Entropy of fully packed hard rigid rods on d-dimensional hypercubic lattices

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We determine the asymptotic behavior of the entropy of full coverings of a $L \times M$ square lattice by rods of size $k \times 1$ and $1 \times k$, in the limit of large k. We show that full coverage is possible only if at least one of L and M is a multiple of k, and that all allowed configurations can be reached from a standard configuration of all rods being parallel, using only basic flip moves that replace a $k \times k$ square of parallel horizontal rods by vertical rods, and vice versa. In the limit of large k, we show that the entropy per site $S_2(k)$ tends to $Ak^{-2} \ln k$, with $A = 1$. We conjecture, based on a perturbative series expansion, that this large-k behavior of entropy per site is superuniversal and continues to hold on all d-dimensional hypercubic lattices, with $d \geqslant 2$.

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I. INTRODUCTION

Systems of particles with only hard core interactions between them have been studied as prototypical models for phase transitions in equilibrium statistical mechanics as well as for understanding aspects of nonequilibrium statistical mechanics. In equilibrium statistical mechanics, hard sphere systems serve as minimal models of solid to fluid transition in molecular solids [1–3], and in colloidal crystals [4]. Dimer models are equivalent to the Ising model, and anisotropic hard particles can effectively model different phases and phase transitions in liquid crystals [5–10]. In nonequilibrium statistical mechanics, hard core models like symmetric or asymmetric exclusion processes provide basic models for driven systems and jamming in granular systems [11–13].

Lattice models of hard-core particles have been of particular interest, as they are analytically more tractable. The phases of assemblies of particles of many different shapes have been studied. Examples include squares [14–19], triangles [20], hexagons [21], long rods [22–24], rectangles [25–27], Y-shaped molecules [28–30], tetraminoes [31], lattice gases with exclusion up to kth nearest neighbors [32–37], cubes [38], plates [39], etc. An analytical exact solution has been possible only for the case of hard hexagons so far [21]. Phase transitions have also been studied in mixtures of different shapes, for example squares and dimers [17,40], rods of different lengths [41,42], polydispersed spheres [43], etc. For the mixture of squares and dimers, it was shown that the critical exponents of the order-disorder transition depend continuously on the relative concentration of the components. Despite a long history, many basic questions about these systems remain open; for example, for a given shape of particles, what are the possible ordered phases, and in which sequence will they appear on increasing the density?

Systems of hard rods and cylinders have attracted a lot of interest, starting with the pioneering work of Onsager, who showed that a system of thin, long cylinders in a three-dimensional continuum undergoes a phase transition from a disordered phase to an orientationally ordered nematic phase [45]. The study of lattice models of linear $k \times 1$ hard rods (k-mers) started with the work of Flory [22] and Zwanzig [44]. On a d-dimensional hypercubic lattice, rods can only orient in one of the d directions. It was realized in Ref. [23], based on Monte Carlo simulations and high-density expansions, that nematic order is present at intermediate densities for large enough k, and that the lattice model at high densities must undergo a second disordering transition at a critical density $1 - \rho_c \sim k^{-2}$ for large k, when the nematic order is lost. Usual Monte Carlo techniques with local moves are rather inefficient in sampling states at high density due to high rates of rejection of moves due to jamming, but recently introduced strip-update Monte Carlo technique has made it possible to reach densities within a few percent of maximum packing density [46,47]. Using these techniques, it is found that on the square lattice, for $k < 6$, there is no phase transition, but for $k > 6$, as density is increased, there are three phases: a low-density disordered phase, an intermediate-density nematic phase, and a high-density phase in which there is no long ranged positional or orientational order [47]. The existence of the transition may be rigorously proved [48]. The first phase transition belongs to the Ising [49–51] or three-state Potts universality classes [49,50,52] depending on whether the rods are on a square or triangular or honeycomb lattice. The nature of the second transition is not so clear. There is some indication of the high-density phase having power law correlations [47] with the second transition not being in the Ising universality class [47,53], while the exact solution of soft repulsive rods on a treelike lattice [54] suggests otherwise. More recently, the transitions in two

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dimensions have been studied using measures such as the classical "entanglement" entropy, mutability, Shannon entropy, and data compression [53,55,56].

In three dimensions, there is no phase transition for $k \leqslant 4$. For $k \geqslant 7$, the system undergoes phase transitions from disordered to nematic to a layered disordered phase as density is increased. In the layered disordered phase, the system breaks up into very weakly interacting two-dimensional planes within which the rods are disordered. For $4 < k < 7$, there is no nematic phase, and a single phase transition from a disordered to a layered disordered phase [57,58].

In this paper, we focus on the fully packed limit of linear rods on the square lattice and give heuristic arguments to extend the results to higher dimensions. In particular, we focus on the entropy per site $S_d(k)$. We note that, in addition to understanding phase transitions in lattice systems of rods with finite density of vacancies, the study of the fully packed phase is relevant for other physical systems. For instance, it would help us understand the tetratic order in self-assembly of squares and rectangles in the continuum [59]. It may also help in our understanding of phase transitions in other strongly correlated systems. For example, the binding-unbinding transition of quarks as a function of the density of hadrons in nuclear matter, studied in QCD, is similar to the binding-unbinding transition of k species of holes during the transition from the disordered high-density phase to the nematic phase of k-mers.

For the case of dimers ($k = 2$)—the only case that is exactly solvable [60–63]—the entropy per site for the square lattice is $S_2(2) = G/\pi = 0.29156\ldots$, where G is Catalan's constant [60]. On the square lattice, the orientation-orientation correlation of two dimers separated by a distance r decays as a power law $r^{-1/2}$ for large r [64], while on a triangular lattice these correlations are short ranged [65]. A review of the method of solution of dimer problems on planar lattices may be found in Ref. [66]. In three dimensions, there is a class of lattices (not cubic lattice) for which an exact solution can be found and the correlations are strictly finite ranged [67], while for the cubic lattice the orientational correlations decay as a power law [6]. The entropy of fully packed trimer ($k = 3$) tilings on a square lattice have also been studied [68]. By numerically diagonalizing the transfer matrices for strips, the entropy per site was found to be $S_2(3) = 0.158\,520 \pm 0.000\,015$. Much less is known for higher values of k. It is known that the tilings admit a vector height field representation [69]. For larger values of k, Gagunashvili and Priezzhev obtained an upper bound for the entropy on the square lattice: $S_2(k) \leqslant k^{-2}\ln(\gamma k)$, where $\gamma = \exp(4G/\pi)/2$, with G being Catalan's constant [70]. It is clear that the full packing constraint induces strong correlations in the orientations of rods, and one would generally expect orientation-orientation correlations to decrease with distance as a power law.

The full packing constraint severely limits the allowed configurations. One way to generate a large number of such configurations, satisfying all these constraints, is to break the system into parallel two-dimensional layers, and fully pack each layer with rods. Since rods on different layers do not interact, configurations on different layers can be independently generated, giving a large entropy. Indeed, there is evidence from Monte Carlo simulations (the simulations are done not at full packing, but for densities close to full packing) that the high-density phase of long rods in three dimensions shows two-dimensional layering [57], and our perturbation expansion suggests that, in the fully packed limit, configurations in even higher dimensions would be dominated by layered two-dimensional configurations.

