive of a first order phase transition with a discontinuity in both density and order parameter as $\mu$ crosses $\mu_c$. The discontinuity in the density is denoted by the shaded regions of Fig. 12. The chemical potential at which the I-C transition occurs is given by, $\mu^{\text{IC}}_c \approx 3.93$. Similar behavior is seen near the I-C transition for rectangles of size $3 \times 3k$ with $k = 2, 3, 4$ and 5. We observe that the discontinuity in the density increases with $k$.

C. Critical behavior of the isotropic-nematic phase (I-N) transition

As for $m = 2$, for $m = 3$ we find the existence of the nematic phase only for $k \geq 7$. We study the I-N transition for $k = 7$ with the order parameter $Q_1$. It is expected to be in the Ising universality class since there are two possible choices of the orientation: either horizontal or vertical. We are unable to obtain good data collapse for $|Q_1|$, $\chi_1$ and $U_1$ as the relaxation time increases with increasing $m$ and $k$. Instead, we present some evidence for the transition being continuous and belonging to the Ising universality class. In Fig. 14(a), the distribution of the order parameter $Q_1$ near the I-N transition is shown. The two symmetric peaks of the distribution come closer with decreasing $\mu$ and merge to a single peak, this being a signature of a continuous transition. The Binder cumulant $U_1$ for different system sizes cross at $\mu_c \approx 2.92$ ($\rho_c \approx 0.79$) [see Fig. 14(b)]. The value of $U$ at $\mu_1$ is very close to the $U_c$ value (0.61) for the Ising universality class.

D. The nematic-columnar phase (N-C) transition

The N-C transition is studied for $k = 7$ using the order parameter $Q_3$. Contrary to our expectation that the N-C transition should be in the q=3 Potts universality class, we observe a first order transition. The temporal dependence of the density near the N-C transition is shown in Fig. 15(a). Density jumps between two well separated values corresponding to the two different phases near the coexistence. Fig 15(b) shows the discontinuity in the order parameter $|Q_3|$ near the transition. $P(|Q_3|)$ shows two peaks of approximately equal height near $\mu^{\text{NC}}_c \approx 3.12$. However, we are limited in our ability to obtain reliable data for $3 \times 21$ rectangles for larger system sizes, and the observed first order nature could be spurious.
The isotropic-columnar phase (C-S) transition

The C-S transition is studied by choosing \( k = 2 \). We use the order parameter \( Q_4 \) which is nonzero only in the S phase. The probability distribution of the density \( \rho \) and the order parameter \( |Q_4| \) for \( 3 \times 6 \) rectangles near the C-S transitions is shown in Fig. 16. The distributions are again double peaked at and near the transition point, making the C-S transition first order. These peaks become sharper with increasing system size. The discontinuity in the density near the C-S transition is very small and can also be seen in the shaded portions of Fig. 12.

We estimate \( \mu_{c,S}^L \approx 9.33 \). Similar behavior near the C-S transitions is also observed for \( k > 2 \), but the relaxation time increases with \( k \).

VI. ESTIMATION OF THE PHASE BOUNDARIES USING ANALYTICAL METHODS

In this section we obtain the asymptotic behavior of the phase diagram for large \( k \) using theoretical arguments.

A. The isotropic–nematic phase boundary

The critical density for the I-N phase transition, for fixed \( m \) and \( k \gg 1 \) may be determined by making an analogy with the continuum problem. The limit \( k \to \infty \), keeping \( m \) fixed corresponds to the system of oriented lines in the continuum. For this problem \( c_1 \approx A_1/k \) [18, 53]. The constant \( A_1 \) is estimated to be \( \approx 6.0 \) [18, 53]. Thus, we expect \( \rho_c^{IN} \approx A_1/k \), where \( A_1 \) is independent of \( m \). For \( k = 7 \), we observe only a weak dependence of \( \rho_c^{IN} \) on \( m \) with the critical density being \( 0.745 \pm 0.005 \) (\( m = 1 \)), \( 0.744 \pm 0.008 \) (\( m = 2 \)) and \( 0.787 \pm 0.010 \) (\( m = 3 \)).

