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Site percolation and random walks on d-dimensional Kagomé lattices

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Abstract. The site percolation problem is studied on d-dimensional generalizations of the Kagomé lattice. These lattices are isotropic and have the same coordination number q as the hyper-cubic lattices in d dimensions, namely $q = 2d$. The site percolation thresholds are calculated numerically for $d = 3, 4, 5$, and 6. The scaling of these thresholds as a function of dimension d, or alternatively q, is different than for hypercubic lattices: $p_c \sim 2/q$ instead of $p_c \sim 1/(q-1)$. The latter is the Bethe approximation, which is usually assumed to hold for all lattices in high dimensions. A series expansion is calculated, in order to understand the different behaviour of the Kagomé lattice. The return probability of a random walker on these lattices is also shown to scale as $2/q$. For bond percolation on d-dimensional diamond lattices these results imply $p_c \sim 1/(q-1)$.

1. Introduction

The Kagomé lattice is one of the most interesting lattices in two dimensions. It is one of the eleven Archimedean tiling lattices, where all the vertices are of the same type (see e.g. Weisstein 1997). In the case of the Kagomé lattice each vertex touches a triangle, hexagon, triangle, and a hexagon. All these polygons are regular. Moreover, the Kagomé lattice is closely related to the other lattices in two dimensions. The sites of the Kagomé lattice correspond to the bonds of the honeycomb lattice, which in turn is the dual of the triangular lattice. Therefore, since the bond percolation threshold of the honeycomb lattice is $1 - 2\sin(\pi/18)$, the site percolation threshold of the Kagomé lattice is $1 - 2\sin(\pi/18) = 0.652\,7036\ldots$ too (Sykes and Essam 1964). The bond percolation threshold is not known exactly, but has been calculated numerically with high precision to be $0.524\,4053 \pm 0.000\,0003$ (Ziff and Suding 1997).

Although these percolation thresholds have been known for quite some time, it is not clear why this site percolation threshold is high, compared to other lattices. For instance, it is much higher than the threshold $0.592\,7460 \pm 0.000\,0005$ for the square lattice (Ziff and Sapoval 1986, Ziff 1992), although its coordination number $q = 4$ is equal to that of the Kagomé lattice. What is more striking is that even the pentagonal lattice, which has a low average coordination number of $q = 3\frac{1}{3}$, has a lower site percolation threshold 0.6471 ± 0.0006 than the Kagomé lattice (Van der Marck 1997a). In other words, the site percolation thresholds are not ordered according to the coordination number q. This runs contrary to common intuition, which leads one to expect that a lattice with a higher connectivity has a lower percolation threshold. If one searches for general formulae that correlate percolation thresholds with dimension and coordination number, the Kagomé lattice therefore poses a problem. Galam and Mauger (1996) introduced different classes of lattices

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to avoid this problem, and they used different correlations for these classes. Although this enabled them to derive good correlations, it prompts the question why certain lattices belong to one class and others to another class.

An analogue in three dimensions was found recently: there is a lattice with $q = 6$ and percolation threshold 0.3898 ± 0.0008 (Van der Marck 1997c). Compared to the simple cubic lattice, which also has $q = 6$, but a threshold of $0.311\,604 \pm 0.000\,006$ (Grassberger 1992), this threshold is much higher. It is even higher than the threshold for several lattices with coordination number $q = 5$ (Van der Marck 1997a).

In this paper, a generalization of the Kagomé lattice to higher dimensions is given (section 2), and numerical calculations of the site percolation thresholds for three, four, five, and six dimensions are presented (section 3). The scaling of these thresholds as a function of dimension appears to be different than for hypercubic lattices. For the latter, Gaunt *et al* (1976) calculated a series expansion in $1/(2d-1)$, where d is the number of dimensions. The leading term in their series is $p_c(d) = 1/(2d-1)$, which is the so-called Bethe approximation. This approximation holds exactly for Bethe lattices (see, e.g., Stauffer and Aharony 1992). For hypercubic lattices, the approximation underestimates the percolation threshold in low dimensions, but improves in accuracy in higher dimensions. In section 4 the series expansion for the d-dimensional Kagomé lattices is studied. It is suggested that in this case the leading term in the series is $1/d$, not $1/(2d-1)$.

The return probability of a random walker on d-dimensional Kagomé lattices is discussed in section 5. Ishioka and Koiwa (1978) conjectured that this probability is a good estimator for the percolation threshold. Indeed, it is shown here that this return probability also scales as $1/d$. Section 6 contains a discussion of the results. These results give some insight into the problem why the two-dimensional Kagomé lattice has a high site percolation threshold.