In this paper, we determine the asymptotic behavior of the entropy of the fully packed configurations in the limit of large rod lengths k: first in two dimensions, and then generalized to higher dimensions. The number of coverings depends strongly on the boundary conditions imposed. We will consider configurations of a finite $L \times M$ rectangular portion of a square lattice fully covered by rectangles of size $k \times 1$ or $1 \times k$. Equivalently, we can consider this a lattice model, with all sites covered using straight rigid rods of length k. We will call this open boundary conditions. We prove that full coverage in the open boundary case is possible only if at least one of L and M is a multiple of k. All the allowed configurations for this case can be reached from the standard configuration of all horizontal rods, using only basic flip moves that flip a $k \times k$ square of parallel horizontal rods by vertical rods, and vice versa. Using rigorous upper and lower bound estimates, we show that $S_2(k)$, to leading order in k, equals $Ak^{-2}\ln k$ with $A = 1$.

Based on a perturbation series expansion, we conjecture that in higher dimensions the entropy for the fully packed phase, for large k, would be dominated by configurations where the rods arrange themselves in stacked two-dimensional layers. Thus, we conjecture that the large-k behavior of entropy per site is "superuniversal," and continues to hold on d-dimensional hypercubical lattices for all $d > 2$ and

$$\lim_{k\to\infty} \frac{k^2 S_d(k)}{\ln k} = 1, \tag{1}$$

independent of d.

The remainder of the paper is organized as follows. In Sec. II, we define the problem precisely. We derive some basic properties of the fully packed phase by showing that an $L \times M$ rectangle can be completely covered by k-mers, only if at least one of L or M is a multiple of k and that all full packing configurations on an open $L \times M$ rectangle can be obtained from the standard configuration of all horizontal rods by a combination of basic flip moves. In Sec. III, we obtain lower bounds for entropy by solving exactly for the entropy of rods on semi-infinite strips $k \times \infty$ and $2k \times \infty$. These results are generalized to arbitrary strips $lk \times \infty$ by considering truncated generating functions. In Sec. IV, we combine the lower bounds for entropy with existing upper bounds to obtain Eq. (1). In Sec. V, we use heuristic arguments based on perturbation theory to support the conjecture that that this result should also hold for all d-dimensional hypercubical lattices with $d > 2$. Section VI contains some concluding remarks.

II. PRELIMINARIES

We consider tilings of a $L \times M$ rectangle, with L, M positive integers, by $k \times 1$ and $1 \times k$ rectangles (k-mers). Each k-mer can only be in one of two orientations: horizontal or

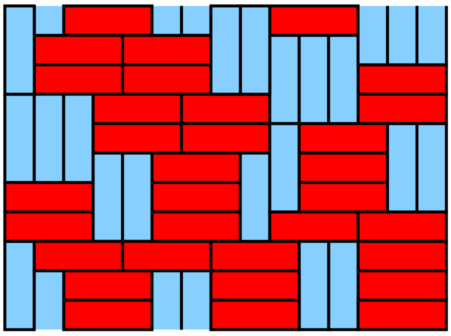

FIG. 1. A tiling of the Euclidean plane by k-mers, with $k = 3$. Only a part of the tiling is shown here, and some k-mers do not fully fall in the region shown.

vertical. An example is shown in Fig. 1 for the case $k = 3$. Equivalently, we can consider this a lattice model, with all sites covered using straight rigid rods of length k. Let $N(L, M)$ be the number of such tilings.

A. Divisibility of L, M by k

We first show that $N(L, M)$ is nonzero, if and only if at least one of L and M is divisible by k. The "if" part is trivial. For the other part, clearly LM has to be a multiple of k, for full coverage. We now argue that in this case at least one of L and M has to be a multiple of k.

Assign one of the k colors, called here $0, 1, 2, \dots, (k-1)$, to each of the squares of the lattice, with square (x, y) given color $q = (x - y) \mod k$. The coloring of the squares for the case $k = 3$ is shown in Fig. 2. Then each k-mer covers exactly one square of each color. Let $L = k\,\ell + \alpha$, $M = k\,m + \beta$, with $0 < \alpha, \beta \leqslant k - 1$. Divide the rectangle into three smaller rectangles of sizes $k\ell \times M, \alpha \times km$, and $\alpha \times \beta$, as shown in Fig. 3. Then, clearly the rectangles of size $k\ell \times M$ and $\alpha \times km$ can be covered by k-mers, implying that the numbers of squares of different colors in these two rectangles are equal. However, the small rectangle of size $\alpha \times \beta$ has $\min(\alpha, \beta)$ squares of same color along the diagonal. To cover them would require at least $\min(\alpha, \beta)$ rods, with total area $k \min(\alpha, \beta)$. Equating this to the total area $\alpha\beta$, we obtain $k = \max(\alpha, \beta)$. This contradicts the assumption that $\alpha, \beta < k$. Hence, the rectangle cannot be fully covered by k-mers, unless either L or M is divisible by k.

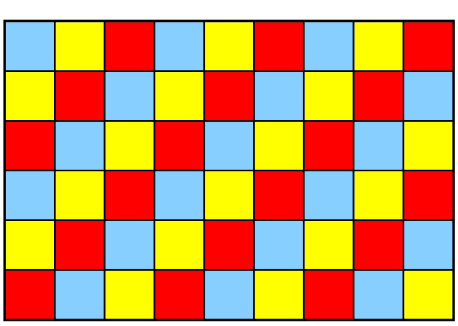

FIG. 2. Assigning colors to 1×1 squares for the case $k = 3$.

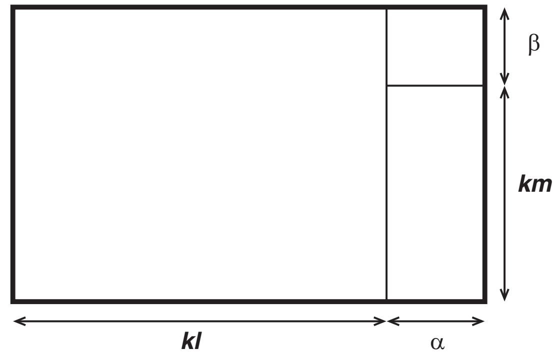

FIG. 3. Dividing an $(k\ell + \alpha) \times (km + \beta)$ rectangle, where $0 < \alpha$, $\beta \leqslant k - 1$, into smaller rectangles.

For simplicity of presentation, in the following, we shall assume that both L and M are multiples of k.

B. Ergodicity of the flip moves

In this subsection, we show that all configurations of rods can be reached from any configurations by just using the flip move (defined below).

We define the standard tiling configuration of a $k\ell \times M$ rectangle by k-mers as one using only horizontal k-mers. A basic flip move is defined as replacing a $k \times k$ square filled with vertical k-mers by one with horizontal k-mers, and vice versa, as illustrated in Fig. 4.

A combination of two flip moves defines a "slide" move, where a vertical k-mer next to a $k \times k$ flippable square exchanges position (see Fig. 5), and the vertical k-mer will be said to slide across the flippable square.

We now argue that any full tiling of a $k\ell \times M$ rectangle by k-mers may be reached from the standard configuration by using only the basic flip and slide moves.