B. The nematic–columnar phase boundary

To obtain the asymptotic behavior of the N-C phase boundary, we use an ad hoc Bethe approximation scheme for rods due to DiMarzio [54], adapted to other shapes [52]. To estimate the phase boundary of the nematic–columnar transition of \( m \times m \) rectangles on the square lattice with \( M = L \times L \) sites, we require the entropy as a function of the occupation densities of the \( m \) types of rows/columns. The calculations become much simpler, if we consider a fully oriented phase with only horizontal rectangles. Now, the nematic phase corresponds to the the phase where there is equal occupancy of each of the \( m \) types of rows, while the columnar phase breaks this symmetry and preferentially occupies one type of row. For this simplified model with only one orientation, we estimate the entropy within an ad hoc Bethe approximation as detailed below. We present the calculation for \( m = 2 \), classifying the rows as even and odd rows. Generalization to higher values of \( m \) is straightforward.

Let there be \( N_e \) (\( N_o \)) number of rectangles whose heads (left bottom site of the rectangle) occupy even (odd) rows. We first place the \( N_e \) rectangles one by one on the even rows. Given that \( j_e \) rectangles have already been placed, the number of ways in which the \((j_e + 1)^{th}\) rectangle can be placed may be estimated as follows. The head of the \((j_e + 1)^{th}\) rectangle has to be placed on an empty site of an even row. We denote this site by \( A \) (see Fig. 17). The site \( A \) can be chosen at random in \((M/2 - 2k_j_e)\) ways, \( M/2 \) being the number of sites in even rows and \( 2k_j_e \) being the number of occupied sites in the even rows by the \( j_e \) rectangles. We now require that the \(2k - 1\) consecutive sites to the right of \( A \) are also empty. The probability of this being true is \( [P_e(B|A)]^{2k-1} \), where \( P_e(B|A) \) is the conditional probability that \( B \) (see Fig. 17) is empty given that \( A \) is empty. In terms of \( M \) and \( j_e \), \( P_e(B|A) \) is given by

\[
P_e(B|A) = \frac{M - 2k_j_e}{M - 2k_j_e + j_e}.
\]

To place the \((j_e + 1)^{th}\) rectangle, we also require that the site \( C \) (see Fig. 17) and the \(2k - 1\) consecutive sites to the right of \( C \) are also empty. The probability of this being true is \( P_y(C|A) \times P_{xy}(D|B \cap C)^{2k-1} \), where \( P_y(C|A) \) is the conditional probability that \( C \) is empty given \( A \) is empty, and \( P_{xy}(D|B \cap C) \) is the conditional probability that \( D \) (see Fig. 17) is empty given that both \( B \) and \( C \) are empty. Sites \( C \) and \( D \) belongs to an odd row. Since both \( A \) and \( B \) are empty, \( C \) and \( D \) can be occupied only by rectangles with heads in the same odd row. But, there are no such rectangles. Therefore, \( P_y(C|A) = 1 \), and \( P_{xy}(D|B \cap C) = 1 \). Thus, given that \( j_e \) rectangles have been placed, the \((j_e + 1)^{th}\) rectangle may be placed in

\[
\nu_{j_e+1} = \left( \frac{M}{2} - 2k_j_e \right) \times [P_e(B|A)]^{2k-1}
\]
we denote this site by \( e \). The probability of this being true is \( \frac{M/2 - 2kN_e - 2kj_o}{M/2 - 2kj_o} \), where \( P_y(G|E) \) is the conditional probability that \( G \) is empty given \( E \) is empty, and \( P_{xy}(H|F \cap G) \) is the conditional probability that \( H \) (see Fig. 17) is empty given that both \( F \) and \( G \) are empty. Ignoring correlations, \( P_y(G|E) \) is given by
\[
P_y(G|E) = \frac{M/2 - 2kN_e - 2kj_o}{M/2 - 2kj_o}.
\]

If we calculate \( P(H|F \cap G) \) following the procedure developed by DiMarzio in Ref. [53], then the resultant entropy is not symmetric with respect to \( N_e \) and \( N_o \) and depends on the order of placement. To overcome this shortcoming, we follow the Bethe approximation proposed in Ref. [53] as follows:
\[
P(H|F \cap G) = \frac{P(F \cap G|H)P(H)}{P_{xy}(G|F)} = \frac{P_x(G|H)P_y(F|H)}{P_{xy}(G|F)},
\]
where in Eq. (9), we used \( P(H) = P(F) \) and in Eq. (10), we replaced \( P(F \cap G|H)P(H) \) by \( P_x(G|H)P_y(F|H) \), which is an approximation.

