Columnar order and Ashkin-Teller criticality in mixtures of hard-squares and dimers

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Particles with only hard-core interactions can exhibit interesting high-density phases. The cases of particles in the shape of $2 \times 2$ squares, and $2 \times 1$ dimers on a square lattice have been studied for a long time. Here, we study the interesting and more general problem of a mixture of such dimers and squares. In the fully-packed limit of no vacancies, increasing the fraction of squares enhances the power-law columnar (stripe) order present in the pure dimer limit and eventually leads to a Kosterlitz-Thouless-type (KT) phase transition to a square-rich phase with long-range columnar order. With vacancies allowed, the entire phase boundary between this columnar ordered phase and the low-density fluid phase has continuously varying exponents and is in the Ashkin-Teller universality class. These results, which we confirm by Monte-Carlo simulations, make explicit the Ashkin-Teller nature of the density-driven transition in the $2 \times 2$ hard-square gas.

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The covering of lattices by non-overlapping $2 \times 1$ dominos (dimers), with only excluded-volume interactions, is a classical problem in lattice statistical mechanics [1–3]. The rich physics of such dimer models, particularly the presence of power-law correlations in the fully-packed limit on several lattices, has been explored for many years now [4–8]. There have been many studies of the geometrical phase transition as a function of density of particles, for different shapes of particles. The cases of squares, long rectangles, triangles, hexagons, and more complicated shapes have been studied on various two-dimensional lattices [9–16]. The problem is also related to the Lee-Yang edge singularity problem [17], and the statistics of directed [18] and undirected branched polymers [19].

The case of $2 \times 2$ hard-squares on the square lattice has been of particular interest. Here, the crystalline phase with sublattice order has a sliding instability, and the the high-density phase shows not sublattice order, but columnar (stripe) order [20–28]. While general symmetry arguments [29, 30] suggest that the transition to columnar order should provide an example of Ashkin-Teller-type (AT) of critical behaviour with a non-universal correlation length exponent [31–34], large-scale Monte-Carlo simulations [25–27] yield critical properties that are very close to those of a two-dimensional Ising model. Indeed, some authors [25] have concluded in favour of an Ising critical point, while others have found small deviations from Ising behaviour [26, 27].

In this Letter, we consider the more general problem of a mixture of $2 \times 2$ squares and $2 \times 1$ dimers on a square lattice (Fig. 1). Our main results are displayed in the schematic phase diagram of Fig. 2. The well-studied hard-square lattice-gas and square-lattice dimer model correspond to the bounding lines $VS$ and $VD$ in this schematic phase-diagram. Along $VD$, the dimer model has exponentially decaying correlations [2] except the fully-packed model (point $D$) which has power-law columnar order [4], while the hard-square gas goes from a low-density fluid phase to a high-density columnar-ordered phase along $VS$. Here, we note that the third boundary $SD$, corresponding to a fully-packed mixture of squares and dimers, admits a height representation. This allows us to argue that adding hard-squares to a system of fully-packed dimers on the square lattice initially enhances the power-law columnar order present in the fully-packed dimer limit, and eventually drives this vacancy-free mixture to a hard-square-rich phase with long-range columnar ordered via a Kosterlitz-Thouless (KT) transition.

When vacancies are allowed in this mixture, this KT transition represents the beginning of an Ashkin-Teller (AT) critical line which ends in the density-driven transition of the hard-square lattice gas along $VS$ (Fig. 2). We argue that the entire phase-boundary between the hard-square-rich columnar ordered phase and the low-density fluid phase is in the Ashkin-Teller universality class. We also develop a correspondence between microscopic hard-square and dimer variables and the Ising ($XY$) fields of a coarse-grained AT (KT) description and use it to confirm our theoretical predictions via large-scale Monte Carlo simulations. Returning to the original hard-square transition along $VS$, our results also lead us to some in-
teresting observations about correlations between vacant sites, and the effect of inter-vacancy interactions at this transition. We begin by defining a lattice-gas of hard-squares that occupy the four elementary plaquettes of a square lattice, dimers that occupy two plaquettes, and vacant single plaquettes (vacancies or monomers). We consider a $L \times L$ square lattice generated by unit lattice translations $\tilde{e}_x$ and $\tilde{e}_y$, with sites labeled by $\vec{R} \equiv (m, n)$ $(m, n)$ integers and corresponding plaquettes labeled by their center: $\vec{r} \equiv \vec{R} + (\tilde{e}_x + \tilde{e}_y)/2$. We use periodic boundary conditions and associate activities $z_s$, $z_d$ and $z_v$ with each square, dimer and vacancy respectively. The grand partition function of the system is then given by

$$Z_{dsv} = \sum_{C_{dsv}} z_s^{N_s} z_d^{N_d} z_v^{N_v}.$$  \hspace{1cm} (1)