Proof. Look at the lowest row. If it consists of only horizontal k-mers, then we ignore this row, and the problem reduces to one with a smaller M. Else, it would have $\ell' = \ell - \Delta$ horizontal k-mers, and $k\Delta$ vertical k-mers. In Fig. 6, we have shown an example of a 4-mer tiling of a 48×12 rectangle, where $\ell = 12$, $\Delta = 1$. We move to the left any $k \times k$ block of horizontal flippable rods we find between these $k\Delta$ vertical k-mers, using the slide move, and make the vertical rods closer to each other. If now there is any block of consecutive vertical k-mers, we can flip these to horizontal, and reduce the problem to one with a fewer number of vertical k-mers.

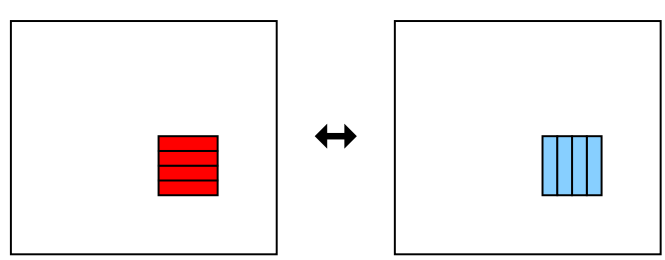

FIG. 4. The basic flip moves consist of replacing a small $k \times k$ square in the configuration covered by k horizontal k-mers, by vertical k-mers, and vice versa.

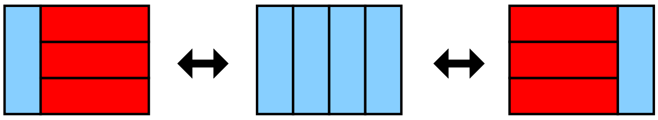

FIG. 5. The slide move consists of transposing a rod and an adjacent flippable square, i.e., sliding the rod across the square, which may be thought of as a combination of two flip moves.

If there is no such horizontal flippable block of rods, we look at the bottom row. Let us say that it has segments of $i_1, i_2, \dots, i_s$ horizontal rods, interspersed with vertical rods. (In Fig. 6, there are four segments, with $i_1 = 1, i_2 = 3, i_3 = 4, i_4 = 3$). Clearly, these are bordered by vertical k-mers at the ends, unless the segment itself is at the end of the rectangle. Then we look at the subrectangles of sizes $i_1 k \times M, i_2 k \times M, \dots$ made up of these segments and bounded by vertical boundaries. In the example shown in Fig. 6, these rectangles are shown with orange boundaries.

We now argue that there will be a flippable $k \times k$ block within each of these small rectangles. This is clear if the width of the rectangle is exactly k. Then the sites just above can only be covered by a horizontal rod, or k vertical rods. In the latter case, it forms a vertical flippable rectangle. If not, then eventually, we will have k horizontal rods just above each other, and form a horizontal flippable rectangle.

If the width is greater than k, and the row just above is not made of all horizontal rods, then it will be made up of a number of horizontal segments, separated by vertical rods. And we can repeat the argument with this smaller set. This process cannot continue for ever, as the total width is finite, and the width decreases at each step.

Thus, we will be able to find a flippable $k \times k$ box at each stage, and eventually the number of vertical rods becomes zero, and the standard tiling of all horizontal k-mers is reached. Since all moves are reversible, and any valid configuration of full packing can be changed to standard configuration, we can go from any full packing configuration on the rectangle to any other using only flip moves.

III. LOWER BOUND FOR ENTROPY FOR LARGE k

We first show that at full packing there is a finite entropy per site. We divide the lattice into $k \times k$ squares. There are LM/k^2 such squares, and each can be tiled in two ways, independent of the others. Then the total number of such tilings is $2^{LM/k^2}$ (see Fig. 7). Of course, more complicated tilings are possible, as shown in Fig. 1, and the above only provides a lower bound. We define entropy per site:

$$S_2(k) = \lim_{L,M\to\infty} \frac{\ln N(L,M)}{LM}. \tag{2}$$

Then, $S_2(k) \geqslant k^{-2} \ln 2$.

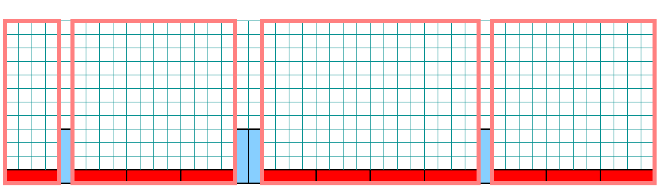

FIG. 6. A tiling of a 48×12 rectangle with rods of length $k = 4$, where only the rods in the bottom row are shown. The vertical rods split the rectangles into smaller rectangles, and aid in finding a block of flippable k-mers (see text for details).

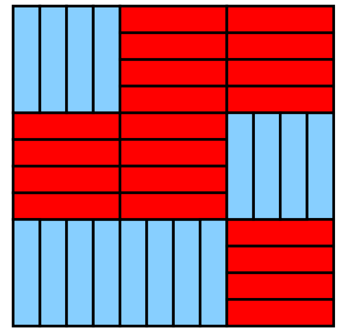

FIG. 7. Dividing a rectangle into $k \times k$ squares (here, $k = 4$).

A. Entropy of strips $k \times \infty$

We can easily obtain a better lower bound on $S_2(k)$. Break the $L \times kM$ lattice in M strips of width k each. Let $N(L,k)$ be denoted by F_L. Since by breaking into strips of width k we disallow configurations where rods cross the boundary, leading to undercounting, we obtain the inequality

$$N(L,kM) \geqslant [F_L]^M. \tag{3}$$

F_L obeys a simple recursion relation. Consider the packing of a $k \times L$ rectangle. The first row can be covered by a horizontal k-mer (reducing L by one) or the first $k \times k$ square can be covered by k parallel vertical k-mers (reducing L by k). Thus, F_L's satisfy the recursion relation

$$F_L = F_{L-1} + F_{L-k}. \tag{4}$$

This implies that F_L increases as λ^L where λ is the largest root of the equation

$$\lambda^k = \lambda^{k-1} + 1. \tag{5}$$

For large k, to leading order $\lambda = 1$. A little bit of algebra shows that in the limit of large k the subleading terms take the form

$$\lambda = 1 + \frac{W(k)}{k} + \mathcal{O}(k^{-2}), \tag{6}$$

where $W(k)$ is the solution of the equation

$$W(k)\exp[W(k)] = k. \tag{7}$$

The function $W(k)$ is called the Lambert function [71]. To leading order, $W(k) \sim \ln k$ for large k [to see this, take the logarithm on both sides of Eq. (7) and compare the terms of leading order]. The subleading term can be similarly obtained to give for large k

$$W(k) \approx \ln\left(\frac{k}{\ln k}\right), \tag{8}$$

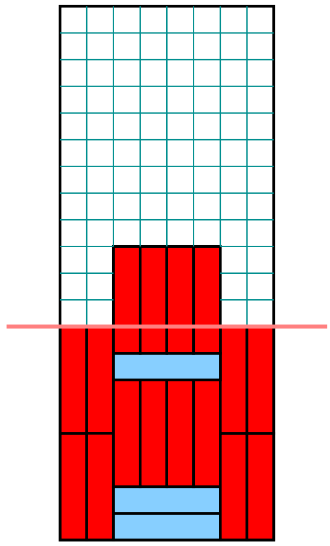

FIG. 8. A partial filling of the strip $2k \times \infty$ by rods for the case $k = 4$. The horizontal red line shows the reference line. The boundary of the configuration is specified by the projection to the top of the reference line—in this case $\{0, 0, 3, 3, 3, 3, 0, 0\}$, or in a more compact notation $\{0^2 3^4 0^2\}$.