In Eq. (10), from symmetry, it is easy to see that \( P_x(G|H) = P_x(F|E) \) and \( P_y(F|H) = P_y(G|E) \) and can be read off from Eqs. (7) and (8). To obtain an expression for \( P_{xy}(G|F) \), the probability that \( G \) is empty, given that the site \( F \) is empty, we again ignore correlations. We then obtain
\[
P_{xy}(G|F) = \frac{M/2 - 2kN_e - 2kj_o}{M/2 - 2kj_o}.
\]

The number of ways of placing the \((j_o + 1)^{th}\) rectangle is
\[
\nu_{j_o+1} = \left( \frac{M}{2} - 2kN_e - 2kj_o \right) \times P_x(F|E)^{2k-1} \times P_y(G|E) \times [P(H|G \cap F)]^{2k-1}.
\]
Substituting for each of the quantities on the right hand side, we obtain the total number of ways of placing the \( N_o \) rectangles on the odd rows as
\[
\Omega_o = \frac{1}{N_o!} \prod_{j_o=0}^{N_o-1} \nu_{j_o+1} = \frac{1}{N_o!} \prod_{j_o=0}^{N_o-1} \left( \frac{M}{2} - 2kN_e - 2kj_o \right)^{4k} \times \left( \frac{M}{2} - 2kN_e - 2kj_o \right)^{2k-1}.
\]

We would like to express the entropy in terms of the total density \( \rho \) and the densities of occupied sites in even
and odd rows, given by $\rho_e$ and $\rho_o$ respectively. Clearly,
\[
\rho_e = \frac{4k N_e}{M}, \quad \rho_o = \frac{4k N_o}{M}, \quad \rho = \rho_e + \rho_o. \tag{16}
\]
The entropy per site $s(\rho_e, \rho_o)$ in the thermodynamic limit is given by
\[
s(\rho_e, \rho_o) = \lim_{M \to \infty} \frac{1}{M} \ln \left( \Omega_0 \Omega_e \right). \tag{17}
\]

Substituting for $\Omega_e$ and $\Omega_o$ from Eqs. (6) and (13), we obtain
\[
s(\rho_e, \rho_o) = - \sum_{i=0,e} \frac{\rho_i}{4k} \ln \left[ \frac{\rho_i}{2k} \right] - (1 - \rho) \ln(1 - \rho) + \left( 1 - \rho + \frac{\rho}{2k} \right) \ln \left( 1 - \rho + \frac{\rho}{2k} \right) + \frac{1 - \rho_i}{2} \ln(1 - \rho_i) - \frac{1}{2} \sum_{i=0,e} \left( 1 - \rho_i + \frac{\rho_i}{2k} \right) \ln \left( 1 - \rho_i + \frac{\rho_i}{2k} \right). \tag{18}
\]

We express the entropy $s(\rho_e, \rho_o)$ in terms of density $\rho$ and the order parameter $\psi_{NC}$, defined as
\[
\psi_{NC} = \frac{\rho_e - \rho_o}{\rho}. \tag{19}
\]
$\psi_{NC}$ is zero in the nematic phase and non-zero in the columnar phase. For a fixed value of $\rho$, the equilibrium values of $\rho_o$ and $\rho_e$ are determined by maximizing the entropy $s(\rho, \psi_{NC})$ with respect to $\psi_{NC}$. In Fig. 13, we show the variation of entropy $s(\rho, \psi_{NC})$ with $\psi_{NC}$ for different densities. For small values of $\rho$, the entropy is dominated by $\psi_{NC} = 0$, i.e., $\rho_e = \rho_o$. Beyond a critical density $\rho_{NC}^c$, $s(\rho, \psi_{NC})$ is maximized by $\psi_{NC} \neq 0$, i.e., $\rho_e \neq \rho_o$. $\psi_{NC}$ grows continuously with $\rho$ for $\rho > \rho_c$, and thus the transition for $m = 2$ is continuous.