2. Kagomé lattices in d dimensions

The Kagomé lattice can be defined in d dimensions as follows. The lattice has a $(d+1)$-point basis, and these points form a regular d-dimensional polytope. In figure 1(a) the situation in two dimensions is depicted. All the points of this basis are direct neighbours of each other. Let us denote the basis points by $\boldsymbol{b}_i$, for $i = 0, \ldots, d$. The lattice can be constructed by translation of the basis in $\frac{1}{2}d(d+1)$ directions. These translations are given by the vectors $2(\boldsymbol{b}_j - \boldsymbol{b}_i)$ for $j \neq i$. This is a dependent set of vectors. One can select a minimal set of d vectors by setting, for example, $i = 0$, $j = 1, \ldots, d$.

A site of the lattice can be identified by its number i within the base polytope (runs from 0 to d), and the translation $\boldsymbol{x}$ with respect to a reference position. Consider a site $\{i, \boldsymbol{x}\}$. This site has d neighbours in the same polytope, $\{j \neq i, \boldsymbol{x}\}$, and another d neighbours in adjacent polytopes, $\{j \neq i, \boldsymbol{x} + 2(\boldsymbol{b}_i - \boldsymbol{b}_j)\}$. Therefore, the coordination number of this lattice is $q = 2d$. Also, because there is no preferential direction in the construction, all the directions are equivalent for this lattice, i.e. it is an isotropic lattice.

So the Kagomé lattice resembles the cubic lattice in the sense that both are isotropic d-dimensional lattices with coordination number $q = 2d$. However, we already know that in two and three dimensions the site percolation thresholds of these lattices are distinctly different.

In two dimensions the site percolation problem on the Kagomé lattice is equivalent to the bond percolation problem on the honeycomb lattice (Sykes and Essam 1964). This was shown by means of the star-triangle transformation. Analogous to the star-triangle transformation, one can use a 'star-tetrahedron' transformation in three dimensions, see figure 2. The site percolation problem on the tetrahedron ABCD, i.e. the three-dimensional

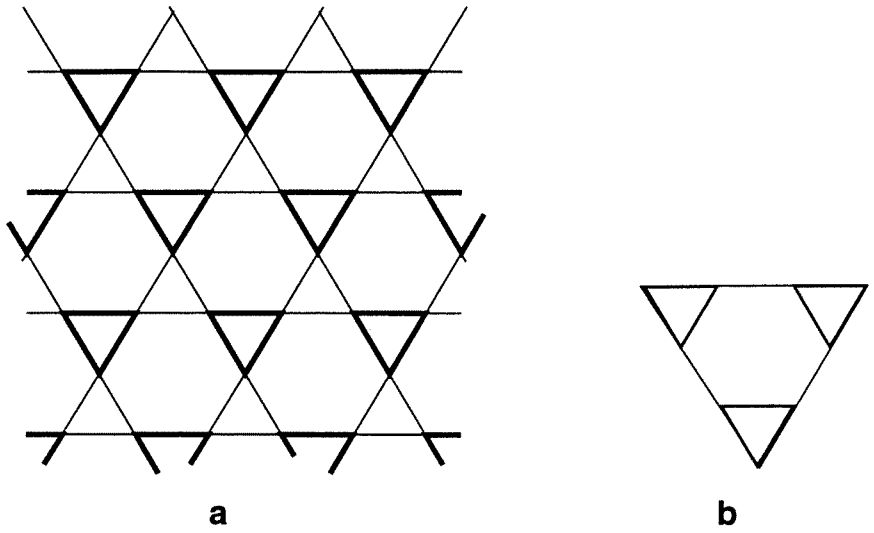

Figure 1. (a) A description of the Kagomé lattice as a lattice with a three-point basis. The basis points form a (regular) triangle. (b) Three base triangles define a larger triangle, which truncates to a hexagon.

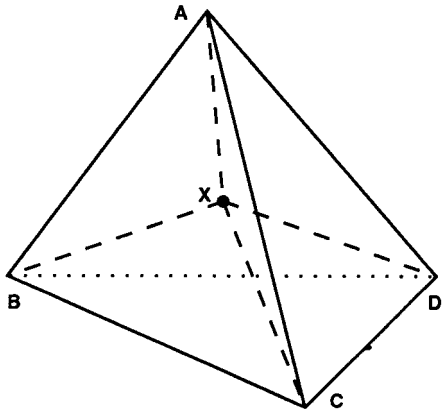

Figure 2. The star-tetrahedron transformation. The dashed lines AX, . . . , DX, that come together in the point X, form the diamond lattice.

Kagomé lattice, is equivalent to the bond percolation problem on the dashed lattice. This dashed lattice is the diamond lattice, for which $p_{c,b} = 0.3893 \pm 0.0003$ has been calculated (Van der Marck 1997b). Generalizing to d dimensions, the site percolation on the d-dimensional Kagomé lattice is equivalent to bond percolation on the d-dimensional diamond lattice, which has $q = d + 1$.