with corrections that only grow slower than $\ln(\ln k)$. Thus we obtain

$$\lambda = 1 + \frac{1}{k} \ln\left(\frac{k}{\ln k}\right) + \text{higher-order terms}. \tag{9}$$

The entropy per site for the $k \times \infty$ strip is $(\ln \lambda)/k$. Thus,

$$S_{k\times\infty} = \frac{\ln k}{k^2}\left(1 - \frac{\ln \ln k}{\ln k} + \dots\right). \tag{10}$$

Since $S_{k\times\infty}$ is a lower bound for $S_2(k)$, we obtain the leading behavior:

$$\lim_{k\to\infty} \frac{k^2 S_2(k)}{\ln k} \geqslant 1. \tag{11}$$

B. Entropy of strips $2k \times \infty$

In this subsection, we describe the exact calculation of the entropy of tilings of the semi-infinite $2k \times \infty$ stripe with k-mers, where the y coordinate is $\geqslant 1$, and the x coordinate lies in the range $[1, 2k]$. We define the generating function $\Omega_{2k}(x)$ as the sum over all covering of rectangles of size $2k \times r$, summed over all positive integer values of r, where the weight of a covering with n tiles is z^n. Then, we have

$$\Omega_{2k}(z) = \sum_{r=0}^{\infty} N(2k, r) z^{2r}. \tag{12}$$

We also define a partial covering of the strip with rods below some reference line $y = s > 0$, so that no site with y coordinate less than s is left uncovered (see Fig. 8), and all rods must cover at least one site with y coordinate less than s. Clearly, all rods that do not lie completely below $y = s$ must be vertical. A partial covering is a rectangular covering if and only if no site with y coordinate larger than s is covered.

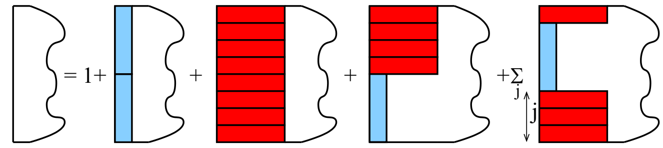

FIG. 9. Recursion equation for $\Psi(\{0^{2k}\})$, shown for $k = 4$. Each subfigure is rotated clockwise by 90° for conserving space. The jagged boundary at the right end indicates summing over all possible configurations on the right.

A partial covering may be characterized by its top boundary $\{h_x\}$, for $x = 1$ to $2k$, where h_x specifies how many sites to the top of the reference line $y = s$ are covered in the column with coordinate x. We will choose s to be as large as possible, so that at least one of the h_x's has to be zero, and $h_x \leqslant k - 1$, for all x. For example, the boundary of the configuration shown in Fig. 8 is specified by $\{0, 0, 3, 3, 3, 3, 0, 0\}$. In a more compact notation, we will write this as $\{0^2 3^4 0^2\}$.

Not all height configurations are allowed. A bit of thought shows that for a partial covering of the $2k \times L$ stripe the only allowed height configurations are $\{0^{2k}\}$, $\{h^k 0^k\}$, $\{0^k h^k\}$, $\{h^j 0^k h^{k-j}\}$, and $\{0^j h^k 0^{k-j}\}$, with h and j taking values from 1 to $k - 1$.

We define the generating functions $\psi(\{h_j\})$ as the generating function of all possible ways of completing a partial tiling with a given height profile $\{h_j\}$, where the completed covering is rectangular, and the weight of the tiling in which we add n extra rods is z^n. Therefore, for example,

$$\psi(\{0^{2k}\}) = \Omega_{2k}(z) = 1 + z^2 + z^4 + \cdots, \tag{13}$$

$$\psi(\{0^k 1^k\}) = z + z^3 + \cdots. \tag{14}$$

Consider a particular height configuration $\{h_x\}$. We can write recursion equations for the corresponding generating function $\psi(\{h_x\})$, by considering all possible ways of filling the column of sites immediately to the top of the reference line by k-mers, such that the top edge of the full tiling is horizontal, and no sites are left uncovered.

For example, it is easily seen that (see Fig. 9)

$$\begin{aligned}\Psi(\{0^{2k}\}) = {} & 1 + (z^2 + z^{2k})\Psi(\{0^{2k}\}) + 2z^{k+1}\Psi(\{0^k(k-1)^k\}) \\ & + \sum_{j=1}^{k-1} z^{k+1}\Psi(\{(k-1)^j 0^k (k-1)^{k-j}\}).\end{aligned} \tag{15}$$

The different terms in this equation correspond to the cases where the next row is left empty, or filled by two horizontal rods, or by $2k$ vertical rods, or by first j vertical rods, then a horizontal rod, then $k - j$ vertical rods.

Writing such generating functions for all possible height configurations, we obtain a set of inhomogeneous linear equations in approximately $2k^2$ variables. This may be written as a transfer matrix of dimension $2k^2 \times 2k^2$. However, using the symmetries of the problem, this number can be considerably reduced.

We note that the recursion equation for the generating function $\Psi(\{h^j 0^k h^{k-j}\}$ is

$$\Psi(\{h^j 0^k h^{k-j}\} = z\Psi(\{(h-1)^j 0^k (h-1)^{k-j}\}) + z^k \Psi(\{0^j (k-h)^k 0^{k-j}\}), \quad 1 \leqslant h < k. \tag{16}$$

This equation has no j dependence. Hence, we may expect that $\Psi(\{h^j 0^k h^{k-j}\}$ is independent of j. It can be checked that this ansatz is consistent with the remaining recursion equations. Similarly, we find that $\Psi(\{0^j h^k 0^{k-j}\})$ is also independent of j. With this simplification, the number of independent variables reduces to approximately $2k$.

The remaining recursion equations are easily written down; we obtain for all $1 \leqslant h \leqslant k-1$

$$\Psi(\{0^j h^k 0^{k-j}\}) = z^k \Psi(\{(k-h)^j 0^k (k-h)^{k-j}\}), \tag{17}$$

and

$$\Psi(\{0^k h^k\}) = z\Psi(\{0^k (h-1)^k) + z^k \Psi(\{0^k (k-h)^k\}). \tag{18}$$

Substituting for $\Psi(\{0^j (k-h)^k 0^{k-j}\})$ in Eq. (16) from Eq. (17), we obtain

$$\Psi(\{h^j 0^k h^{k-j}\} = \frac{z}{(1-z^{2k})} \Psi(\{(h-1)^j 0^k (h-1)^{k-j}\}, \tag{19}$$

which is immediately solved to give

$$\Psi(\{h^j 0^k h^{k-j}\}) = \frac{z^h}{(1-z^{2k})^h} \Psi(\{0^{2k}\}), \quad 1 \leqslant h, j \leqslant k-1. \tag{20}$$

Substituting for $\Psi(\{(k-1)^j 0^k (k-1)^{k-j}\})$ in Eq. (15) from Eq. (20) and simplifying, we obtain

$$[1 - z^2 - z^{2k} - (k-1)z^{2k}(1-z^{2k})^{-k+1}]\Psi(\{0^{2k}\}) = 1 + 2z^{k+1}\Psi(\{0^k (k-1)^k\}). \tag{21}$$