Here, the sum is over all allowed configurations $C_{dsv}$ that respect the geometric constraint that no two objects overlap, and $N_s$, $N_d$ and $N_v$ are the total numbers of squares, dimers and vacancies in $C_{dsv}$ (Fig. 4). As $4N_s + 2N_d + N_v = L^2$, we can parameterize the problem with two parameters, which we choose to be $v = z_v z_s^{-1/4}$, and $w = z_d/z_s$. The case $v = 0$ (boundary DS) corresponds to monomer-free mixture of squares and dimers with partition function $Z_{ds}$. If $z_s = 0$ (point D), $Z_{ds}$ equals $Z_{dimers}$, the partition function of a fully-packed square-lattice dimer model with dimer fugacity $z_d$. $Z_{dimers}$ is characterized by a power-law tendency to columnar order manifested in the connected correlation function of horizontal (vertical) dimers, which decays as $(-1)^l/l^{2}$ for large separation $l$ along the $x$ ($y$) axis.

For small but non-zero $w^{-1}$, the partition sum $Z_{ds}$ involves configurations with a finite-density of squares. Using the procedure of Ref. [49] to map $Z_{ds}$ to an interacting dimer-model with $k$-dimer interactions $(k = 2, 3, \ldots)$, we see [50] that the leading interaction is a two-body attraction of strength $V_2(w) = \log[1 + 1/(2w^2)]$ between two dimers whose long sides touch. Drawing upon earlier work [15-17], we expect that this interaction enhances the power-law columnar order present in the dimer-limit, with power-law exponent $\eta(w)$ decreasing from $\eta(w = \infty) = 2$ as $V_2$ increases in strength. Furthermore, the net effect of the $k > 2$ interaction terms [50] also favours columnar ordering as $w$ is reduced. Therefore, as $w$ is reduced to go into a square-rich regime, we expect that the system will eventually be driven into a phase with long-range columnar order for $w$ less than a critical value $w_c^*$. In the columnar state, the system spontaneously breaks lattice translation symmetry along $\tilde{e}_x$ or along $\tilde{e}_y$. This four-fold symmetry-breaking is best characterized in terms of a complex order parameter $\psi(\vec{r})$ defined on plaquettes $\vec{r}$ (Fig. 3). With this definition, the mean value of $\psi$ takes values $\pm a$, $\pm ia$ in the four columnar-ordered states, where $a$, the modulus of $\psi$, depends on the densities of squares and dimers, while $\langle \psi^* (\vec{r}) \psi(0) \rangle \sim 1/r^{\eta(w)}$ for large $r$ (note the absence of any oscillatory pre-factor) in the $w > w_c^*$ phase with power-law columnar order at full-packing.

For understanding the nature of the transition at $w_c^*$, our key observation is that our model admits a scalar height representation along DS, i.e. the local configuration can be reconstructed from lattice-gradients of a single-valued scalar height $H(\vec{R})$. To construct the height field $H(\vec{R})$, we assign the height at the origin $H(\vec{0}) = 0$, define $\eta_{mn} \equiv (-1)^m-n$, and traverse any sequence of links to go from $\vec{O}$ to $\vec{R} \equiv (m, n)$. When traversing a vertical link from $(m, n)$ to $(m, n+1)$ (horizontal link from $(m+1, n)$ to $(m, n)$), $H$ increases by $3\eta_{mn}/4$ if this link is fully covered by a dimer, by $\eta_{mn}/4$ if fully covered by a square, and by $-\eta_{mn}/4$ otherwise. When there are no squares, this reduces to the well-known height representation for the fully-packed dimer model [47, 51, 58].

In the $w > w_c^*$ power-law ordered phase, long-wavelength fluctuations of the height-field are well-described by the effective action [47, 51, 54, 58]:

$$S_{\text{eff}} = \int_{\Lambda} d^2r [\pi g(\nabla h)^2 + \sum_{n=1,8,12\ldots} u_n \int d^2r \cos(2\pi nh)].$$  \hspace{1cm} (2)

Here $h(\vec{r})$ is a coarse-grained version of the microscopic height field (the distinction between sites $\vec{R}$ and plaquettes $\vec{r}$ is not necessary in this coarse-grained description), the starting values (at cutoff scale $\Lambda$) of the stiffness $g$ and $n$-fold anisotropy terms $u_n$ are input parameters in this description, and the form of these cosine terms in the action are fixed [47, 51, 58] by the transformation properties of $h(\vec{r})$ under lattice-symmetries of the original partition function.

The utility of this coarse-grained height-representation lies in two observations: First, since $\exp(2\pi ih(\vec{r}))$ transforms under lattice-symmetries of the same way as $\psi(\vec{r})$, we expect long-distance properties of correlators of $\psi(\vec{r})$ in $Z_{dsv}$ to correspond to those of $\exp(2\pi ih(\vec{r}))$ in the coarse-grained theory $S_{\text{eff}}$. Second, $S_{\text{eff}}$ with all $u_n$ set to zero represents a line of critical fixed-points parameterized by a variable stiffness $g$. All allowed cosine terms $u_n$ are irrelevant perturbations of this fixed-line for $g < 4$ [54].