The Kagomé lattice defines a tiling of d-dimensional space. In two dimensions, the Kagomé lattice defines a tiling of the plane in terms of a regular triangle and a regular hexagon. One can construct this hexagon from the base triangle: take three neighbouring base triangles, as in figure 1(b). These three form a larger regular triangle. The hexagon appears when one truncates the larger triangle by taking away the three smaller triangles.

Table 1. The site percolation thresholds of the cubic and Kagomé lattices in three, four, five, and six dimensions, as a function of the linear lattice size L. By comparison, some values for the cubic lattices given in the literature are 0.311 604(6) (Grassberger 1992), 0.197(6), 0.141(3), and 0.108(3) (Gaunt *et al* 1976). In the last row, marked 'rw', the values for the return probability of a random walker are given. The estimated error margins concerning the last digits are indicated between brackets.

$d=3$			$d=4$			$d=5$			$d=6$		
L	cubic	Kagomé	L	cubic	Kagomé	L	cubic	Kagomé	L	cubic	Kagomé
			8	0.2088(2)	0.2787(2)	8	0.1425(2)	0.2080(3)	6	0.1043(2)	0.1630(2)
16	0.3233(2)	0.3952(2)	12	0.2037(2)	0.2753(2)	12	0.1413(2)	0.2076(2)	8	0.1049(2)	0.1643(3)
32	0.3171(2)	0.3924(2)	16	0.2014(2)	0.2736(2)	16	0.1412(2)	0.2078(2)	10	0.1060(2)	0.1652(3)
64	0.3139(2)	0.3908(2)	25	0.1989(2)	0.2726(2)	20	0.1407(2)	0.2080(2)	12	0.1064(2)	0.1660(3)
128	0.3125(2)	0.3903(2)	32	0.1987(2)	0.2724(2)	24	0.1406(2)	0.2081(2)	14	0.1067(2)	0.1664(3)
250	0.3119(2)	0.3897(2)	50	0.1974(2)	0.2719(2)	32	0.1406(2)		16	0.1070(2)	
∞	0.3114(2)	0.3895(2)	∞	0.1967(3)	0.2715(3)	∞	0.1407(3)	0.2084(4)	∞	0.1079(5)	0.1677(7)
rw	0.343(1)	0.417(1)	rw	0.195(1)	0.274(1)	rw	0.136(1)	0.208(1)	rw	0.105(1)	0.170(1)

In two dimensions this is a rather complicated description of the tiling, but the advantage is that one can use an identical procedure in d dimensions. One can start with the regular base polytope of $(d+1)$ points in d dimensions, $\boldsymbol{b}_i$ (for $i = 0, \ldots, d$). This polytope is shifted in d directions by the vectors $2(\boldsymbol{b}_i - \boldsymbol{b}_0)$ for $i = 1, \ldots, d$. This defines a larger regular polytope, which is then truncated by taking away the $(d+1)$ small polytopes. In three dimensions, for example, the resulting polyhedron is the truncated tetrahedron (see, e.g., Weisstein 1997). The d-dimensional space is filled with the base regular polytope and the larger truncated polytope.

In view of the considerations in sections 4 and 5, it is helpful to discuss one more important property of the d-dimensional Kagomé lattice: two adjacent sites have $d-1$ *common neighbours*. This is demonstrated by the following arguments. When the two sites are within the same base polytope, characterized by $\{i, \boldsymbol{x}\}$ and $\{j, \boldsymbol{x}\}$ $(j \neq i)$, all the other $d-1$ sites of that polytope are common neighbours. When the two sites are *not* within the same base polytope, they are characterized by $\{i, \boldsymbol{x}\}$ and $\{j, \boldsymbol{x} + 2(\boldsymbol{b}_i - \boldsymbol{b}_j)\}$. Note that j cannot be equal to i for two adjacent sites. The $d-1$ common neighbours of these two sites are $\{k, \boldsymbol{x} + 2(\boldsymbol{b}_i - \boldsymbol{b}_k)\}$ with the restriction that $k \neq i, j$. This is because they are one step $\boldsymbol{b}_i - \boldsymbol{b}_k$ away from $\{i, \boldsymbol{x}\}$, and one step $\boldsymbol{b}_k - \boldsymbol{b}_j$ from $\{j, \boldsymbol{x} + 2(\boldsymbol{b}_i - \boldsymbol{b}_j)\}$.

