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Percolation processes in two dimensions I. Low-density series expansions

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Abstract. The derivation of low-density series expansions for the mean cluster size in random site and bond mixtures on a two-dimensional lattice is described briefly. New data are given for the triangular, simple quadratic and honeycomb lattices and their matching lattices.

1. Introduction

In this paper we describe the derivation of series expansions required for a study of random mixtures of sites (or bonds) in the low-density region on a two-dimensional lattice. We give new data for the perimeter polynomials and the mean cluster size expansion for the more usual lattices. We assume a general familiarity with the problem; recent reviews are by Shante and Kirkpatrick (1971) and Essam (1972); earlier general articles are by Frisch and Hammersley (1963), Fisher and Essam (1961) and Fisher (1964). The critical index, γ, for the mean cluster size is of importance in the theory of scaling (Kastelyn and Fortuin 1969, Essam and Gwilym 1971, Essam 1972). In a previous publication (Sykes *et al* 1973) we reported on a pilot study of the simple quadratic site problem; we now derive data for a comprehensive study of site and bond problems in two dimensions. The analysis of the new data is given in a companion paper (Sykes *et al* 1976).

2. Series expansions for the mean cluster size at low densities: site problem

The application of series expansions to a study of random mixtures and percolation processes was first introduced by Domb (conference on *Fluctuation Phenomenon and Stochastic Processes, Birkbeck College, London, March* 1959 and briefly reported in *Nature, Lond.* **184** 509) at a Symposium of the Physical Society and the method we describe is essentially based on notes taken by one of us. To illustrate the basic ideas we take as specific example a random mixture of black and white sites on the triangular lattice. We define as the primary species the black sites (probability p) and as the secondary species the white sites (probability $q = 1-p$). The low-density region corresponds to $p < p_c$ and in the very-low-density region as $p \to 0$ the only black clusters will be small. We illustrate the possible clusters of up to three sites in figure 1. Each cluster of black sites must be surrounded by sites of the opposite species. Denoting the expectation

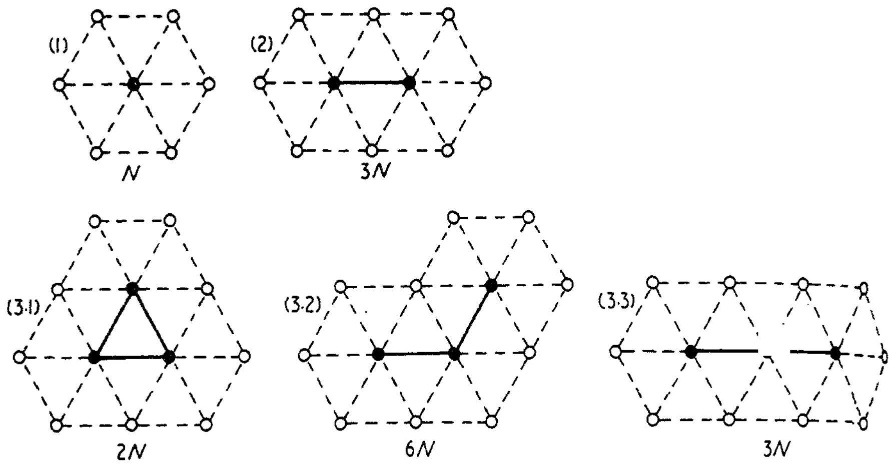

Figure 1. Clusters of up to three sites on the triangular lattice. ●, black sites; ○, white sites. The counts are for an N-site lattice.

(or mean number) per lattice site of clusters of size s (size being measured by the number of sites) by $\langle n_s \rangle$ we readily obtain by inspection:

$$\langle n_1 \rangle = pq^6$$
$$\langle n_2 \rangle = 3p^2q^8 \qquad (2.1)$$
$$\langle n_3 \rangle = 2p^3q^9 + 9p^3q^{10}$$