Along this fixed-line, we have $\langle e^{2\pi ih(\vec{r})}e^{-2\pi ih(0)} \rangle = 1/r^{1/g}$ [54]. Since $\langle e^{2\pi ih(\vec{r})}e^{-2\pi ih(0)} \rangle \sim \langle \psi^* (\vec{r}) \psi(0) \rangle$, this implies power-law columnar order with exponent $\eta = g^{-1}$. Therefore, we may identify the $w \to \infty$ limit ($Z_{\text{dimers}}$) with the point $\eta = 1/4$ on this fixed-line, consistent with $\eta(\infty) = 2$. Since we have already argued that $\eta(w)$ reduces as $w^{-1}$ is increased from 0, we expect that the corresponding value of $g$ increases on this fixed-line until it hits $g = 4$ corresponding to $\eta = 1/4$. At this point, $u_4$ becomes marginally relevant, driving a Kosterlitz-Thouless (KT) transition to a four-fold symmetry-breaking state with long range order for $\exp(2\pi ih(\vec{r}))$, i.e. a columnar ordered state with
FIG. 2: (Color online) Schematic phase diagram of the squares-dimers-vacancies model (not to scale) in the \( \rho_s, \rho_d, \rho_v \) plane \( \rho_s + \rho_d + \rho_v = 1 \), where \( \rho_s, \rho_d \), and \( \rho_v \) are the fractional areas covered by squares, dimers, and vacancies respectively. The vertices \( S, D \), and \( V \) correspond to \( \rho_s = 1, \rho_d = 1, \rho_v = 1 \) respectively. The phase transition along \( \rho_v = 0 \) is a Kosterlitz-Thouless transition. The transition is studied along the lines \( (I, II \) and \( III) \) in Monte-Carlo simulations.

\[
\langle \psi \rangle \neq 0 \text{. Furthermore, this irrelevance of all cosine terms in the power-law ordered phase implies that the phase of } \Psi_L = \sum_\mathbf{r} \psi(\mathbf{r}) / L^{1-\eta(w)/2} \text{ (where the sum is over a large } L \times L \text{ box) will be uniformly distributed in } (0, 2\pi) \text{ throughout the power-law ordered phase and at the KT point, reflecting an emergent } U(1) \text{ symmetry at large length scales.}
\]

We now argue that this \( (w = w_c^v, v = 0) \) KT transition represents the beginning of an Ashkin-Teller (AT) critical line in the \( (w, v) \) phase-diagram of \( Z_{dsv} \), at whose other end \( (w = 0, v = v_c^d) \) lies the density-driven transition of the hard-square lattice gas. To establish this, we first note that it is enough to keep a non-zero \( u_4 \) and set all other \( u_n \) in \( S_{\text{eff}} \) to zero in the vicinity of this KT transition at \( g = 4 \) \cite{34}; the \( v = 0 \) KT transition can be thus thought of as a transition to four-fold symmetry breaking order in a vortex-free XY model with four-fold anisotropy. Next, we note that an isolated vacancy on plaquette \( \mathbf{r} = (m, n) + (e_x + e_y)/2 \) causes the phase of the XY order parameter \( e^{2\pi i h} \sim \psi(\mathbf{r}) \) to wind by \( 2\pi \times (-1)^{m+n} \) along a circuit that encloses the vacancy at \( (m, n) \) once, while \( \psi = 0 \) on the vacant plaquette itself, as befits the core of a vortex in an XY order parameter. Thus, a non-zero density of vacancies in \( Z_{dsv} \) corresponds to perturbing this vortex-free, four-fold anisotropic XY model with a non-zero density of vortices and anti-vortices. As is well-known from the work of Kadanoff and others on such XY models with four-fold anisotropy \cite{33, 38, 41, 42, 43, 44}, vorticity and four-fold anisotropy “balance” each other along a line of fixed points that starts at this vortex-free KT point. This fixed-line describes the continuously-varying critical properties of the Ashkin-Teller (AT) universality class \cite{33, 38}, \textit{i.e.} the non-universal critical behaviour of
two Ising models whose energy densities are coupled to each other.