3. Percolation thresholds

The site percolation thresholds of the Kagomé lattice in three, four, five, and six dimensions are show in table 1 as a function of the lattice size. The method given by Stauffer and Aharony (1992) has been used. This method is simple to program, but in its simplest form it has the drawback that one needs to have all $N = (d+1)L^d$ sites of a network resident in memory. Therefore, the calculation is restricted to relatively low values of L, the linear size of the lattice. Especially in higher dimensions this is rather restrictive: the highest L-value used was $L = 14$ for the six-dimensional Kagomé lattice. One can check in a scaling plot, figure 3, that the used lattices are indeed large enough to be in the scaling regime, and hence allow extrapolation to infinite lattice sizes.

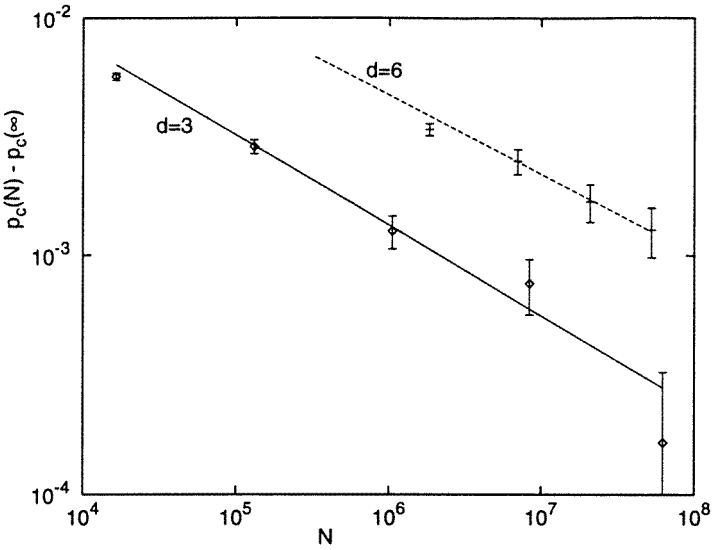

Figure 3. The scaling of the percolation threshold with network size $N = (d+1)L^d$.

For each of the lattices, percolation in only one direction, say the x_1-direction, was checked. The lattice was defined to be percolating whenever the two boundaries $\{i = 0, x_1 = 1\}$ and $\{i = d, x_1 = L\}$ were connected. The boundary conditions in the other directions were not periodic.

The percolation thresholds of a lattice of size N obey the scaling relation

$$|p_c(N) - p_c(\infty)| \sim N^{-1/(\nu d)}. \tag{1}$$

Here the critical exponent ν is 0.88 in three dimensions and 0.68, 0.57, 0.5 in four, five, and six dimensions, respectively (Stauffer and Aharony 1992). The results quoted in the row marked ∞ in table 1 are fits of $p_c(N)$ to this scaling relation, using the last three points in the table.

The data and the fits are shown in figure 3 for $d = 3$ and $d = 6$. From the figure it can be concluded that the input values for the fits are indeed within the scaling regime, and that the fits are therefore sensible. For $d = 6$ the difference $p_c(N) - p_c(\infty)$ is larger than for lower dimensions, because the number of lattice sites that are near to a boundary increases with dimension.

Also shown in table 1 are results for the percolation thresholds of the cubic lattice. These numbers agree with the literature (Stauffer and Aharony 1992) and can be seen as a check that the programs used in the present work are correct.

The difference between the percolation threshold for the Kagomé lattices and the (hyper-) cubic ones increases with dimension. This is illustrated in figure 4. In the next section a series expansion is studied, in order to understand this behaviour.

4. Series expansion

One could conjecture, based on the numerical estimates of the percolation thresholds, that the scaling of these thresholds as a function of dimension is different for the Kagomé lattice than for the cubic lattice. The scaling behaviour of the cubic lattice was studied by

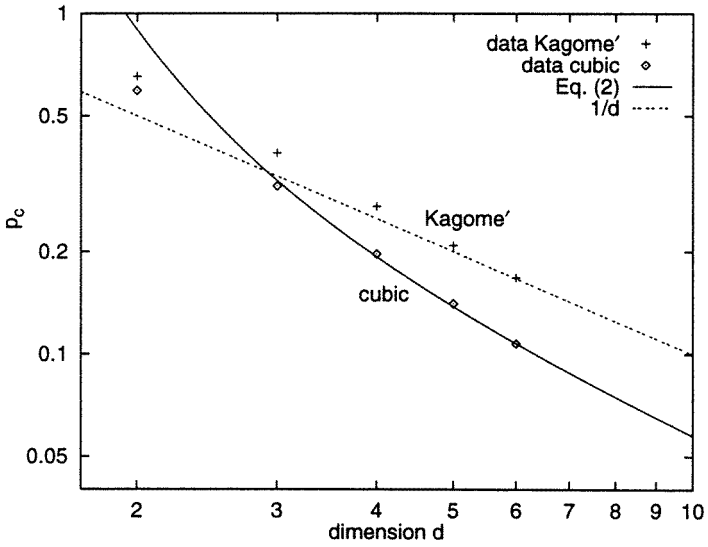

Figure 4. The percolation thresholds as a function of dimension d. Equation (2) is the result of Gaunt *et al* (1976) for the thresholds of the cubic lattices. The thresholds for the Kagomé lattices scale as $1/d$.