The expansion of $s(\rho, \psi_{NC})$ in powers of $\psi_{NC}$ has only even powers of $\psi_{NC}$ since $s(\rho, \psi_{NC})$ is invariant when
\[
s(\{\rho_i\}) = - \sum_{i=1}^m \frac{\rho_i}{m^2 k} \ln \left[ \frac{\rho_i}{mk} \right] - (1 - \rho) \ln(1 - \rho) + \left( 1 - \rho + \frac{\rho}{mk} \right) \ln \left( 1 - \rho + \frac{\rho}{mk} \right) + \frac{1 - \rho + \rho_i}{m} \ln(1 - \rho + \rho_i) - \frac{1}{m} \sum_{i=1}^m \left( 1 - \rho + \rho_i + \frac{\rho - \rho_i}{mk} \right) \ln \left( 1 - \rho + \rho_i + \frac{\rho - \rho_i}{mk} \right). \tag{21}
\]

Here, we define the order parameter to be
\[
\psi_{NC} = \frac{\rho_1 - \rho_2}{\rho}, \tag{22}
\]
where we set $\rho_2 = \rho_3 = \ldots = \rho_m$. Now, $s(\psi_{NC}, \rho)$ is not invariant when $\psi_{NC} = -\psi_{NC}$. Thus, when expanded in powers of $\psi_{NC}$, $s(\psi_{NC}, \rho)$ has cubic terms, making the transition first order. This is illustrated in Fig. 13, which shows the variation of entropy with $\psi_{NC}$ for different $\rho$ near the N-C transition. For low densities $s(\psi_{NC})$ exhibit a single peak at $\psi_{NC} = 0$, but with increasing $\rho$ a secondary maximum gets developed at $\psi_{NC} \neq 0$. For $\rho = \rho_{NC}^c$ the maximum at $\psi_{NC} = 0$ and $\psi_{NC} \neq 0$ becomes of equal height. Beyond $\rho_{NC}^C$ the global maximum of $s(\psi_{NC}, \rho)$ jumps to $\psi_{NC} \neq 0$, making the N-C transition to be first order.

Unlike the $m = 2$ case, there is no way to obtain an analytic expression for $\rho_{NC}^C$. For $m = 3$, the numerically determined $\rho_{NC}^C$ for different $k$ is shown in Fig. 20.
We note that this expression has the same form as for \( m = 2 \) [see Eq. (20)].

For \( m > 3 \), we proceed as follows. The transition density \( \rho_{NC}^c \) is bounded from above by the spinodal density \( \rho_{sNC} \), the density at which the entropy at \( \psi_{NC} = 0 \) changes from a local maximum to local minimum. \( \rho_{sNC} \) is obtained from the condition \( \frac{d^2 s}{d \psi_{NC}^2} \Big|_{\psi_{NC}=0} = 0 \) and we obtain

\[
\rho_{sNC} = \frac{-m + 2km^2 - m\sqrt{1 - 4k + 4k^2m}}{2(1 - m - km + km^2)} \geq \rho_{NC}^c \tag{24}
\]

\[
= \frac{\sqrt{m}}{1 + \sqrt{m}} + \frac{B_1(m)}{k} + O\left(k^{-2}\right), \quad k \to \infty, \tag{25}
\]

\[
= 1 - \frac{1}{\sqrt{m}} + \frac{B_2(k)}{m} + O\left(m^{-3/2}\right), \quad m \to \infty \tag{26}
\]

where \( B_1(m) = \frac{1}{2(m + \sqrt{m})} \) and \( B_2(k) = (1 + \frac{1}{2k}) \). The spinodal density is compared with \( \rho_{NC}^c \) in Fig. 20. From Eq. (26), it follows that \( \rho_{sNC} \leq 1 \) and tends to one when \( m, k \to \infty \). The limit \( m \to \infty \) corresponds to the continuum limit. In this limit \( \rho_{sNC} \to 1 \). Thus, it is not clear whether the nematic-columnar phase will exist in the continuum.