and in general

$$\langle n_s \rangle = p^s D_s(q). \qquad (2.2)$$

The coefficients of each power of p are polynomials D_s in q that summarize the average environmental situation for all the clusters of s sites. Unfortunately the problem presented by these *perimeter polynomials* is one of classical difficulty. Direct enumeration is difficult because of the rapid growth in the total number of possible clusters. We give in table 1 the values of $D_s(1)$ for the triangular, simple quadratic and honeycomb lattices. These total counts of the number of connected clusters (per site) have application to many other problems. They arise in the graph theoretic treatment of the cell growth problem (see the article by Harary 1967 for a bibliography) where they are often called *animals*; they have application to the enumeration of aromatic hydrocarbons and the theory of chemical graphs (Balaban and Harary 1968 and references there cited): as a pure mathematical problem they have been studied under the name of *polyominoes* (see the articles by Lunnon 1971†, 1972 and Golomb 1965). The numbers in table 1 correspond to *fixed* polyominoes; *free* polyominoes correspond to an enumeration of space-types (Domb 1960). For example there are three possible free polyominoes of size 3 illustrated in the figure by (3.1–3).

The asymptotic behaviour of the total number of connected clusters appears to be approximately represented by

$$D_s(1) \simeq As^{-\theta}\lambda^s \qquad (2.3)$$

† The number of clusters with 17 sites on the simple quadratic lattice there given is incorrect.

Table 1. Total number of connected clusters grouped by sites

Sites	Triangular	Simple quadratic	Honeycomb
1	1	1	1
2	3	2	$1\frac{1}{2}$
3	11	6	3
4	44	19	7
5	186	63	18
6	814	216	47
7	3 652	760	125
8	16 689	2 725	$337\frac{1}{2}$
9	77 359	9 910	919
10	362 671	36 446	$2\,526\frac{1}{2}$
11	1 716 033	135 268	7 008
12	8 182 213	505 861	$19\,584\frac{1}{2}$
13	39 267 086	1 903 890	55 097
14	189 492 795	7 204 874	$155\,875\frac{1}{2}$
15	918 837 374	27 394 666	443 080
16	4 474 080 844	104 592 937	1 264 630
17		400 795 844	3 622 431
18		1 540 820 542	10 409 249
19		5 940 738 676	29 997 257
20			86 669 481
21			250 997 035
22			$728\,445\,773\frac{1}{2}$

where θ is a constant and λ a lattice-dependent parameter. From a Padé approximant analysis (Gaunt and Guttmann 1974) we estimate that θ is very close to unity (corresponding to a logarithmic singularity in the generating function) and the indicated values of λ are:

$$\begin{aligned} &\text{Triangular} && \lambda = 5{\cdot}19 \pm 0{\cdot}03 \\ &\text{Simple quadratic} && \lambda = 4{\cdot}06 \pm 0{\cdot}02 \\ &\text{Honeycomb} && \lambda = 3{\cdot}04 \pm 0{\cdot}02 \end{aligned} \tag{2.4}$$

in good agreement with the estimates of Lunnon (1971, 1972).

Heap (1963) applied computers to the generation of perimeter polynomials and using the technique described by Martin (1974) we have generated perimeter polynomials for the more usual lattices. We quote those for the site problem on the triangular, simple quadratic and honeycomb lattices in the appendix. Perimeter polynomials summarize the basic configurational data but they can be usefully supplemented by the application of some general considerations whose practical application we describe briefly. (For a detailed theoretical treatment see, for example, Essam (1972) and Sykes and Essam (1964).)

At low densities the mean density of black sites, p, is obtained by weighting the mean number of clusters of size s by s and summing over all values of s. We have the formal relation

$$p = \sum_s s\langle n_s\rangle. \tag{2.5}$$

For any finite graph the right-hand side of (2.5) must reduce to p identically. For an infinite graph the perimeter polynomials provide a double series in p and q; we follow

Domb and suppose the expansion converges up to some $p' > 0$ and therefore that the mean density of black sites derived in this way is p if p is small enough. Formally the substitution $q = 1-p$ in (2.5) interpreted by (2.2) yields p identically as illustrated by the following scheme:

$$
\begin{aligned}
\langle n_1\rangle &= p-6p^2+15p^3-20p^4\ldots+\alpha_{1,n}p^n+\ldots\\
2\langle n_2\rangle &= \quad 6p^2-48p^3+168p^4\ldots+2\alpha_{2,n}p^n+\ldots\\
3\langle n_3\rangle &= \quad 33p^3-324p^4\ldots+3\alpha_{3,n}p^n+\ldots\\
4\langle n_4\rangle &= \quad 176p^4\ldots+4\alpha_{4,n}p^n+\ldots\\
&\vdots\\
\sum_s s\langle n_s\rangle &= p+0p^2+0p^3+0p^4\ldots+0p^n+\ldots.
\end{aligned}
\tag{2.6}
$$