Gaunt *et al* (1976). Their result for the percolation threshold was

$$p_c(d) = \frac{1}{2d-1}\left(1 + \frac{3/2}{2d-1} + \frac{15/4}{(2d-1)^2} + \frac{83/4}{(2d-1)^3} + \cdots\right). \tag{2}$$

The leading term is the percolation threshold of a Bethe lattice with coordination number $q = 2d$. Equation (2) agrees well with the known numerical estimates for the cubic lattices for $d \geqslant 3$, as is clear from figure 4.

Gaunt *et al* (1976) used cluster counting to calculate a series expansion for the mean size S of clusters at low probabilities p. Since the mean cluster size diverges at the percolation threshold, they studied the radius of convergence of the series expansion of S. They argued that this radius of convergence will be determined predominantly by the singularity at $p = p_c$, which enabled them to derive equation (2). In this section these techniques are used to study the percolation thresholds of the Kagomé lattice in higher dimensions. At the basis of the approach are the 'perimeter polynomials', as described by Sykes and Glen (1976). Denoting the mean number per lattice site of clusters of s sites by $\bar{n}_s$, we have for example

$$\bar{n}_1 = pq^{2d} \qquad \bar{n}_2 = dp^2q^{3d-1}. \tag{3}$$

Here p is the probability that a site is occupied, and $q = 1 - p$ the probability that a site is empty. One can interpret $p(s) = s\bar{n}_s$ as the probability that a site is occupied by a cluster of size s. When one sums $p(s)$ over all cluster sizes, one gets the probability that a site is occupied by *any* cluster, i.e. p:

$$\sum_{s=1}^{\infty} s\bar{n}_s = \sum_{s=1}^{\infty} p(s) = p. \tag{4}$$

The power $3d - 1$ of q in the expression for $\bar{n}_2$ indicates that all clusters of two sites are surrounded by $3d - 1$ neighbours. Already we see a difference with the cubic lattice, which

has $\bar{n}_2 = dp^2q^{4d-2}$. So even though a site on the Kagomé lattice has as many neighbours as a site on the cubic lattice (namely $2d$), a two-site cluster has less neighbours on a Kagomé lattice than on a cubic lattice. This is because on the Kagomé lattice two adjacent sites have $d-1$ common neighbours, whereas on the cubic lattice they have none.

A relatively simple counting procedure by hand reveals the next few perimeter polynomials to be

$$\begin{aligned}
\bar{n}_3 &= \tfrac{1}{3}d(4d-1)p^3q^{4d-2} \\
\bar{n}_4 &= \tfrac{1}{12}d(5d-1)(5d-2)p^4q^{5d-3}, \\
\bar{n}_5 &= [\tfrac{1}{60}d(6d-1)(6d-2)(6d-3) - 2d(d-1)]p^5q^{6d-4} \\
&\quad +2d(d-1)p^5q^{6d-5}.
\end{aligned} \tag{5}$$

In figures 5–7 the contributing graphs are depicted in two dimensions. In the expressions for $\bar{n}_1, \ldots, \bar{n}_4$ a clear pattern seems to emerge. The coefficient of $\bar{n}_s$ has factors $(s+1)d-1$, $(s+1)d-2, \ldots$, and the power of q is always $(s+1)d-(s-1)$.

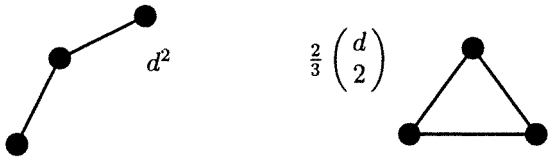

Figure 5. The clusters of three sites.

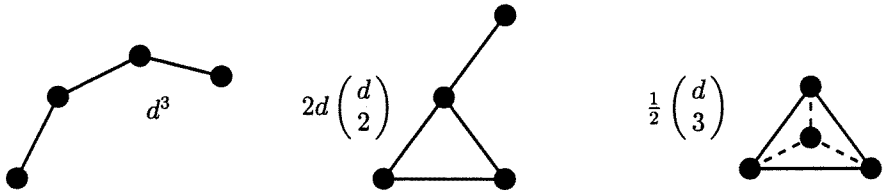

Figure 6. The clusters of four sites.

