Predictions of bond percolation thresholds for the kagomé and Archimedean (3,12^2) lattices

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Here we show how the recent exact determination of the bond percolation threshold for the martini lattice can be used to provide approximations to the unsolved kagomé and (3,12^2) lattices. We present two different methods, one of which provides an approximation to the inhomogeneous kagomé and (3,12^2) bond problems, and the other gives estimates of $p_c$ for the homogeneous kagomé (0.5244088...) and (3,12^2) (0.7404212...) problems that respectively agree with numerical results to five and six significant figures.

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Percolation [1, 2] has provided some of the most intriguing and difficult problems in statistical mechanics. Devised in 1957 by Broadbent and Hammersley [3], it has served as the simplest example of a lattice process exhibiting a phase transition, and its study provides insight into more complicated physical models.

The problem is very simply stated. Given any lattice, such as either of those shown in Fig. 1, we declare each bond to be in one of two states; open or closed. If a bond (although we could just as well consider sites) is open with probability $p$ and closed with probability $1-p$, then clusters of various sizes will appear, with the average cluster size increasing as a function of $p$. In the limit of an infinite lattice there exists a critical value of this parameter, denoted $p_c$, and referred to as the percolation or critical threshold, where an infinite cluster will appear with probability 1. The value of $p_c$ is specific to each lattice.

While the problem can be easily and precisely defined, exact solutions for thresholds (or anything else for that matter) have historically proved elusive, with results being limited to a small set of lattices. Recent work [4, 5] has significantly expanded this set, and in fact it was shown in [6] that an infinite variety of problems are exactly solvable so long as their basic cells are contained between three vertices and are stacked in a particular self-dual way. Despite this recent progress, the most perplexing unsolved problems still remain. In particular, the exact site percolation thresholds of the square and honeycomb (also called hexagonal) lattices, and the bond threshold of the kagomé lattice are still unknown after nearly half a century of research in the field. The latter problem is one of the subjects of this Communication.

The square, honeycomb, and kagomé problems belong to an important subset of two dimensional lattices called the Archimedean lattices [6], in which all sites are equivalent. There are 11 such graphs, and although both site [7] and bond [8] thresholds have been studied numerically for all of them, the only exactly solved problems are the bond thresholds of the square, honeycomb, and triangular [9] lattices, and the site thresholds of the triangular, kagomé, and (3,12^2) lattices. Note that finding the site threshold is a completely different problem from finding the bond threshold, and these last two site values are known only because of a trivial transformation from the honeycomb bond lattice — a transformation that does not help us in solving the bond problems. However, the (3,12^2) lattice bears enough similarity to the kagomé that the methods we present here will provide us with estimates for that bond threshold as well, one of which agrees with a recent numerical result [8] to its limit of precision, which is six significant figures.

The bond threshold for the kagomé lattice has previously been the subject of several conjectures [10, 11, 12, 13]. Using a method that predicted correct critical frontiers for the Potts model [14] on other lattices, Wu...
conjectured that it would also work for the kagomé, and, using the fact that percolation is the $q \to 1$ limit of the Potts model, proposed that $p_c = 0.524430\ldots$, the solution of a polynomial we will encounter below. A few years afterward, and also in the context of the Potts model, Tsallis [11, 12] offered the competing conjecture $p_c = 0.522372\ldots$, employing an argument that also made correct predictions for other lattices. It was not until much later that both of these propositions were ruled out numerically [13] though fairly high precision was required to exclude Wu’s estimate. Tsallis also considered the $(3,12^2)$ lattice, and proposed $p_c(3,12^2) = 0.739830\ldots$

Aside from these various speculative methods, in which one makes conjectures that must be verified or rejected numerically, there are some rigorous results for the kagomé and $(3,12^2)$ thresholds in the form of bounds on the values of $p_c$. This work is largely carried out by Wierman and co-workers [19, 21], using a technique called substitution. The method is such that continual refinements are possible and the most current rigorous bounds are [21]:

$$0.522197 < p_c(\text{kagomé}) < 0.526873 , \quad (1)$$

and

$$0.739773 < p_c(3,12^2) < 0.741125 . \quad (2)$$

Various other quantities besides the standard percolation threshold have also been studied on the kagomé lattice such as the mixed site-bond threshold [22], a correlated percolation threshold [23], and an exact solution for the average cluster number on a kagomé lattice strip [24], among others. As already mentioned, the kagomé Potts model has also received, and continues to receive, attention. In addition to the work already cited, some recent examples include [25], and [26] in which the conjectures of Wu and Tsallis are discussed for various values of $q$.