The condition that the coefficient of p^4 must vanish determines the total number of clusters of four sites in conjunction with the perimeter polynomials (2.1) through D_3: this result generalizes to the statement that the formal identity (2.5), in conjunction with the perimeter polynomials through D_{n-1} determines the total number of clusters of n sites, $\alpha_{n,n} = D_n(1)$. For most two-dimensional lattices the expansion of the mean number of clusters

$$\sum_s \langle n_s\rangle = \sum_n k_n p^n \tag{2.7}$$

can be obtained by special methods. (A detailed treatment is given by Sykes and Essam 1964, 1966). By graph theoretic methods, or by expanding the perimeter polynomials of the corresponding matching lattice in powers of q, the expansion (2.7) is readily extended well beyond the availability of the perimeter polynomials. This yields an additional constraint on (2.6); from the relations

$$\sum_{s=1}^{n} s\alpha_{s,n} = 0 \qquad n > 1 \tag{2.8}$$

$$\sum_{s=1}^{n} \alpha_{s,n} = k_n \tag{2.9}$$

it follows that the total number of clusters of n sites is determined by the perimeter polynomials through D_{n-2} in conjunction with the identity (2.6) and the expansion (2.7) through p^n. We have exploited this property in deriving the data for table 1; the total number of clusters in each case has been obtained two orders further than the perimeter polynomials quoted in the appendix.

The mean size of clusters at *low* densities, $S(p)$, is defined as the mean number of black sites connected to any black site:

$$S(p) = \frac{1}{p}\sum_s s^2\langle n_s\rangle = \sum_n b_n p^n. \tag{2.10}$$

The successive coefficients b_n are determined by the $\alpha_{s,n}$ of (2.6) and the same economies exploited to derive the total number of clusters apply to the derivation of these coefficients. The coefficients quoted in table 2 have all been derived from perimeter polynomials supplemented in this way, two extra coefficients having been added in every case. If the total number of clusters at the next order were known, then in conjunction with (2.8)

Table 2. Coefficients for expansion of $S(p) = \Sigma b_r p^r$. Site problem.

r	Triangular	Simple quadratic	Honeycomb	Simple quadratic matching	Honeycomb matching
1	6	4	3	8	12
2	18	12	6	32	66
3	48	24	12	108	312
4	126	52	24	348	1 368
5	300	108	33	1 068	5 685
6	750	224	60	3 180	23 034†
7	1 686	412	99	9 216	90 288†
8	4 074	844	156	26 452†	350 124†
9	8 868	1 528	276	73 708†	1 318 767†
10	20 892	3 152	438	206 872†	4 986 324†
11	44 634†	5 036†	597	563 200†	
12	103 392†	11 984†	1 134†	1 555 460†	
13	216 348†	15 040†	1 404†		
14	499 908†	46 512†	2 904†		
15	1 017 780†	34 788†	3 522†		
16		197 612†	6 876†		
17		4 036†	7 548†		
18		929 368†	16 680†		
19			18 153†		
20			39 846†		
21			41 805†		

† New coefficient.

and (2.9) an extra coefficient could be derived for $S(p)$; in general although computer enumeration of the total number of clusters is faster than the generation of perimeter polynomials (which is of necessity more detailed) it is not fast enough to exploit this possibility.

3. Series expansions for the mean cluster size at low densities: bond problem

For a random mixture of *bonds* it is sometimes convenient to consider the corresponding bond problem separately; however because of the bond-to-site transformation (Fisher and Essam 1961) bond problems may always be treated as site problems on the corresponding *covering lattice*. In general the covering lattice will have crossing bonds but the bond problem on the honeycomb lattice corresponds to the site problem on the Kagomé lattice. Thus if γ is a function of dimension only we must expect the same value for two-dimensional site problems as for two-dimensional bond problems. We have derived data for the bond problem on the honeycomb, simple quadratic and triangular lattices; these lattices have the advantage that their critical concentrations are known (Sykes and Essam 1964). Unfortunately the corresponding values of the cluster growth parameter λ in (2.3):