For $Z_{dsv}$, this implies that the $(w = w^*_v, v = 0)$ KT transition represents the start of an AT critical line that separates a square-rich columnar-ordered phase from a low-density fluid phase (Fig. 2). The density-driven transition at $(w = 0, v = v^*_c)$ in the hard-square lattice gas thus represents the other end of this AT line. The two scalar fields $\sigma$ and $\tau$ of this alternate Ashkin-Teller description are related to the $XY$ order parameter $\psi$ defined earlier via

$$\psi(\vec{r}) = \frac{\sigma(\vec{r}) + \tau(\vec{r})}{2} + i \frac{\sigma(\vec{r}) - \tau(\vec{r})}{2}.$$  \hspace{1cm} (3)

The emergent $U(1)$ symmetry of the KT point, and of the fixed line controlling the power-law columnar-ordered phase of the vacancy-free mixture, makes the $XY$-order parameter $\psi(\vec{r})$ a natural variable at $v = 0$, while the scalar fields $\sigma$ and $\tau$ are more natural variables away from $v = 0$. From their expressions in terms of microscopic variables, it is clear that lattice symmetries guarantee $(\sigma(\vec{r})\tau(\vec{r})) = 0$ and $(\psi^*(\vec{r})\psi(0)) = (\sigma(\vec{r})\sigma(0)) = (\tau(\vec{r})\tau(0))$. As we shall see below, $\psi^*(\vec{r})\psi(0))$ and correlators of $\text{Re}(\psi^2(\vec{r})) \equiv \sigma(\vec{r})\tau(\vec{r})$ play a key role in characterizing the nature of the phase-boundary.

Several interesting predictions for these correlators follow immediately from our knowledge of the long-wavelength physics of the AT line and its KT end-point. First, in the $v = 0$ power-law ordered phase, as well as at the $v = 0$ KT transition, the emergent $U(1)$ symmetry implies that $\langle \text{Re}(\psi^2(\vec{r}))\text{Re}(\psi^2(0)) \rangle$ and $\langle \text{Im}(\psi^2(\vec{r}))\text{Im}(\psi^2(0)) \rangle$ both decay as $1/v^{2\nu(0)}$, where $\eta(w)$ is the power-law exponent for correlations of $\psi$: $\langle \psi^*(\vec{r})\psi(0) \rangle \sim 1/v^{\eta(w)}$. Along the AT phase boundary at non-zero $v$, $\langle \psi^*(\vec{r})\psi(0) \rangle \sim 1/v^{1/4}$, while $\langle \text{Re}(\psi^2(\vec{r}))\text{Re}(\psi^2(0)) \rangle \sim 1/v^{\eta(2)}$, with $\eta_2(v)$ varying continuously, starting from the $v = 0$ value $\eta_2(v = 0) = 1$. Thus $\eta_2$ is a convenient and natural coordinate in terms of which one can specify the position along the AT line. The correlation-length exponent $\nu$, which characterizes the divergence of the correlation length for $\sigma$ and $\tau$ correlations in the vicinity of the AT line, is related to $\eta_2$ via $2\nu = (1 - \eta_2)^{-1}$.

In order to test this picture, we have performed Monte-Carlo simulations of $Z_{dsv}$ on $L \times L$ periodic lattices (with $L$ up to 1024) using a modified [54] version of the transfer-matrix algorithm of Ref. [61] which does not suffer from jamming. Our modification works at full-packing as well, and can be generalized to a large class of similar problems. Our simulations provide clear evidence for the existence of a $v = 0$ power-law ordered phase for $w > w^*_v \approx 0.198(2)$, with $\langle \psi^*(\vec{r})\psi(0) \rangle \sim 1/v^{\eta(w)}$ and $\langle \text{Re}(\psi^2(\vec{r}))\text{Re}(\psi^2(0)) \rangle \sim \langle \text{Im}(\psi^2(\vec{r}))\text{Im}(\psi^2(0)) \rangle \sim 1/v^{4\nu(0)}$ (Fig. 4). Additionally, we confirm $\eta(w^*_v) = 1/4$ (Fig. 4). At an intermediate point (Fig. 4 and Fig. 5) on the phase-boundary, we confirm that $\eta = 1/4$ provide a good account of our data (Supplemental Material [59]), and find $\eta_2 \approx 0.70(5)$ and $\nu \approx 1.70(5)$ (Fig. 5); within errors, these exponents satisfy the Ashkin-Teller relation $\eta_2 = 1 - 1/(2\nu)$. Finally, for the density-driven transition of hard-squares at $w = 0 \neq v^*_v = 0.3181(2)$, our data is well-fit by $\eta = 1/4$, and $\nu \approx 0.92(2)$ (Supplemental Material [59]), consistent with some of the earlier studies [26, 27].

For the transition in the original hard-square gas, the foregoing picture implies that a small density of dimers will drive this transition towards the decoupled Ising point, while attractive interaction between next-nearest neighbour vacancies will move it towards the four-state Potts point on the AT line. Although $\text{Re}(\psi^2(\vec{r})) = 0$ identically at $z_d = 0$, we can also learn about certain correlations between vacancies at the hard-square critical point by considering the limiting value of $\langle \text{Re}(\psi^2(\vec{r})) \rangle$ as the hard-square transition is approached along the AT line: The leading term in this limit is proportional to $\langle N_{xx} + N_{yy} - N_{xy} \rangle_0$, where $N_{xx}$, $N_{yy}$ and $N_{xy}$ are respectively the number of ways of adding two horizontal dimers, two vertical dimers, and one horizontal and one vertical dimers on vacant plaquettes, and the average is taken at the hard-square critical point. Since $\langle \text{Re}(\psi^2(\vec{r})) \rangle \sim L^{4-\eta_2} \sim L^{3+1/4\nu}$ along the AT line and $\nu \approx 0.92(2)$ for the hard-square transition, we expect $\langle N_{xx} + N_{yy} - N_{xy} \rangle_0 \sim L^{3.54}$ at the hard-square critical point.