Here we show how a recent exact solution on a similar lattice, the martini lattice [Fig. 2(a)], can be used to provide precise estimates of the kagomé and $(3,12^2)$ thresholds.

The starting point of our analysis is the bond threshold for the martini lattice [Fig. 2(b)]. For the general martini generator of Fig. 2(b), the method outlined in [1] gives for the inhomogeneous critical surface

$$1 - p_1p_2t_3 - p_2p_3t_1 - p_1p_3t_2 - p_1p_2t_1 \to$$

$$- p_1p_2t_3 - p_2p_3t_1 - p_1p_3t_2$$

$$+ p_1p_2p_3t_1 - p_1p_2p_3t_2 + p_1p_2p_3t_3$$

$$+ p_1p_2p_3t_1 + p_1p_2p_3t_2 + p_1p_2p_3t_3 = 0 \quad (3)$$

which was also reported recently in [10]. Taking $r_i = 1$, we get the result for the critical surface of the general honeycomb lattice [3]:

$$1 - p_1p_2 - p_1p_3 - p_2p_3 + p_1p_2p_3 = 0 \quad (4)$$

and taking $p_i = 1$ we get the following formula for the critical surface of the general triangular lattice [3]:

$$1 - r_1 - r_2 - r_3 + r_1r_2r_3 = 0 \quad (5)$$

For the first approach to the kagomé lattice, we start with the inhomogeneous double-bond honeycomb lattice, whose unit cell is shown in Fig. 3(a). Replacing the bond with probability $p_i$ in the honeycomb lattice with a pair of bonds in series with probability $p_i$, we find from [1] that the critical surface is given by

$$1 - p_1p_2t_1t_2 - p_2p_3t_1t_3 - p_1p_3t_1t_3 + p_1p_2p_3t_1t_2t_3 = 0 \quad (6)$$

Now consider the progression shown in Fig. 3. Starting with the double honeycomb lattice (a), changing every up star into a triangle gives the martini lattice (b), and changing the down stars gives the kagomé lattice (c). The fact that the thresholds of the first two stages of this transformation are now known allows us to make guesses as to the way to reach the third.

Comparing (6) with (3), it can be seen that the transformation

$$t_1t_2 \to r_3 + r_1r_2(1 - r_3) \quad (7)$$

$$t_1t_3 \to r_2 + r_1r_3(1 - r_2) \quad (8)$$

$$t_2t_3 \to r_1 + r_2r_3(1 - r_1) \quad (9)$$

$$t_1t_2t_3 \to r_1r_2r_3 + r_1r_2(1 - r_3) + r_2r_3(1 - r_1) + r_1r_3(1 - r_2) \quad (10)$$

effectively turns the double honeycomb critical surface into the martini critical surface. These substitutions can be interpreted in terms of probabilities of connections between vertices on a triangle, i.e., $t_1t_2$ is the probability that a particular pair of vertices are connected on the star, and $r_1 + r_1r_2(1 - r_3)$ is the probability of the same thing on the triangle. The same transformations will also change the critical surface of the honeycomb lattice [4] into that of the triangular [5] — but note that we are not applying the star-triangle transformation here. In fact, these manipulations are largely formal, as the
we conjecture that if we transform the down star the same
equation (10) is not implied by (7) — (9). Nevertheless,
FIG. 3: The transformation from the (a) double honeycomb,
to the (b) martini, to the (c) kagomé lattice.

There are nine probabilities in this case and the resulting

\[ p_1 \text{ in Fig. 2(b)], and setting all} \]

\[ \text{probabilities equal gives the condition} \]

\[ 1 - 3p^2 - 6p^3 + 12p^4 - 6p^5 + p^6 = 0, \] (11)

with solution in \([0, 1]\) \(p_c = 0.5244297175\). This result
turns out to be identical to the conjecture made several
years ago by Wu \cite{Wu15} by different means. Subsequently,
this value was found to be high numerically, but by only
3 \cdot 10^{-5} \cite{Wu15}. Note that (11) is a plausible form for the
kagomé threshold: all the bonds are equivalent, setting
any one probability to 0 gives the correct threshold for the
A lattice [the lattice that results when \(p_1\) is set to 1 in Fig. 2(b)], and setting all \(p_1 = 1\) reduces the expression
to the triangular critical surface. It is difficult
to imagine any other form that satisfies these conditions and
remains linear in the probabilities, suggesting that
the true general formula for the kagomé lattice will not
be linear in this way.