To close the equations, we have to determine $\Psi(\{0^k h^k\})$ in terms of $\Psi(\{0^{2k}\})$. The values of $\Psi(\{0^k h^k\})$ for one value of h are related by Eq. (18) to arguments $(h-1)$ and to $(k-h)$. This seems complicated, but it is easily checked that the ansatz

$$\Psi(\{0^k h^k\}) = C\alpha^h + D\alpha^{-h}, \quad \text{for} \quad 0 \leqslant h \leqslant k-1 \tag{22}$$

satisfies Eq. (18), so long as

$$\left(1 - \frac{z}{\alpha}\right)C = z^k \alpha^{-k} D, \quad (1 - z\alpha)D = z^k \alpha^k C. \tag{23}$$

Eliminating C/D from Eq. (23), we obtain

$$(1 - \alpha z)\left(1 - \frac{z}{\alpha}\right) = z^{2k}. \tag{24}$$

This is a quadratic equation in α, and determines α for any given value of z. Explicitly, we obtain

$$\alpha^{\pm 1} = \frac{1 + z^2 - z^{2k} \pm \sqrt{[(1-z)^2 - z^{2k}][(1+z)^2 - z^{2k}]}}{2z}. \tag{25}$$

Using Eq. (23), we can express C and D in terms of a single variable κ:

$$C = \kappa \alpha^{-k/2} \sqrt{1 - z\alpha}, \tag{26}$$

$$D = \kappa \alpha^{k/2} \sqrt{1 - z/\alpha}. \tag{27}$$

The actual values of C and D can be determined from the boundary condition at $h = 0$:

$$C + D = \Psi(\{0^{2k}\}). \tag{28}$$

We obtain

$$\kappa = \frac{\Psi(\{0^{2k}\})}{\alpha^{-k/2}(1 - z\alpha)^{1/2} + \alpha^{k/2}(1 - z/\alpha)^{1/2}}. \tag{29}$$

Substituting for κ in Eqs. (26) and (27), we obtain C and D in terms of z:

$$C = \frac{1 - z\alpha}{1 - z\alpha + z^k \alpha^k} \Psi(\{0^{2k}\}), \tag{30}$$

$$D = \frac{\alpha^k z^k}{1 - z\alpha + z^k \alpha^k} \Psi(\{0^{2k}\}). \tag{31}$$

Finally, substituting the value of C and D in Eq. (22), we obtain

$$\psi(\{0^k (k-1)^k\}) = \frac{(1 - z\alpha)\alpha^{k-1} + z^k \alpha}{1 - z\alpha + z^k \alpha^k} \Psi(\{0^{2k}\}). \tag{32}$$

Equation (32) may be simplified by substituting for z^k from Eq. (24):

$$\Psi(\{0^k (k-1)^k\}) = \Psi(\{0^{2k}\}) \left[\frac{\alpha^{k/2-1}\sqrt{1 - z\alpha} + \alpha^{-k/2+1}\sqrt{1 - z/\alpha}}{\alpha^{-k/2}\sqrt{1 - z\alpha} + \alpha^{k/2}\sqrt{1 - z/\alpha}} \right]. \tag{33}$$

Note the explicit symmetry of the expression under the exchange of $\alpha \leftrightarrow 1/\alpha$.

Substituting the expressions for α, $\Psi(\{0^k (k-1)^k\})$ in Eq. (21), we obtain an explicit expression for $\Psi(\{0^{2k}\})$ of the form

$$\Psi(\{0^{2k}\}) = \frac{1}{E(z)}, \tag{34}$$

where the denominator $E(z)$ equals

$$E(z) = 1 - z^2 - z^{2k} - \frac{(k-1)z^{2k}}{(1 - z^{2k})^{k-1}} - 2z^{k+1} \left[\frac{\alpha^{k/2-1}\sqrt{1 - z\alpha} + \alpha^{-k/2+1}\sqrt{1 - z/\alpha}}{\alpha^{-k/2}\sqrt{1 - z\alpha} + \alpha^{k/2}\sqrt{1 - z/\alpha}} \right]. \tag{35}$$

The entropy $S_{2k\times\infty}$ is given by $-k^{-1} \ln z^*_{2k}$, where z^*_{2k} is the singularity of $\Psi(\{0^{2k}\})$ that is closest to the origin. We will show below that asymptotic behavior of entropy for strips of width $2k$ is the same as that of strips of width k. The explicit values of the entropies for strips $k \times \infty$ and $2k \times \infty$ for k up to 2^{31} are given in Table I, and compared with the asymptotic result $k^{-2} \ln k$ in Eq. (1).

We now determine the leading singularity z^*_{2k} of $\Psi(\{0^{2k}\})$ in the limit $k \gg 1$. To do so, consider the denominator $E(z)$. It has a square root singularity at z_c when the discriminant in Eq. (25) equals zero. By factorizing the discriminant and writing in terms of the modulus of z_c, we obtain that z_c satisfies the equation

$$1 - z_c - z_c^k = 0, \tag{36}$$

TABLE I. Entropy S for full packing of rods of length k on strips $k \times \infty$ and $2k \times \infty$, compared with the leading asymptotic result $k^{-2} \ln k$ in Eq. (1).

k	$S_{k\times\infty}$	$S_{2k\times\infty}$	$k^{-2}\ln k$
2^1	2.406059×10^{-1}	2.609982×10^{-1}	1.732868×10^{-1}
2^3	2.608540×10^{-2}	2.929916×10^{-2}	3.249127×10^{-2}
2^5	2.503880×10^{-3}	2.797511×10^{-3}	3.384508×10^{-3}
2^7	2.190142×10^{-4}	2.429123×10^{-4}	2.961444×10^{-4}
2^9	1.791444×10^{-5}	1.975853×10^{-5}	2.379732×10^{-05}
2^{11}	1.396705×10^{-6}	1.532938×10^{-6}	1.817851×10^{-06}
2^{13}	1.051617×10^{-7}	1.148760×10^{-7}	1.342731×10^{-07}
2^{15}	7.714252×10^{-9}	8.388809×10^{-9}	9.683154×10^{-09}
2^{17}	5.546713×10^{-10}	6.006134×10^{-10}	6.858901×10^{-10}
2^{19}	3.925774×10^{-11}	4.234237×10^{-11}	4.791144×10^{-11}
2^{21}	2.743428×10^{-12}	2.948320×10^{-12}	3.309672×10^{-12}
2^{23}	1.897264×10^{-13}	2.032237×10^{-13}	2.265549×10^{-13}
2^{25}	1.300702×10^{-14}	1.389037×10^{-14}	1.539096×10^{-14}
2^{27}	8.851686×10^{-16}	9.426769×10^{-16}	1.038890×10^{-15}
2^{29}	5.985929×10^{-17}	6.358717×10^{-17}	6.974028×10^{-17}
2^{31}	4.025907×10^{-18}	4.266698×10^{-18}	4.659372×10^{-18}

identical to that satisfied by z^* for the strip $k \times \infty$ [see Eq. (5) with $\lambda = 1/z$]. For large k, it has the solution

$$\ln z_c = -\frac{\ln k}{k}\left(1 - \frac{\ln \ln k}{\ln k} + \cdots\right), \quad k \gg 1. \tag{37}$$

We now show that $E(z)$ has a zero at $z^*_{2k} \lesssim z_c$. Following a bit of algebra, it can be shown that

$$E(z_c) = \frac{-(k-1)z_c(1-z_c)}{(2-z_c)^{k-1}} \approx \frac{-\ln k}{k}, \quad k \gg 1. \tag{38}$$

Clearly, $E(z_c) < 0$, as $z_c < 1$. At the same time, it is clear that $E(0) = 1$ since $\Psi(\{0^{2k}\})|_{z=0} = 1$. Therefore, there must be a zero z^*_{2k} in $(0, z_c)$, leading to a higher entropy for strips $2k \times \infty$, as evident in Table I. Also as $E(z_c) \to 0$ for large k, we expect that $z^*_{2k} \to z_c$ for large k.