To summarize, we have elucidated the phase diagram of a lattice-gas of non-overlapping $2 \times 2$ squares and $2 \times 1$ dimers on the square lattice. Our study makes explicit
the Ashkin-Teller nature of the transition to columnar order in a gas of $2 \times 2$ hard-squares, and yields new insights about the nature of vacancy-pair correlations and the effect of inter-vacancy interactions at this well-studied transition.

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Supplemental Material for “Columnar order and Ashkin-Teller criticality in mixtures of hard-squares and dimers”

In this document we present details of our Monte Carlo algorithm and additional results from our simulations which support the key findings highlighted in the main text.

TRANSFER-MATRIX BASED ALGORITHM

Update Scheme

To simulate the system of dimers and squares on the square lattice, we use the following transfer-matrix based Monte Carlo algorithm which is a variant of the technique developed in Refs. [14–16, 60, 61]. Our variant is designed to ensure that we can work directly in the full-packing limit if needed. In our scheme, we update all objects fully contained in a $2 \times N$ track (two adjacent rows/columns of plaquettes) at once, with the correct weights in the partition function. The steps involved in each update are as follows:

- We empty out all objects that are fully contained within a randomly chosen $2 \times N$ track (horizontal or vertical).

- The remaining objects either lie outside the chosen track (this includes objects which share an edge with the long boundary of the track) or protrude partially into the track. The latter class of objects, which protrude partially into the track, provide excluded-volume constraints that need to be respected when the track is refilled.

- To refill the track with objects lying entirely within the track, we compute the partition function of the track subject to the constraints imposed by objects that protrude into the track. This is done using a standard transfer matrix technique.

- Using this partition function, we generate a configuration with the correct Botzmann weight consistent with the constraints, and re-populate the track. We summarize these steps in Fig. 6 below.

![FIG. 6: Steps in the transfer-matrix based algorithm.](image)

To evaluate the weights of the allowed configurations for the purpose of refilling a track, we need to calculate the restricted partition function of this track subject to constraints imposed by objects protruding into the track. We do this by using a standard transfer matrix technique. Below we provide details of this update for a horizontal track.
Details of the Transfer Matrices

We break up the track into a sequence of two-plaquette “rungs”, defined as two vertically adjacent plaquettes. After the track is emptied of all objects lying completely within it, these rungs still have areas covered by objects protruding into the track from above and below (as shown in Fig. 6). These protrusions preclude the occupation of some objects on the rung, and thereby provide constraints on which objects can be re-populated. The four possible types of protrusions (represented by shaded areas) on a given rung are shown in Fig. 7. Based on this underlying “morphology”, we assign an index $\sigma$ to each rung, with $\sigma = 1, 2, 3, 4$ chosen with the convention of Fig. 7.

![Fig. 7: The four possible underlying morphologies $\sigma = 1, 2, 3, 4$ of a two-plaquette rung, arising from objects protruding into the track from above and below (represented by the shaded areas). $\sigma = 4$ corresponds to a complete blockade.](image)

Next, in order to fill the rung with objects, we focus on the “state” $C$ of a rung, the ways in which objects can be placed on this rung. When the underlying morphology is ignored, there are six possible ways of filling a two-plaquette rung, as shown in Fig. 8.

![Fig. 8: The six possible states of a two-plaquette rung.](image)

To unambiguously assign objects to each rung, we use the convention that objects are on the rung, if their left edge coincides with the left edge of the rung (represented by open circles in Fig. 8). Our convention is also designed to ensure that the allowed states are influenced only by the morphology of the given rung and the one immediately to the right. When the underlying morphology is considered, not all states are allowed. For example, state $C = 3$ is disallowed if the morphology of the rung is $\sigma = 2, 3, 4$, the state $C = 6$ is disallowed if the morphology of the rung OR of the rung immediately to the right is $\sigma = 3, 4$, and so on.