$$\begin{aligned}
&\text{Triangular} && \lambda = 8{\cdot}626 \pm 0{\cdot}006 \\
&\text{Simple quadratic} && \lambda = 5{\cdot}210 \pm 0{\cdot}004 \qquad (3.1) \\
&\text{Honeycomb} && \lambda = 3{\cdot}368 \pm 0{\cdot}002
\end{aligned}$$

are somewhat larger than for the corresponding site problems and this restricts the number of perimeter polynomials that can be obtained for a given expenditure of computer time. The general observations of the previous section apply to these problems and we give the expansion coefficients for $S(p)$ in table 3.

Table 3. Coefficients for expansion of $S(p) = \Sigma b_r p^r$. Bond problem.

r	Triangular	Simple quadratic	Honeycomb
1	10	6	4
2	46	18	8
3	186	48	16
4	706	126	32
5	2 568	300	54
6	9 004	762	100
7	30 894	1 668	182
8	103 832	4 216	328
9	343 006	8 668	494
10	1 123 770†	21 988	984
11		43 058	1 572
12		110 832†	2 656
13		202 432†	4 212
14		561 020†	8 162
15			11 176†
16			21 704†
17			30 994†
18			60 548†

† New coefficient.

Acknowledgment

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Appendix. Perimeter polynomials for the site problem

Triangular lattice

$D_1 = q^6 \qquad D_2 = 3q^8 \qquad D_3 = 2q^9 + 9q^{10}$

$$D_4 = 3q^{10} + 12q^{11} + 29q^{12}$$

$$D_5 = 6q^{11} + 21q^{12} + 66q^{13} + 93q^{14}$$

$$D_6 = 14q^{12} + 43q^{13} + 153q^{14} + 298q^{15} + 306q^{16}$$

$$D_7 = q^{12} + 30q^{13} + 111q^{14} + 366q^{15} + 840q^{16} + 1\,290q^{17} + 1\,014q^{18}$$

$$D_8 = 6q^{13} + 69q^{14} + 291q^{15} + 957q^{16} + 2\,349q^{17} + 4\,299q^{18} + 5\,310q^{19} + 3\,408q^{20}$$

$$D_9 = 27q^{14} + 166q^{15} + 803q^{16} + 2\,592q^{17} + 6\,734q^{18} + 13\,634q^{19} + 20\,469q^{20} + 21\,372q^{21} + 11\,562q^{22}$$

$$D_{10} = 3q^{14}+86q^{15}+492q^{16}+2\,157q^{17}+7\,484q^{18}+19\,416q^{19}+42\,963q^{20}$$
$$+72\,256q^{21}+93\,747q^{22}+84\,468q^{23}+39\,599q^{24}$$

$$D_{11} = 24q^{15}+255q^{16}+1\,542q^{17}+6\,111q^{18}+21\,810q^{19}+58\,164q^{20}+133\,380q^{21}$$
$$+247\,974q^{22}+364\,314q^{23}+415\,422q^{24}+330\,414q^{25}+136\,623q^{26}$$

$$D_{12} = 2q^{15}+117q^{16}+801q^{17}+4\,771q^{18}+18\,608q^{19}+63\,804q^{20}+179\,186q^{21}$$
$$+417\,270q^{22}+829\,725q^{23}+1\,348\,139q^{24}+1\,762\,933q^{25}$$
$$+1\,800\,147q^{26}+1\,282\,260q^{27}+474\,450q^{28}$$

$$D_{13} = 27q^{16}+426q^{17}+2\,858q^{18}+14\,442q^{19}+58\,902q^{20}+192\,626q^{21}+554\,523q^{22}$$
$$+1\,331\,286q^{23}+2\,746\,954q^{24}+4\,819\,800q^{25}+6\,996\,003q^{26}$$
$$+8\,279\,398q^{27}+7\,664\,811q^{28}+4\,948\,374q^{29}+1\,656\,656q^{30}$$

$$D_{14} = 3q^{16}+168q^{17}+1\,524q^{18}+10\,029q^{19}+46\,119q^{20}+185\,220q^{21}+605\,766q^{22}$$
$$+1\,730\,943q^{23}+4\,287\,699q^{24}+9\,131\,949q^{25}+16\,871\,550q^{26}$$
$$+26\,571\,525q^{27}+35\,061\,399q^{28}+37\,965\,417q^{29}+32\,198\,928q^{30}$$
$$+19\,012\,074q^{31}+5\,812\,482q^{32}.$$