We now show that the leading behaviors of z^*_{2k} and z_c are identical for large k. We look for solutions

$$z^*_{2k} = e^{-\eta/k}, \tag{39}$$

where $\eta/k^\theta \to 0$ for any $\theta > 0$, and $\eta \to \infty$ for $k \gg 1$. In this limit, $\alpha \approx 1 + \sqrt{4\eta/k}$, and after some algebra $E(z^*)$ may be simplified to give

$$E(z^*_{2k}) \approx \frac{2\eta}{k} - ke^{-2\eta} - 2e^{-\eta}. \tag{40}$$

Equating $E(z^*_{2k})$ to zero, we obtain

$$\frac{2\eta}{k} = ke^{-2\eta} + 2e^{-\eta}. \tag{41}$$

From direct substitution, it is straightforward to check that Eq. (41) is satisfied to leading order by $\eta = \ln k[1 - \ln(\ln k)/(2\ln k]$. Equation (39) then gives

$$\ln z^*_{2k} = -\frac{\ln k}{k}\left[1 - \frac{\ln \ln k}{2\ln k} + \text{lower-order terms}\right]. \tag{42}$$

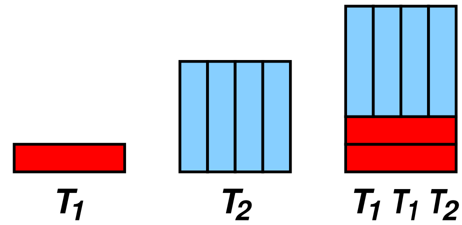

FIG. 10. A schematic diagram illustrating the procedure of vertical concatenation. Here T_1 and T_2 are two admissible tilings, and the concatenated tiling $T_1T_1T_2$ is obtained by putting two T_1s and one T_2 from bottom to top in the specified order.

Since the entropy is given by $-\ln z^*_{2k}/k$, we obtain

$$S_{2k\times\infty} = \frac{\ln k}{k^2}\left(1 - \frac{\ln \ln k}{2\ln k} + \cdots\right). \tag{43}$$

The leading behavior of $S_{2k\times\infty}$ coincides with that of $S_{k\times\infty}$ [see Eq. (10)]. The subleading term is different. We thus obtain the same lower bound as given in Eq. (11).

C. Entropy of strips $L \times \infty$

For general $L \times \infty$, though one can write down the recursion relations obeyed by different generating functions, it is not possible to find a closed form solution for them. Here, we provide an alternate analysis by determining a lower bound for the asymptotic behavior of entropy of $L \times \infty$ strips, which will happen to coincide with the exact results for the strips $k \times \infty$ and $2k \times \infty$

We define the generating function

$$\Omega_L(z) = \sum_{M=0}^{\infty} N(L, M) z^{LM/k}, \tag{44}$$

with $N(L, 0) = 1$, by convention. Then, by direct enumeration,

$$\Omega_1(z) = 1 + z + z^2 + z^3 + \cdots, \tag{45}$$

$$\Omega_2(z) = 1 + z^2 + z^4 + z^6 + \cdots, \; k > 2. \tag{46}$$

$\Omega_L(z)$ is the sum of weights of all configurations of rods on a semi-infinite strip of width L, with the weight of a configuration of n rods being z^n. We have the further constraint that all rods must lie fully in a rectangular region, with both bottom and top edge horizontal, and no uncovered regions within the rectangle. As a slightly more complicated example, it is easily seen that $\Omega_k(z)$ is the generating function for $k \times \infty$ strips, and hence,

$$\Omega_k(z) = \frac{1}{1 - z - z^k}. \tag{47}$$

In determining admissible tilings, a useful concept is that of *concatenation*. Given two tilings of rectangles of sizes $L \times M_1$ and $L \times M_2$, we define the vertical concatenation of these tilings as the tiling of size $L \times (M_1 + M_2)$, obtained by just putting the rectangles on top of each other in the order of concatenation. An illustration of vertical concatenation of three tilings is shown in Fig. 10. A horizontal concatenation is defined similarly.

A tiling is said to be vertically indecomposable, if it cannot be expressed as a vertical concatenation of two admissible tilings. For a vertically decomposable tiling, there is a horizontal line that divides the rectangle into two smaller tilings, such that no rod crosses the horizontal line.

We now define $R_L(z)$ as the sum of weights of all vertically indecomposable tilings of rectangles of width L. Clearly, $R_L(z)$ is a series in powers of z, with all coefficients as nonnegative integers. Then, we have

$$\Omega_L(z) = \frac{1}{1 - R_L(z)}. \tag{48}$$

Let the radius of convergence of the power series of $\Omega_L(z)$ be z_L^*. Then,

$$R_L(z_L^*) = 1. \tag{49}$$

Since $R_L(z)$ is a series of positive coefficients, we may truncate the series at any order, and obtain an upper bound estimate of z_L^*, and hence of z^*, the limit of z_L^*, for large L. This, in turn, will provide a lower bound for the entropy.

We will take L to be a multiple of k, as these give the best bounds. The simplest case is $L = k$. In this case, $R_k(z)$ is a finite polynomial, and we have

$$R_k(z) = z + z^k. \tag{50}$$

We see that this is consistent with Eq. (47).

Now, let us consider the more complicated case $L = 2k$. In this case, $R_{2k}(z)$ is not a finite polynomial. But it has an interesting structure: the lowest order term is z^2, corresponding to a configuration of two horizontal k-mers side by side. But, then terms of order $z^4, z^6, \ldots$ are all zero, as the corresponding tilings are decomposable. The first nonzero term is of order z^{2k}, which corresponds to configurations consisting of a plaquette of k aligned horizontal rods and k vertical rods tiling the remaining area, and another of $2k$ vertical k-mers. With a small amount of brute force enumeration, it is easily seen that the plaquette can be placed in $(k+1)$ ways to give

$$R_{2k}(z) = z^2 + (k+2)z^{2k} + \mathcal{O}(z^{2k+2}). \tag{51}$$

If we truncate the equation at order z^{2k}, we obtain an upper bound estimate for z_{2k}^*. It turns out that for large k the terms that have been dropped make only a negligible contribution to $R_{2k}(z)$ at $z = z_{2k}^*$. We will verify this claim later. First, we solve the truncated equation for z_{2k}^*:

$$z_{2k}^{*2} + (k+2)z_{2k}^{*2k} = 1. \tag{52}$$

Writing $z_{2k}^* = \exp(-B/k)$, we see that $(1 - z_{2k}^{*2}) \approx 2B/k$; if k is large, to leading order in k, B satisfies the equation

$$2B\exp(2B) \approx k(k+2), \tag{53}$$

which has the solution $B \approx (1/2)W(k(k+2))$ [$W(z)$ being the Lambert function], which for large k has the leading behavior

$$B \approx \ln\left[\sqrt{\frac{k(k+2)}{2\ln k}}\right] \approx \ln\left(\frac{k}{\sqrt{2\ln k}}\right). \tag{54}$$

Since $S_{2k\times\infty} \geqslant -\ln(z_{2lk}^*)/k$, we obtain

$$S_{2k\times\infty} \geqslant \frac{\ln k}{k^2}\left(1 - \frac{\ln\ln k}{2\ln k} + \cdots\right). \tag{55}$$

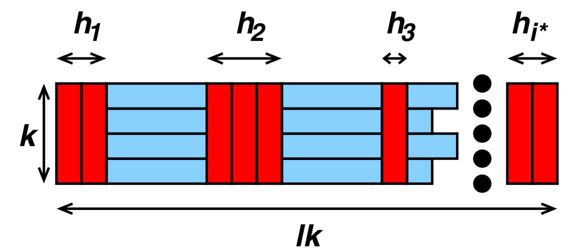

FIG. 11. A schematic representation of configurations that contribute to C_l to leading order in k. Here, there must be exactly k vertical k-mers so that $h_1 + h_2 + \cdots + h_{i^*} = k$.