We next construct the partition function of the track subject to these constraints and also the excluded volume constraints provided by the objects on the track. Our transfer matrix formalism transfers the state of a two-plaquette rung to the next two-plaquette rung to its left, subject to these constraints. So, let $Z_n(C', \sigma')$ be the partition function of an $n$-rung track, where the leftmost rung is filled with the state $C'$, and has an underlying morphology $\sigma'$. Then, the partition function of the ($n+1$)-rung track, $Z_{n+1}(C, \sigma)$ is given by the recursion relation:

$$Z_{n+1}(C, \sigma) = \sum_{C'} T_{\sigma, \sigma'}(C, C') Z_n(C', \sigma'),$$

(4)

where $T_{\sigma, \sigma'}(C, C')$ is a $6 \times 6$ transfer matrix, consistent with the excluded volume constraints of $C$ and $C'$ and also with the constraints provided by the underlying morphology $\sigma, \sigma'$. We therefore have 16 possible transfer matrices, based on these indices $\sigma, \sigma'$. However, we note that if there is a complete disruption in the track ($\sigma = 4$), the partition function of the track breaks up into a product over partition functions of open chains. We deal with these cases separately since, as we show later, the computational cost is greatly reduced in this case.

Hence, based on the possible combinations $\sigma, \sigma' = 1, 2, 3$ (shown in Fig. 9), there are nine possible transfer matrices. We list them below:
If one or more of the rungs on the track is completely blocked \( (T_{\sigma,\sigma'} = 1, 2, 3) \), appearing asymmetrically, the partition function of an open chain is given by

\[
Z_{\text{track}}^{\text{open}} = \langle \mathcal{L}_{\sigma_N} | T_{\sigma_{N-1}} T_2 T_1 | \mathcal{R}_{\sigma_1} \rangle, \tag{7}
\]

where \( L \) is the size of the lattice and the matrices \( T_i \) are chosen according to the underlying morphology as described above. Here \( T_1 = T_{\sigma_1,\sigma_1}, T_2 = T_{\sigma_1,\sigma_2}, \ldots, T_L = T_{\sigma_1,\sigma_L} \).

If one or more of the rungs on the track is completely blocked (\( \sigma = 4 \)), then the partition function of the track is given by a product of partition functions of open chains. For an open chain where \( N < L \) consecutive rungs are allowed for occupation, the partition function is given by

\[
Z_{\text{track}}^{\text{closed}} = \text{Tr}(T_L \cdots T_2 T_1). \tag{6}
\]
where $\sigma_1$ and $\sigma_N$ represent the morphology of the first and $N$-th rung respectively. The three right vectors are given by (formally $\mathcal{R}_\sigma(C) = \mathcal{T}_{\sigma,1}(C, 4)$)

\[
|\mathcal{R}_1\rangle = \begin{pmatrix} 0 \\ 0 \\ z_d \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\mathcal{R}_2\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\mathcal{R}_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{pmatrix},
\]

and the three left vectors are given by (formally $\mathcal{L}_\sigma(C) = \mathcal{T}_{1,\sigma}(4, C)$)

\[
\langle \mathcal{L}_1 | = (1 \ 1 \ 1 \ z_v^2 \ z_v \ z_v), \quad \langle \mathcal{L}_2 | = (0 \ 0 \ 0 \ z_v \ 0 \ 1), \quad \langle \mathcal{L}_3 | = (0 \ 0 \ 0 \ z_v \ 1 \ 0).
\]

### Choosing a New Configuration

In order to choose a new configuration of objects on this track, we use the following recursive technique.

**Open Chain**

For an open chain, the state $C_N$ of the leftmost rung is chosen with the probability

\[
p(C_N = i) = \frac{\langle \mathcal{L}_{\sigma_N} | i \rangle \langle i | \mathcal{T}_{N-1} \ldots \mathcal{T}_5 \mathcal{T}_2 \mathcal{T}_1 | \mathcal{R}_{\sigma_i} \rangle}{\sum_i \langle \mathcal{L}_{\sigma_N} | i \rangle \langle i | \mathcal{T}_{N-1} \ldots \mathcal{T}_5 \mathcal{T}_2 \mathcal{T}_1 | \mathcal{R}_{\sigma_i} \rangle},
\]

where $|i\rangle$ are the standard $6 \times 1$ basis vectors. Given this state $i$ of the leftmost rung, the state $S_{N-1}$ of the next rung to the right, is then chosen with the probability

\[
p(C_{N-1} = j) = \frac{\langle \mathcal{L}' | j \rangle \langle j | \mathcal{T}_{N-2} \ldots \mathcal{T}_5 \mathcal{T}_2 \mathcal{T}_1 | \mathcal{R}_{\sigma_j} \rangle}{\sum_j \langle \mathcal{L}' | j \rangle \langle j | \mathcal{T}_{N-2} \ldots \mathcal{T}_5 \mathcal{T}_2 \mathcal{T}_1 | \mathcal{R}_{\sigma_j} \rangle},
\]

where $\langle \mathcal{L}' | = \langle i | \mathcal{T}_{N-1}$, acts as the new left vector. We can then recursively populate the entire track using this procedure. Clearly, starting from a given right vector $|\mathcal{R}_{\sigma_i}\rangle$, depending on the morphology of the rightmost rung, one only needs to store the partial products $\mathcal{T}_L \ldots \mathcal{T}_3 \mathcal{T}_2 \mathcal{T}_1 | \mathcal{R}_{\sigma_i}$, of $6 \times 1$ vectors at each rung in this algorithm.