**C. The columnar–sublattice phase boundary**

The dependence of the C-S phase boundary on \( m \) and \( k \) may be determined by estimating the entropy for the C and S phases close to full packing. We approximate the entropy of the C phase by the entropy of the fully aligned C phase. Since the heads of the rectangles are all in either even or odd rows/columns, by ignoring the unoccupied rows/columns, the calculation of entropy reduces to an one-dimensional problem of rods. The mean number of holes in a row is \( L(1 - \rho) \), and the mean number of rods (of length \( mk \)) in a row is \( \frac{\rho L}{m} \). There are \( L/m \) such rows. The number of ways of arranging the rods and holes on
a row is

$$\Omega_{\text{row}} = \frac{[L(1-\rho) + \rho A_k]!}{[L(1-\rho)]!(\rho A_k)!},$$

(27)

such that the total number of ways of arranging the rectangles is $\Omega_{\text{row}}^{L/m}$. Hence, $S_C$, the entropy per site of the columnar phase is given by $S_C = (Lm)^{-1} \ln \Omega_{\text{row}}$, which for densities close to 1 is

$$S_C \approx \frac{1-\rho}{m} \ln \left[ \frac{e}{km(1-\rho)} \right] + O[(1-\rho)^2].$$

(28)

We now estimate the entropy for the sublattice phase. At full packing, the head of each rectangle is on one of $m^2$ sublattices. Ignoring the sites belonging to other sublattices, it is easy to see that each configuration of rectangles can be mapped on to a configuration of rods of length $k$ on a lattice of size $L/m \times L/m$. When $k \gg 1$, by solving the full packed problem of rods on strips, it is known that the entropy per unit site is $k^{-2} \ln k^{18}$. For rectangles of size $m \times mk$ we obtain

$$S_S(\rho = 1) \approx \frac{\ln k}{m^2 k^2}, \quad k \gg 1,$$

(29)

where $S_S$ is the entropy per site of the S phase. For densities close to 1 ($\rho = 1-\epsilon$) we estimate the correction term to $S_S(\rho = 1)$ by removing $\epsilon/(m^2k)$ fraction of rectangles at random from the fully packed state. Here, we ignore the entropy of the holes, assuming that the holes form bound states. This gives the entropy of the sublattice phase, close to the full packing to be approximately

$$S_S \approx \frac{\ln k}{m^2 k^2} - \frac{1}{m^2 k^2}[(1-\rho) \ln(1-\rho) + \rho \ln \rho], \quad k \gg 1,$$

(30)

Comparing Eqs. (28) and (30) up to the leading order we obtain the critical density for the C-S transition to be

$$\rho_C^{CS} \approx 1 - \frac{A_2}{mk^2}, \quad k \gg 1,$$

(31)

where $A_2 > 0$ is a constant.

VII. SUMMARY AND DISCUSSION

To summarize, we obtained the rich phase diagram of a system of $m \times mk$ hard rectangles on a square lattice for integer $m, k$ using a combination of Monte Carlo simulations and analytical calculations. We improve an existing cluster Monte Carlo algorithm by implementing the plaquette flip move, which reduces the autocorrelation time considerably. For $k \geq 7$, we show that the system undergoes three entropy driven transitions with increasing density. For $m = 2$, we find that the I-N, N-C and C-S transitions are continuous, but the I-C transition may be continuous or first order, depending on $k$. The critical exponents for the continuous transitions were obtained using finite size scaling. The I-N and N-C transitions are found to be in the Ising universality class, while the C-S transition in the Ashkin-Teller universality class. The I-C transitions are also found to be in the Ashkin-Teller universality class when continuous. For larger $m$, the number of possible ordered states increase and the corresponding transitions become first order.

Surprisingly, our numerical data suggests that the nematic-columnar phase transition for $m = 3$ is first order. However, once a nematic phase with orientational order exists, there are only three possible choices for the columnar phase. By analogy with the three state Potts model, we would expect a continuous transition, in contradiction with the numerical result. We also performed simulations for a system where the activity for vertical rectangles is zero (only horizontal rectangles are present) and observed again a first order transition. However, for $3 \times 21$ rectangles, the autocorrelation time is high and it becomes increasingly difficult to obtain reliable data. Simulations of larger systems are required to resolve this puzzle in the future.

When $m = 2$, the I-C transition is found to be continuous for $k = 4$ and 5, but first order for $k = 6$. For $k = 6$, it is a weak first order transition and it is difficult to see the jump in density for small system sizes. It would be interesting to reconfirm the first order nature by either simulating larger systems or doing constant density Monte Carlo simulations at the transition point so that phase separation may be seen. Also, determining a method to map $k$ and $\rho$ to the Ashkin Teller model parameters would be useful in clarifying this issue.