However, this trend is broken in $\bar{n}_5$. Although the sum of the two coefficients appearing here still has the factors $(s+1)d-1$, etc, there are now terms with different powers of q. In other words, in $\bar{n}_5$ we encounter for the first time that there are clusters with different numbers of neighbours; clusters with $6d-4$ neighbours and clusters with $6d-5$ neighbours. The latter ones are depicted in figure 8. They are the type of cluster that 'bites itself in the tail'. At first sight, one would think that this would occur already for clusters of two sites, but in those cases the number of neighbours is not affected. This number is only affected for the clusters depicted in figure 8. On the cubic lattice this occurs for the first time for clusters of three sites. Another difference is that for the cubic lattice the leading power of q is $2sd-2(s-1)$, compared to $(s+1)d-(s-1)$ for the Kagomé lattice.

The identity (4) can be exploited to determine one more mean cluster number, namely $\bar{n}_6$, albeit in the limit of $q \to 1$. Following Sykes and Glen (1976) we substitute equations (3) and (5) into the identity (4), and set $q = 1-p$. This yields a power series in p, of which the coefficient of p is 1, and the coefficients of $p^2, \ldots, p^5$ vanish identically. The higher-order

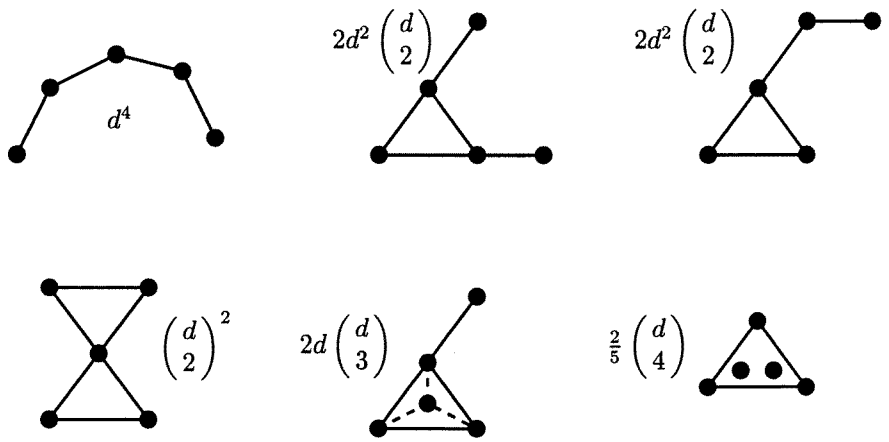

Figure 7. The clusters of five sites.

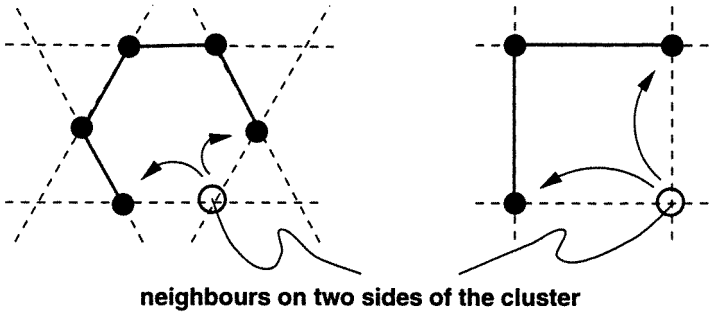

Figure 8. On the Kagomé lattice the first instance of a cluster with fewer than usual neighbours occurs for clusters of five sites (left picture). On a cubic lattice it occurs for clusters of three sites (right picture).

coefficients do not vanish, because the number of clusters of six or more sites were not included. Because $\bar{n}_6$ is the only missing term that can contribute terms of order p^6, we can conclude that

$$\bar{n}_6|_{q\to 1} = [\tfrac{1}{360}d(7d-1)(7d-2)(7d-3)(7d-4) - \tfrac{5}{3}d(d-1)]p^6. \tag{6}$$

The mean size of clusters at low probabilities, S, is defined as

$$S = \frac{\sum_s sp(s)}{\sum_s p(s)} = \frac{1}{p}\sum_s s^2\bar{n}_s. \tag{7}$$

Again equations (3) and (5) can be used, and $q = 1 - p$, to derive a power series

$$S(p) = 1 + 2(dp) + 2(dp)^2 + 2(dp)^3 + 2(dp)^4 + 2(dp)^5\left[1 + \frac{10}{d^3}\left(1 - \frac{1}{d}\right)\right] + \mathcal{O}(p^6). \tag{8}$$

The first few terms in this low-density expansion of $S(p)$ are remarkably simple. It is almost a geometric series, until the fifth power. The extra terms in the coefficient of $(dp)^5$ are due to the clusters that 'bite in their own tail'.