**Closed Chain**

For a closed chain, the state $S_L$ of the first rung is chosen with the probability

\[
p(C_L = i) = \frac{\langle i | \mathcal{T}_L \ldots \mathcal{T}_3 \mathcal{T}_2 \mathcal{T}_1 | i \rangle}{\sum_i \langle i | \mathcal{T}_L \ldots \mathcal{T}_3 \mathcal{T}_2 \mathcal{T}_1 | i \rangle}.
\]

Given this state $i$ of the first rung, the state $S_{L-1}$ of the next rung to the right is then chosen with the probability

\[
p(C_{L-1} = j) = \frac{\langle i | \mathcal{T}_L | j \rangle \langle j | \mathcal{T}_{L-1} \ldots \mathcal{T}_3 \mathcal{T}_2 \mathcal{T}_1 | i \rangle}{\sum_j \langle i | \mathcal{T}_L | j \rangle \langle j | \mathcal{T}_{L-1} \ldots \mathcal{T}_3 \mathcal{T}_2 \mathcal{T}_1 | i \rangle},
\]

and similarly for the rest of the chain (as for the open chain), until the entire track is filled. Thus, in the case of a closed chain, one needs to store the partial products of $6 \times 6$ matrices at each rung.

We note that the algorithm described above does not reject any configurations. This is particularly useful when studying high density phases, where local algorithms often encounter “jamming”. This algorithm is naturally extendable to updates of wider tracks, where the size and the number of the transfer matrices grows with the number of rows/columns considered.

We also note that this algorithm is quite computationally efficient. For large lattice sizes and high densities, the probability of encountering a periodic track falls rapidly. To update a single open track, only storage of order $6L$
numbers is required in an $L \times L$ system. In the rare cases when we encounter a periodic track, we need storage of order $36L$ to update it. Naturally, the rarity of periodic tracks also implies that the algorithm does not change winding sectors (defined exactly as in the usual dimer model) easily for a large system. This is in principle a draw-back compared to loop algorithms or pocket-algorithms, both of which can be readily generalized for use in the present problem, and may change sectors more easily (we have not explored this in any detail). In our simulations, we always start in the zero-winding sector, and our results for the larger values of $L$ shown in the main text are therefore averages over the zero-winding sector. However, as is well-known in the context of interacting dimer models, the restriction to zero-winding in the microscopic model simply corresponds to periodic boundary conditions for the coarse-grained heights. Therefore, it does not change our conclusions. Finally, we note that a full Monte-Carlo sweep, requiring us to randomly choose $\mathcal{O}(L)$ different tracks and update their interior configurations, requires of order $\mathcal{O}(L^2)$ operations, making the time required comparable to that of other available schemes, while being rejection-free.

### Detailed Balance and Ergodicity

Since the new configurations are chosen with the correct weights from the “restricted” partition function, this algorithm trivially satisfies the detailed balance criterion. The question of ergodicity is more subtle. To check that the algorithm samples all available states of the system, we have performed the following numerical check.

We enumerate all possible states on a $4 \times 4$ lattice with periodic boundary conditions. For the full-packing case (no vacancies), there are 1228 possible configurations of squares and dimers. Using this explicit knowledge of all the states, we monitor the frequency with which each state is sampled in our simulations. We choose activities such that all fully-packed states have unit Boltzmann weight and states with vacancies have zero weight. In this case, we have checked that for a large enough number of Monte Carlo steps, all allowed states are sampled with equal frequency. In addition we have checked that the variance of this frequency decreases as $1/N_{MC}$, where $N_{MC}$ represents the number of Monte Carlo steps. In Fig. 10a, we plot this frequency table for different numbers of Monte Carlo samplings.

We have also enumerated all possible states for this small sample when $v \neq 0$. In this case there are 69941 configurations of dimers, squares and vacancies available to the system. We check explicitly that each one of these states is sampled with the correct probability given by

$$p(C_{dsv}) = \frac{w^{N_d^*} v^{N_v^*}}{\sum_{C_{dsv}} w^{N_d^*} v^{N_v^*}},$$

where $N_d^*$ and $N_v^*$ are the number of dimers and vacancies in the configuration $C_{dsv}$, and $N_d$ and $N_v$ are the number of dimers and vacancies in the configuration $C_{dsv}$. The sum is over all possible configurations of the system. In Fig. 10b, we plot the frequency of the occurrence of each of the 69941 configurations in our simulations, normalized by the above probability. We find that the normalized frequency of each of these states converges to 1, confirming the ergodicity of our algorithm (for small lattice sizes).
ADDIONAL NUMERICAL EVIDENCE