This is a bit larger than the estimate using strips of width k [see Eq. (10)], but for large k the leading behavior remains the same with the difference showing only in the subleading correction of order $(\ln\ln k)/k^2$. We also note that the bound for $S_{2k\times\infty}$ obtained by truncation coincides with the exact analysis [see Eq. (43)].

Now, the term of order z^{2k+2} in R_{2k} is only $2z^{2k+2}$, and its contribution to the sum is smaller than that of the term of order z^{2k} by a factor $(1/k)$. At higher orders, the term of order z^{6k} has a coefficient of order k^3. Using the fact that z^k is of order $1/k$, the net contribution of this term decreases as $1/k^3$. This also does not change the leading order k dependence of z_{2k}^*.

A similar argument works for other values of $R_{lk}(z)$. We will only sketch the arguments here. The series expansion for $R_{lk}(z)$ in powers of z is of the form

$$R_{lk}(z) = z^l + C_l z^{lk} + \text{higher powers of } z^l. \tag{56}$$

Here C_l is an l-dependent coefficient. The leading contribution to this term comes from configurations depicted in Fig. 11, consisting of $(l-1)$ plaquettes of k aligned horizontal k-mers, interspersed with k vertical rods. The number of such configurations is $\binom{k+l-1}{l-1}$. Thus, keeping only the first two nontrivial terms in the expansion for $R_l(z)$, we write

$$z_{lk}^{*l} + \binom{k+l-1}{l-1} z_{lk}^{*kl} = 1. \tag{57}$$

Solving this equation, we see that its smallest positive root has the leading k dependence given by

$$z_{lk}^* \approx \exp\left[-\frac{1}{k}\ln\frac{k}{(l!\ln k)^{1/l}}\right], \quad k \gg m. \tag{58}$$

Since the entropy $S_{lk\times\infty} = -\ln(z_{lk}^*)/k$, we obtain that

$$S_2(k) \geqslant S_{lk\times\infty} \geqslant \frac{\ln k}{k^2}\left(1 - \frac{\ln\ln k}{l\ln k} + \cdots\right), \quad k \gg 1. \tag{59}$$

We conclude that

$$\lim_{k\to\infty} \frac{k^2 S_2(k)}{\ln k} \geqslant 1. \tag{60}$$

IV. UPPER BOUND FOR ENTROPY FOR LARGE k AND THE MAIN RESULT

Gagunashvili and Priezzhev obtained an upper bound for $N(L, M)$ [70]. They considered a subset of sites of the square

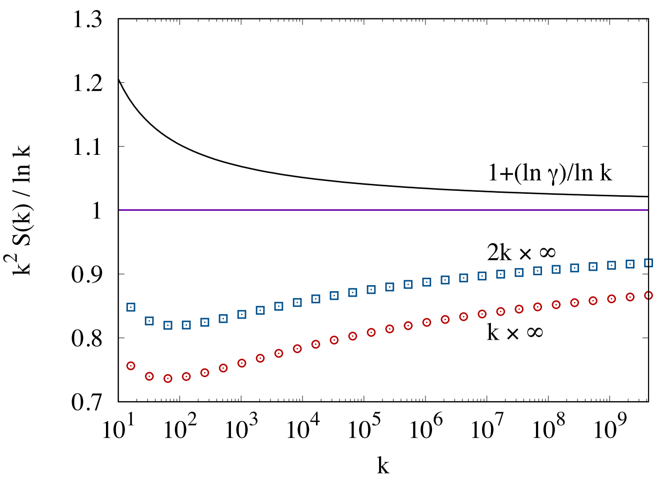

FIG. 12. Bounds for the quantity $k^2S_2(k)/\ln k$, the asymptotic answer of which is 1 [see Eq. (1)]. Lower bounds are provided by the entropies on strips $k \times \infty$ and $2k \times \infty$. An upper bound [70] is provided by $1 + \ln\gamma/\ln k$, where $\gamma \approx 1.605$.

lattice the coordinates of which are multiples of k, and assumed that we are given the configuration of k-mers that cover these sites. Then, they proved that there is at most one way to cover the remaining sites with k-mers. Then, the number of coverings allowed is bounded from above by the number of ways the subset of sites can be covered by k-mers. But each of these can be covered in at most $2k$ ways. Since there are at most N/k^2 such sites, they obtain

$$N(L, M) \leqslant (2k)^{LM/k^2}. \tag{61}$$

This implies that $S_2(k) \leqslant \ln(2k)/k^2$, or equivalently

$$\lim_{k\to\infty} \frac{k^2S_2(k)}{\ln k} \leqslant 1. \tag{62}$$

In fact, Gagunashvili and Priezzhev proved a stronger upper bound which for large k is $S_2(k) \leqslant k^{-2}\ln(\gamma k)$, where $\gamma = \exp(4G/\pi)/2$, with G being Catalan's constant. Numerically, $\gamma \approx 1.605$. However, the weaker bound is adequate for our purpose here

We now combine the lower bound obtained for entropy in Eqs. (11) and (60), and the upper bound obtained for entropy in Eq. (62). Since these two bounds are the same, we conclude that the entropy for fully packed rods on a square lattice has the asymptotic behavior

$$\lim_{k\to\infty} \frac{k^2S_2(k)}{\ln k} = 1, \tag{63}$$

as given in Eq. (1), thus proving our main result.

We now look at how the bounds converge to the asymptotic result. The entropies on the strips $k \times \infty$ and $2k \times \infty$ provide lower bounds for the entropy on infinite lattices. Reference [70] gives an upper bound for large k as $S_2(k) \leqslant k^{-2}\ln(\gamma k)$, where $\gamma \approx 1.605$. Since the leading form is the same for both the upper bounds as well as lower bounds, we divide it out by considering $k^2S(k)/\ln k$, which converges to 1 for large k. The strips provide lower bounds while $\ln\gamma$ provides an upper bound for this quantity. These bounds are shown in Fig. 12.