Although the resemblance of $S(p)$ to a geometric series is not exact, it does suggest that $1/d$ is the obvious candidate for the expansion parameter. This is in contrast to the cubic lattice, where it is $1/(2d-1)$, see equation (2). In fact, the resemblance to a geometric series suggests that a singularity of $S(p)$ should occur in the vicinity of $dp = 1$. Therefore, one can expect the percolation threshold to scale as

$$p_c \sim \frac{1}{d}. \tag{9}$$

In figure 4 the relation $p_c = 1/d$ is shown with a dashed line. The percolation thresholds for $d = 5$ and 6 are already reasonably well approximated by this relation. In an attempt to calculate the percolation threshold for $d = 8$, we computed 0.1059 ± 0.0005 for $L = 5$, 0.1086 ± 0.0006 for $L = 6$, and 0.1117 ± 0.0005 for $L = 7$. Based on the last two points one can fit the percolation threshold to be 0.120 ± 0.003, which is close to the value 0.125 one would expect on the basis of equation (9). However, the point for $L = 5$ does not lie on the same fit, indicating that these lattice sizes are not yet large enough. Therefore, there is probably also a small systematic error in the determination of the value 0.120.

When one wants to refine the scaling behaviour given by equation (9) with terms of the order of $1/d^2$ and further, analogous to equation (2), more terms in the series expansion would be required, plus a careful mathematical analysis of the radius of convergence of the series. This is beyond the scope of the present paper.

5. Random walks

It is interesting to study the return probability P_r of a random walker on a d-dimensional Kagomé lattice. Ishioka and Koiwa (1978) suggested that P_r is an upper bound for the site percolation threshold on any lattice: $P_r \geqslant p_c$. For Bethe lattices, the equal sign holds (Hughes and Sahimi 1982). The arguments given by Ishioka and Koiwa to support their conjecture are not exact, but the relation appears to work fairly well. P_r and p_c lie closer together, the more connected a lattice is. Also Sahimi *et al* (1983) studied the relation between a random walker (not self-avoiding) and percolation, albeit bond percolation.

The return probability of a random walker can be calculated numerically with a simple computer program. One can let N_w walkers perform at maximum N_s steps, and count the number of walkers that have re-visited the site they started from. Alternatively, one can let N_w walkers perform steps until they are either back at the origin or further away from the origin than a certain predefined distance. Both methods have been used to estimate P_r with an estimated inaccuracy of about 0.001. Note that there are two sources of inaccuracy. The first is a statistical uncertainty, which scales as $1/\sqrt{N_w}$; the second is a systematic error, because each walker is stopped at a certain moment (after N_s steps or at a given distance from the origin). For each of these walkers there is a finite probability that they would have reached the origin, when given enough time. As a result, the numerical estimates have a systematic error to the downside. This bias can be made smaller by using a large number of steps, or a large cut-off distance. In the calculation of the numbers quoted in table 1, $N_s = 10^6$ and higher has been used, and $N_w = 10^5$. The results for the cubic lattices are consistent with Finch (1997) and Flajolet (1995).

The numerical values for P_r are close to the percolation thresholds, especially for $d \geqslant 4$. It looks as if the return probability of a random walker obeys the same scaling relation as the percolation threshold. In the remainder of this section, therefore, a crude approximation for the return probability is calculated using simple arguments. This approximation corroborates the scaling of the return probability as $P_r \sim 1/d$.

Consider a random walker on the d-dimensional Kagomé lattice. Since all directions of the lattice are equivalent, it does not make a difference which step the walker makes first. Assume, without loss of generality, that the walker remains within the base polytope $\{i, \mathbf{0}\}$. Assume further, as a first approximation, that he stays within this polytope for a number of steps, and then returns to the origin. The walker can take an arbitrary number of steps within this base polytope, with a probability $(d-1)/(2d)$ (the walker can choose from $2d$ directions, d of which are outside the base polytope, and one of the $2d$ is the origin). After a number of steps the walker should step back to the origin, which happens with a probability $1/(2d)$. This approximation yields

$$P_{\mathrm{r},1} = \sum_{s=2}^{\infty} \frac{1}{2d} \left(\frac{d-1}{2d} \right)^{s-2} = \frac{1}{1+d}. \tag{10}$$

This approximation already reveals an interesting point: in high dimensions, the return probability scales as $P \sim 1/d$. Since the probability $1/(1+d)$ is the exact probability of return via a few selected paths, we also know that the exact probability on return via *any* path will be higher than $1/(1+d)$. It is therefore impossible that it is as low as $1/(2d-1)$, as is the case for cubic lattices.