Another issue that we are not able to resolve completely is the determination of the minimum value of $k$ (say $k_{\text{min}}$) for which two transitions exist. For $m \geq 3$, we show that $k_{\text{min}} = 2$. When $m = 2$, our numerical data suggests that $k_{\text{min}} = 4$, with a direct transition from isotropic to sublattice phase for $k = 2, 3$. However, for $k = 4$, the columnar phase exists in a very narrow window of $\mu$ or $\rho$. Whether the columnar phase is present for $k = 2, 3$, but we are unable to resolve the transitions, is something that requires investigation of much larger system sizes.

We obtained the N-C phase boundary analytically through a Bethe approximation. However, an improvement of the calculations is desirable as the approximations are ad hoc and uncontrolled and there does not appear to be a systematic way of improving it. An exact solution on tree like lattices, for example the random locally layered tree like lattice (RLTL) [5, 23] would be more satisfying. At present, we have not been able to formulate the problem of rectangles on RLTL. This is a promising area for future study.
Several extensions of the problem are possible. An interesting limit is the continuum problem of oriented rectangles of aspect ratio \( k \). This corresponds to the \( m \to \infty \) limit of the lattice model. From the analytical arguments presented in the paper, we would expect an isotropic nematic transition at a critical density proportional to \( k^{-1} \). Within the Bethe approximation, the spinodal density for the nematic–columnar transition tends to 1 in the continuum limit. This being an upper bound for the critical density for the nematic–columnar transition, it is likely that the continuum problem will have a second transition into a columnar phase like phase, a true columnar phase being prohibited by the Mermin Wagner theorem. We expect the C-S transition to be absent in the continuum, as the critical density for the C-S transition tends to 1 as \( m \to \infty \). It would be interesting to verify these claims numerically. Preliminary simulations show an isotropic nematic transition.

One could also consider the model on other lattices like the triangular lattice. Here, the rectangles may orient themselves along three possible lattice directions. In this case, the phase diagram would be qualitatively similar to that for the square lattice. However, as there are three broken symmetry phases corresponding to the three directions, the I-N transition would be in the 3 state Potts universality class, as opposed to Ising universality class for the square lattice. However, the N-C transition would be same as that for the square lattice. The I-C transition is now expected to be first order for all \( m \) since the number of symmetric C phases increases from \( 2m \) to \( 3m \). The number of S phases is still \( m^2 \). Therefore, we expect the I-S transition to be similar to that for the square lattice. It would be interesting to study the C-S transition carefully in detail for the triangular lattice and compare with that for the square lattice.

We have also studied systems with non-integer \( k \) on the square lattice (e.g., \( 2 \times 11 \)). Now, it is straightforward to see that the high density phase cannot have sublattice order. Thus, the high density phase does not possess either translational or orientational order. But, at intermediate densities, we observe the existence of the C phase for \( k \geq k_{\text{min}} \) and N phase for \( k \geq 7 \). When \( m = 2 \) we observe the C phase for \( k \geq 5.5 \) (rectangles of size \( 2 \times 11 \)). In this case the I-C transition is found to be first order. For both \( m = 2 \) and 3, the I-N and N-C transitions are expected to be similar to that for integer \( k \). Unlike integer \( k \), we do not observe any transition for small \( k \) (\( k < 5.5 \) for \( m = 2 \)) and the phase remains isotropic at all densities. We hope to clarify these issues in detail in a future paper.

We argued, based on an analogy with the continuum problem, that \( \rho_{\text{C-N}}^{I} \approx A_1/k \), where \( A_1 \) is independent of \( m \). Can this conjecture be verified analytically or through numerical simulations? We expect that for \( m = 2 \), the critical density can be determined numerically up to a \( k \) large enough to determine \( A_1 \). Comparison with the value of \( A_1 \) for \( m = 1 \) would help in verifying the conjecture.

Extension to three dimensional cubic lattice would result in a much richer phase diagram that remains to be explored. The algorithm used in this paper is easily implementable in three dimensions.

Finally, the \( m = 1 \) case (hard rods) is the only instance where the existence of a nematic phase may be proved rigorously [19]. To the best of our knowledge, there exists no proof of existence of phases with partial translational order like the columnar phase. The hard rectangle model seems an ideal candidate to prove its existence.

ACKNOWLEDGMENTS

We thank Deepak Dhar and J"urgen F. Stilck for helpful discussions. The simulations were carried out on the supercomputing machine Annapurna at The Institute of Mathematical Sciences.

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