Simple quadratic lattice

$D_1 = q^4 \qquad D_2 = 2q^6 \qquad D_3 = 4q^7+2q^8$

$$D_4 = 9q^8+8q^9+2q^{10}$$

$$D_5 = q^8+20q^9+28q^{10}+12q^{11}+2q^{12}$$

$$D_6 = 4q^9+54q^{10}+80q^{11}+60q^{12}+16q^{13}+2q^{14}$$

$$D_7 = 22q^{10}+136q^{11}+252q^{12}+228q^{13}+100q^{14}+20q^{15}+2q^{16}$$

$$D_8 = 4q^{10}+80q^{11}+388q^{12}+777q^{13}+818q^{14}+480q^{15}+152q^{16}+24q^{17}+2q^{18}$$

$$D_9 = 28q^{11}+291q^{12}+1\,152q^{13}+2\,444q^{14}+2\,804q^{15}+2\,089q^{16}+856q^{17}+216q^{18}$$
$$+28q^{19}+2q^{20}$$

$$D_{10} = 4q^{11}+154q^{12}+986q^{13}+3\,676q^{14}+7\,612q^{15}+9\,750q^{16}+8\,192q^{17}+4\,330q^{18}$$
$$+1\,416q^{19}+292q^{20}+32q^{21}+2q^{22}$$

$$D_{11} = 52q^{12}+644q^{13}+3\,530q^{14}+11\,772q^{15}+24\,472q^{16}+33\,336q^{17}+31\,202q^{18}$$
$$19\,532q^{19}+8\,130q^{20}+2\,180q^{21}+380q^{22}+36q^{23}+2q^{24}$$

$$D_{12} = 9q^{12}+325q^{13}+2\,644q^{14}+12\,502q^{15}+38\,694q^{16}+79\,730q^{17}+114\,342q^{18}$$
$$+115\,502q^{19}+83\,183q^{20}+41\,136q^{21}+14\,064q^{22}+3\,208q^{23}+480q^{24}$$
$$+40q^{25}+2q^{26}$$

$$D_{13} = q^{12}+112q^{13}+1\,660q^{14}+10\,480q^{15}+44\,574q^{16}+129\,020q^{17}+264\,482q^{18}$$
$$+391\,432q^{19}+423\,786q^{20}+337\,144q^{21}+193\,820q^{22}+79\,240q^{23}$$
$$+22\,993q^{24}+4\,508q^{25}+592q^{26}+44q^{27}+2q^{28}$$

$$D_{14} = 28q^{13}+828q^{14}+7\,508q^{15}+41\,408q^{16}+158\,532q^{17}+437\,186q^{18}+887\,404q^{19}$$
$$+1\,347\,560q^{20}+1\,538\,558q^{21}+1\,331\,170q^{22}+859\,176q^{23}+410\,302q^{24}$$
$$+142\,624q^{25}+35\,664q^{26}+6\,160q^{27}+716q^{28}+48q^{29}+2q^{30}$$

$$D_{15} = 4q^{13}+332q^{14}+4\,608q^{15}+33\,046q^{16}+160\,296q^{17}+566\,886q^{18}+1\,497\,208q^{19}$$
$$+3\,014\,432q^{20}+4\,655\,776q^{21}+5\,565\,832q^{22}+5\,144\,236q^{23}$$
$$+3\,662\,778q^{24}+1\,978\,664q^{25}+805\,740q^{26}+242\,484q^{27}+53\,286q^{28}$$
$$+8\,152q^{29}+852q^{30}+52q^{31}+2q^{32}$$

$$D_{16} = 106q^{14}+2\,406q^{15}+23\,311q^{16}+140\,111q^{17}+615\,940q^{18}+2\,031\,394q^{19} +5\,185\,083q^{20}+10\,325\,335q^{21}+16\,192\,608q^{22}+20\,054\,044q^{23} +19\,633\,804q^{24}+15\,125\,366q^{25}+9\,086\,116q^{26}+4\,207\,428q^{27} +1\,487\,681q^{28}+393\,736q^{29}+76\,826q^{30}+10\,584q^{31}+1\,000q^{32} +56q^{33}+2q^{34}$$