One can improve on the above approximation by allowing the walker to step outside the base polytope occasionally. Choose, for instance, i sites x_i from which the walker steps outside. If the walker makes s steps within the base polytope before returning to the origin, there are $\binom{s-1}{i}$ possible choices (because the last of the s steps is to the origin):

$$P_{\mathrm{r},2} = \sum_{s=2}^{\infty} \frac{1}{2d} \left(\frac{d-1}{2d} \right)^{s-2} \times \sum_{i=0}^{s-1} \binom{s-1}{i} \left(\frac{1}{4d} \right)^{i}.$$

The factor $1/(4d)$ emerges because the walker has a probability of $1/2$ to step outside the base polytope, and a probability $1/(2d)$ to immediately step back to x_i. One can also allow the walker to make a number of additional steps, as long as he is only one step away from x_i and outside the base polytope. There are $(d-1)$ possibilities out of a total of $2d$ to make such a step

$$\begin{aligned} P_{\mathrm{r},2} &= \sum_{s=2}^{\infty} \frac{1}{2d} \left(\frac{d-1}{2d} \right)^{s-2} \times \sum_{i=0}^{s-1} \binom{s-1}{i} \left[\frac{1}{4d} \sum_{k=0}^{\infty} \left(\frac{d-1}{2d} \right)^{k} \right]^{i} \\ &= \frac{1}{d} \frac{1+3/(2d)}{1+3/(2d)+3/(2d^2)}. \end{aligned} \tag{11}$$

This type of reasoning can be taken a step further, yielding

$$P_{\mathrm{r},3} = \frac{1}{d} \frac{1+2/d+9/(4d^2)}{1+2/d+11/(4d^2)+9/(4d^3)}. \tag{12}$$

All the paths that are included in this way are paths where the walker returns to the origin through the base polytope he started in. The first contributions from paths that return from the opposite side are paths of six steps, see figure 8. As there are $2d(d-1)$ of such paths, the probability to return from the opposite side in six steps is $(d-1)/(2d)^5$, which is of the order $1/d^4$. Thus the conclusion that the return probability scales as $1/d$ remains unchanged.

As a numerical check on this scaling behaviour, the return probability for the eight-dimensional Kagomé lattice was calculated: $P_{\mathrm{r}} = 0.126 \pm 0.001$. This compares well with the approximation 0.124 from equation (12).

6. Discussion

The Kagomé lattice has rather different properties in d dimensions than the cubic lattice: it does not behave as a Bethe lattice in high dimensions, although one usually assumes that all lattices do. The series expansion of section 4 provides some insight into why this is the case. One clear difference with the cubic lattice is that the leading power of q in the expression for the number of clusters of s sites is $(s+1)d-(s-1)$ for the Kagomé lattice, but $2sd-2(s-1)$ for the cubic lattice. The coefficient of sd differs by a factor of two here. The significance of this power of q is that it is the 'coordination number' of a cluster of s sites, just as q is the coordination number of a single site. The underlying reason for the different powers of q is that two adjacent sites on the Kagomé lattice always have $d-1$ common neighbours, whereas two adjacent sites on the cubic lattice have none. In high dimensions this difference does not disappear, but instead becomes more important.

The same difference also explains why the return probability is different for these lattices. Since adjacent sites have $d-1$ common neighbours, there is, in high dimensions, an increasing number of ways to return to the origin in three steps. On a Bethe lattice, such paths do not exist: here a walker can only return to the origin by retracing his steps. Therefore, the Kagomé lattice does not behave as a Bethe lattice in high dimensions.

Going back to the two-dimensional Kagomé lattice, one could say that one of the reasons why it has a much higher site percolation threshold than the square lattice is because of its 'common neighbours'.

We can apply the same reasoning to *bond* percolation. The bond percolation threshold of the Kagomé lattice is also higher than that of the square lattice, but the difference is smaller than for the site percolation threshold. Two adjacent bonds on the square lattice always have two common neighbours. On the Kagomé lattice, two adjacent bonds have, depending on their relative position, two or three common neighbours. The former happens in two thirds of the situations, the latter in one third. Therefore, for *bond* percolation the Kagomé lattice has more resemblance to the square lattice, but still the two lattices are different. This is consistent with the difference in bond percolation thresholds being smaller, but not negligible.

Finally, let us consider the relation to the diamond lattice in d dimensions. Since the site percolation threshold of the Kagomé lattice scales as $p_c \sim 1/d = 2/q$, this holds for the bond percolation threshold of the diamond lattice as well. However, for the diamond lattice $q = d+1$, so $p_{c,\mathrm{dia}} \sim 1/(q-1)$, which is the familiar Bethe result once more. This highlights a more general property. Each bond problem can be mapped onto a site problem (see, e.g., Kesten 1982). When the bond problem is on a lattice with $q = q_b$, the lattice for the corresponding site problem will have $q_s = 2(q_b-1)$. As a consequence, for each class of lattices for which the bond percolation thresholds scale as $p_c \sim f(q)$, there is another class of lattices for which the site percolation thresholds scale as $p_c \sim f(\frac{1}{2}q+1)$. It would, therefore, be more consistent to describe bond percolation in terms of the number of neighbours a bond has, which is $2(q-1)$.

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