The same procedure can also be used to find an approx-
imate solution to the \((3, 12^2)\) lattice. We start with the
\emph{triple}-bond honeycomb lattice, and transform the stars
into triangles in the same manner as before (Fig. 4).
There are nine probabilities in this case and the resulting

\[ 1 - m_1m_2(r_3 + r_1r_2 - r_1r_2r_3)(s_3 + s_1s_2 - s_1s_3) \]
\[ - m_1m_3(r_2 + r_1r_3 - r_1r_2r_3)(s_2 + s_1s_3 - s_1s_2) \]
\[ - m_2m_3(r_1 + r_2r_3 - r_1r_2r_3)(s_1 + s_2s_3 - s_1s_2s_3) \]
\[ + m_1m_2m_3(r_1r_2 + r_1r_3 + r_2r_3 - 2r_1r_2r_3) \]
\[ \times (s_1s_2 + s_1s_3 + s_2s_3 - 2s_1s_2s_3) = 0. \] (13)

Setting all \(m_i = 1\) gives (11) (in factored form), and
setting all \(m_i = m\) and \(r_i = s_i = r\) gives the equation
for an inhomogeneous \((3, 12^2)\) lattice with all triangle
bonds having probability \(r\) and all linking bonds having
probability \(m\):

\[ 1 - 3m^2(r + r^2 - r^3)^2 + m^3(3r^2 - 2r^3)^2 = 0. \] (14)

Finally, letting \(r = m = p\) gives the equation for the
homogeneous \((3, 12^2)\) lattice,

\[ (1 + p - 2p^3 + p^4)(1 - p + p^2 + p^3 - 7p^4 + 4p^5) = 0, \] (15)

with solution on \([0, 1]\) \(p_c = 0.7404233179\ldots\), well within
the bounds of \cite{Wu15}. According to the numerical analysis
of Parviainen \cite{Parviainen8}, \(p_c(3, 12^2) = 0.74042195(80)\). Our result
is high by less than two standard deviations. Yet, we can
get even better agreement with both of these results by
taking a somewhat different route.

In our second approach, we also compare the critical
double honeycomb with the critical martini lattice, but
we consider all bonds equivalent, in which case the double
honeycomb threshold is \(p_0 = \sqrt{1 - 2\sin \pi/18}\) by \cite{Wu15}.
Now, consider the martini lattice with \(p_1 = p_2 = p_3 = p\),
and \(r_1 = r_2 = r_3 = r\). Equation (3) implies that the
critical surface is

\[ 1 - 3p^2(r + r^2 - r^3)^2 + p^3(3r^2 - 2r^3)^2 = 0. \] (16)

and taking \(p = p_0\), we find that the critical value for \(r\) is

\[ r = 0.52440876529769\ldots. \] (17)

That is, when one star with bond probabilities \(p_0\) is
replaced by a triangle with probabilities \(r\), the system
remains at a critical point (even though local correlations
will necessarily be different because this is not a fixed
This result is within the error bars of [8] and falls within the rigorous bounds of [10], which raises the possibility that the result is exact. Clearly, more precise numerical work for both lattices is called for.

We can generalize our argument above for the inhomogeneous $(3, 12^2)$ lattice with two probabilities $m$ and $r$. The critical surface is determined by (16) with $p = p_0 \sqrt{m}$. When $m = 1$, this gives the kagomé estimate (14), when $m = r$ it gives the homogeneous estimate (13), and when $r = 1$ it gives the exact honeycomb result $m = p_0^2$. The formula (10) (with $p = p_0 \sqrt{m}$) can be compared with (14), which though mathematically quite different, gives very similar numerical solutions. Finally, we note one last relation: if we require that the second terms of the two estimates (14) and (15) (which represents two-point correlations) be the same, we get the simple condition

$$p_0^2/m = r + r^2 - r^3$$  \hspace{1cm} (19)$$

which turns out to be identical to Tsallis’ conjecture for this system. As mentioned above, however, the predictions of this formula are much farther from the numerical measurements than the predictions of (14) and (16).

In conclusion, we have shown that the results for the martini and honeycomb lattices can be used to make precise estimates of bond percolation on the kagomé and $(3, 12^2)$ lattices, both long-standing problems in percolation theory. For the kagomé lattice, we have reproduced the conjectures of both Wu and of Hori and Kitahara, while for the $(3, 12^2)$ lattice we have apparently very precise estimates. Perhaps these methods can point the way to finding rigorous thresholds for these lattices, and analyzing other unsolved lattices in percolation.

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