$$D_{17} = 22q^{14}+1\,104q^{15}+14\,385q^{16}+110\,132q^{17}+581\,976q^{18}+2\,346\,548q^{19} +7\,313\,380q^{20}+18\,091\,092q^{21}+35\,693\,692q^{22}+56\,587\,516q^{23} +72\,212\,800q^{24}+74\,161\,528q^{25}+61\,122\,466q^{26}+40\,085\,932q^{27} +20\,749\,892q^{28}+8\,377\,000q^{29}+2\,609\,116q^{30}+614\,816q^{31} +107\,801q^{32}+13\,424q^{33}+1\,160q^{34}+60q^{35}+2q^{36}.$$

Honeycomb lattice

$D_1 = q^3 \qquad D_2 = 1\tfrac{1}{2}q^4 \qquad D_3 = 3q^5$

$D_4 = 7q^6 \qquad D_5 = 3q^6+15q^7$

$D_6 = \tfrac{1}{2}q^6+15q^7+31\tfrac{1}{2}q^8$

$D_7 = 3q^7+60q^8+62q^9$

$D_8 = 37\tfrac{1}{2}q^8+177q^9+123q^{10}$

$D_9 = 12q^8+190q^9+471q^{10}+246q^{11}$

$D_{10} = 1\tfrac{1}{2}q^8+111q^9+744q^{10}+1\,167q^{11}+503q^{12}$

$D_{11} = 39q^9+705q^{10}+2\,361q^{11}+2\,874q^{12}+1\,029q^{13}$

$D_{12} = 9q^9+449\tfrac{1}{2}q^{10}+3\,006q^{11}+7\,078q^{12}+6\,927q^{13}+2\,115q^{14}$

$D_{13} = q^9+207q^{10}+2\,721q^{11}+11\,181q^{12}+20\,160q^{13}+16\,473q^{14}+4\,354q^{15}$

$D_{14} = 69q^{10}+1\,902q^{11}+12\,937\tfrac{1}{2}q^{12}+37\,635q^{13}+55\,794q^{14}+38\,526q^{15}+9\,012q^{16}$

$$D_{15} = 15q^{10}+1\,083q^{11}+11\,758q^{12}+52\,311q^{13}+120\,537q^{14}+149\,349q^{15} +89\,304q^{16}+18\,723q^{17}$$

$$D_{16} = 1\tfrac{1}{2}q^{10}+492q^{11}+8\,895q^{12}+57\,960q^{13}+194\,656\tfrac{1}{2}q^{14}+367\,394q^{15} +390\,750q^{16}+205\,416q^{17}+39\,065q^{18}$$

$$D_{17} = 162q^{11}+5\,796q^{12}+53\,949q^{13}+252\,297q^{14}+674\,724q^{15}+1\,081\,608q^{16} +1\,001\,814q^{17}+470\,322q^{18}+81\,759q^{19}$$

$$D_{18} = 33q^{11}+3\,258q^{12}+43\,728q^{13}+275\,614\tfrac{1}{2}q^{14}+998\,280q^{15}+2\,227\,525\tfrac{1}{2}q^{16} +3\,085\,374q^{17}+2\,531\,651q^{18}+1\,072\,167q^{19}+171\,618q^{20}$$

$$D_{19} = 3q^{11}+1\,522q^{12}+31\,536q^{13}+262\,848q^{14}+1\,248\,556q^{15}+3\,696\,108q^{16} +7\,046\,169q^{17}+8\,595\,792q^{18}+6\,317\,457q^{19}+2\,436\,234q^{20} +361\,032q^{21}$$

$$D_{20} = 565\tfrac{1}{2}q^{12}+20\,355q^{13}+224\,571q^{14}+1\,365\,312q^{15}+5\,186\,827\tfrac{1}{2}q^{16} +12\,951\,117q^{17}+21\,572\,958q^{18}+23\,461\,497q^{19}+15\,606\,471q^{20} +5\,518\,698q^{21}+761\,109q^{22}.$$

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