Finally, we use our Monte Carlo update scheme to perform large scale simulations on the lattice gas of dimers and squares on the square lattice. Recent simulations of the hard-square lattice gas have shown the necessity of simulations on large system sizes to fully understand the nature of scaling in such hard-core systems with columnar ordering. The columnar ordered state is relatively unstable to the presence of vacancies, as compared to sublattice ordering, and is characterised by large correlation lengths. We therefore perform simulations on lattices of sizes up to 1024 × 1024 in order to fully elucidate the phase diagram of this system. We use the convention $v = z_v/\sqrt{z_s}$, $w = z_d/z_s^{1/4}$ and $z_s + z_d^2 + z_v^4 = 1$. In our simulations, we focus on three principle directions of the phase diagram (Fig. 2 of main text)

- **I.** The fully-packed boundary $SD$, ($v = 0$) corresponding to the pure squares and dimers mixture. We find that the system exhibits a KT transition from the square-rich columnar ordered phase to a power-law ordered dimer-rich phase above the critical point $w_\ast^c = 0.198(2)$. The details of these results are provided in Fig. 4 (A) and (B) of the main text.

- **II.** A trajectory passing through a generic point on the phase boundary separating the square-rich columnar ordered phase from the disordered squares-dimers-vacancy fluid phase. In our simulations, we move along the trajectory

$$z_d = \alpha z_v,$$

where $\alpha \approx 2.54947$. This corresponds to the trajectory $w = \alpha v(1 + w^2 + v^4)^{1/4}$. We find that in this case the transition is of second order, with a critical point at $P \equiv (w_\ast, v_\ast) = (0.1600(1), 0.0623(1))$. In Fig. 11 we display the critical crossing of $\frac{\langle |\Psi|^2 \rangle_{L^2}}{L^{1/\nu}}$ at this critical point $P$, consistent with Ashkin-Teller behaviour with $\eta = \frac{1}{4}$. Here $\Psi \equiv \sum \psi(\vec{r})$. We find a good collapse of these curves with the scaling exponent $\nu = 1.70(5)$. We also find a critical crossing at this point $P$ of the real part of the order parameter $\Re(L) = \langle (\sum \psi(\vec{r}))^2 \rangle / L^2$ scaled by $L^{2-\eta_2}$, with $\eta_2 = 0.70(5)$. Once again, these curves show a good collapse with the scaling exponent $\nu = 1.70(5)$. These estimates of $\eta_2$ and $\nu$ satisfy $2\nu \approx (1 - \eta_2)^{-1}$, as argued in the main text.

- **III.** The boundary $VS$, ($w = 0$) corresponding to the hard-square lattice gas. Once again, we find a second order transition at the critical point $v_\ast^c = 0.3181(2)$. We display these results in Fig. 12. The figure shows $\frac{\langle |\Psi|^2 \rangle_{L^2}}{L^{1/\nu}}$ vs. $v$ for different values of the system size $L$. The curves show a critical crossing at $v_\ast^c$, consistent with Ashkin-Teller behaviour with $\eta = \frac{1}{4}$. We also show the scaling collapse of these curves with the exponent $\nu = 0.92(2)$.

**FIG. 11:** The phase transition along II, defined in Eq. 10 (Left) $\frac{\langle |\Psi|^2 \rangle_{L^2}}{L^{1/\nu}}$ vs. $v$, for different values of the system size $L$. Here $\Psi \equiv \sum \psi(\vec{r})$. The curves show a critical crossing at $v_\ast^c = 0.0623(1)$. (Inset) Scaling collapse of this data with exponent $\nu = 1.70(5)$ (Right) $\Re(L) = \langle (\sum \psi(\vec{r}))^2 \rangle / L^2$ scaled by $L^{2-\eta_2}$ vs. $v$ for different values of the system size $L$. The curves show a critical crossing at $v_\ast^c$ with $\eta_2 = 0.70(5)$. (Inset) Scaling collapse of $\Re(L)/L^{2-\eta_2}$ with the scaling exponent $\nu = 1.70(5)$. These estimates of $\eta_2$ and $\nu$ satisfy $2\nu \approx (1 - \eta_2)^{-1}$. 

\[\sum \psi(\vec{r})\]
FIG. 12: Phase transition along III (the boundary VS with $w = 0$), corresponding to the hard-square lattice gas. The figure shows $\langle |\Psi|^2 \rangle / L^{7/4} vs. v$ for different values of the system size $L$. The curves show a critical crossing at $v^*_c = 0.3181(2)$, consistent with Ashkin-Teller behaviour with $\eta = 1/4$. (Inset) Scaling collapse of the order parameter with the scaling exponent $\nu = 0.92(2)$.

Our simulations clearly establish the presence of a KT transition between the square-rich columnar ordered phase and a power-law ordered dimer-rich phase along the boundary SD. They also confirm that with the addition of vacancies the transition between the columnar-ordered and disordered fluid phases is consistent with Ashkin-Teller criticality. Our simulations therefore provide clear corroborating evidence for the arguments presented in the main text.