In addition, it is also possible to put a bound on the subleading corrections to the entropy. Let β be the coefficient of the subleading term $\ln(\ln k)/k^2$ in the asymptotic expansion of the entropy such that

$$S_2(k) = \frac{\ln k}{k^2} + \beta\frac{\ln\ln k}{k^2} + \cdots. \tag{64}$$

From Eq. (59), by taking the limit ł $\to \infty$, it follows that

$$\beta \geqslant 0. \tag{65}$$

V. EXTENSION TO HIGHER DIMENSIONS

We now present a heuristic argument that extends the above result to higher dimensions $d > 2$. For a system of k-mers on a d-dimensional hypercubical lattice, with $d > 2$, we argue below that configurations of rods that are fully layered provide a good starting point to calculate the entropy of the system. In fact, this approach becomes better for larger k and one can develop a series expansion in the number of rods that are between the layered planes. Then, in a typical state, there are only a few such rods, and the full state will show spontaneous symmetry breaking, with most of the rods in the configuration being one of the $\binom{d}{2}$ orientations. In this way, one obtains the full packing constraint satisfied within a two-dimensional layer, and different layers can be occupied independently, leading to a large entropy. We note that the existence of layering in the high-density phase has been seen in simulations at densities close to full packing for rods of length larger than or equal to 5 in $d = 3$ [57].

We first consider the case $d = 3$. The argument is easily extended to higher d.

We will use an adaption of the series expansion technique developed in the context of hard square lattice gases [14–16] and hard rectangle lattice gases [72]. For the simple cubic lattice, we consider different activities w_1, w_2, and w_3 for rods oriented along the x, y, and z directions. Let the corresponding partition function for an $L \times L \times L$ lattice be denoted by $\Omega_L(w_1, w_2, w_3)$.

We will consider a perturbation expansion of this in powers of w_3. We start with the case $w_1 = w_2 = w$, and $w_3 = 0$. The grand partition function of a $L \times L \times L$ cuboid $\Omega_L(w, w, 0)$ can be written as product of two-dimensional partition functions

$$\Omega_L(w, w, 0) = [\Omega_{2d,L}(w)]^L, \tag{66}$$

where $\Omega_{2d,L}(w)$ is the partition function of a full packing of $L \times L \times 1$ layer by k-mers. We write $\Omega_L(w, w, w_3)$ as a perturbation expansion in w_3 about $w_3 = 0$. If this series expansion is well behaved, this implies that for large enough k the full packed configuration will show spontaneous symmetry breaking, and for large k the fraction of nonplanar rods in a random full planar configuration will tend to zero. The first term in w_3 must be proportional to L^d so that the entropy is extensive. We, thus, write the expansion as

$$\Omega_L(w, w, w_3) = \Omega_L(w, w, 0)\big[1 + L^dA_1\,(w_3/w)^k + \mathcal{O}\big((w_3/w)^{2k}\big)\big]. \tag{67}$$

Taking the logarithm and dividing by L^d, we obtain the expansion for the entropy,

$$S_3(w, w, w_3) = S_3(w, w, 0) + A_1(w_3/w)^k + \cdots, \tag{68}$$

and we assume that this systematic expansion is well behaved, and converges for small w_3.

The first nontrivial term in Eq. (67) is proportional to $(w_3/w)^k$, and the coefficient A_1 is determined in terms of the number of configurations of k z-type rods (to be also called vertical rods), with the rest of the rods being of the x and y type. These vertical rods will have to be in the same vertical slab of height k. Let the x and y coordinates of the lowest point of these vertical rods be $\{\alpha_i, \beta_i\}$, $i = 1$ to k. Let the number of possible coverings of rods in one plane, given unoccupied sites $\{x_i, y_i\}$, be $N(\{x_i, y_i\})$. Then the number of coverings of the cuboid is proportional to $[N(\{x_i, y_i\})]^k$, and the relative weight of this term will be $[N(\{\alpha_i, \beta_i\})/\Omega_{2d,L}]^k$. We note that $[N(\{\alpha_i, \beta_i\})/\Omega_{2d,L}]^k$ may be considered as proportional to the probability distribution of the bound state of k holes. We then sum over different possible $\{\alpha_i, \beta_i\}$. We expect $N_{\alpha_i,\beta_i}/\Omega_{2d,L}$ to be less than 1, and to decrease as a power law of the distances between $\{\alpha_i, \beta_i\}$, but with a power large enough so that

$$A_1 = \sum_{\{\alpha_i,\beta_i\}}^{\prime} \left[\frac{N(\{\alpha_i, \beta_i\})}{\Omega_{2d,L}}\right]^k < \infty, \tag{69}$$

where the primed sum is over $i = 2, 3, \ldots, k$, with $\{\alpha_1, \beta_1\}$ fixed. Then the sum over α_1 and β_1 gives a factor proportional to L^3.

This is a complicated problem, for which we do not know the exact closed form expression. However, we note that each term decreases exponentially with k for large k since we expect $N_{\alpha_i,\beta_i}/\Omega_{2d,L} < 1$. We note that $N(\{\alpha_i, \beta_i\})$ would be expected to be largest, when the holes are near each other. In fact, the closest they can be be is in a continuous single line of k points, which may be created by removing a single rod from the $2d$ covering. In this case, the contribution of the term is $[1/(2k)]^{k-1}$.

If we sum to all orders, the dominant contribution will be expected to be of the same form. We thus conclude that for large k

$$S_3(k) = S_2(k) + \text{ terms of order } k^{-k}. \tag{70}$$

Then for $\Omega_L(w_3)$, as a function of w_3, and expanding in powers of $(w_3/w)^k$, order by order, each term in the perturbation series will give an exponentially small contribution in the large-k limit.

Taking the derivative of $\ln \Omega_L(w, w, w_3)$ with respect to $\ln w_3$, we obtain the fractional number of rods in the z direction at full packing in this ensemble, and we see that this fraction tends to zero as k increases, and the departure from perfect layering decreases for larger k.

The argument is immediately extended to higher d, and leads us to the conjecture in Eq. (1).

VI. CONCLUDING REMARKS

In this paper, we studied the tiling of a finite rectangular part of the plane by rectangles of size $k \times 1$ and $1 \times k$. We showed that in order to get a full coverage one of the sides of the rectangle to be covered should be a multiple of k. We also studied the structure of the tilings of rectangles, and showed that all tilings can be obtained from each other by a sequence of basic flip moves that exchanges a small $k \times k$ small square made of k parallel vertical rectangles into horizontal ones, and vice versa. We also provided nonrigorous perturbation theory based arguments for the conjecture that $S_d(k)$, the entropy per site for k-mers on a d-dimensional hypercubical lattice covered by straight rods of length k, for all $d \geqslant 2$ satisfies Eq. (1). We emphasize that while the perturbation theory argument seems quite plausible there is no proof that such a perturbation expansion is convergent. If the series expansion does not converge, or converges to a wrong value, the argument given here would break down.

The fact that this limit is independent of dimension deserves some comment. In general, we would expect the coefficients of logarithms encountered in the study of critical phenomena to be "universal," because by definition they do not change under a change of length scale in a renormalization transformation. But, such coefficients are in general not dimension independent. In fact, here, S_d has a multiplying factor k^{-2}, which indicates that the relevant quantity is the number of allowed configurations per unit square of length k (which is the natural length scale in the problem). This number is proportional to k, and the entropy is proportional to $\ln k$. The fact that this is independent of dimension is only reflecting the fact that for large k the problem essentially reduces to a two-dimensional problem, because of spontaneous symmetry breaking, and most of the configurations at full packing are the ones where the system breaks up into disjoint two-dimensional layers. Consequently, for large k, the leading behavior of entropy in higher dimensions is the same as the two-dimensional case.

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