Revision of upper estimate of percolation threshold on square lattice

Yu.P. Virchenko, Yu.A. Tolmacheva

The more exact upper estimate of the percolation threshold for the site problem on the quadratic lattice \( \mathbb{Z}^2 \) have been found on the basis of the cluster decomposition. It is done by the number estimate of cycles on \( \mathbb{Z}^2 \) which maybe external boundaries of finite clusters.

1. Introduction

Generally, percolation theory studies the connectedness relation for random sets in topological spaces. Problems representing greatest interest in the theory appear in noncompact topological spaces.

The existence of a noncompact connected component in random set realizations with nonzero probability is the crucial question in the theory [1]. In such a general setting of the problem, however, it is impossible to obtain any strong results. That is why the basic objects of the percolation theory are random sets in \( \mathbb{R}^d \) and \( \mathbb{Z}^d \) at \( d = 2, 3 \) generated by stationary random fields [1, 2]. The first case corresponds to so-called continuous percolation theory and the second one – to discrete percolation theory. This limitation is a consequence of the fact that it is the problem set in such a way is mainly needed in physical applications. Therefore, it may be considered as the object of mathematical physics. However, despite the above restriction, the basic problem is very complicated and hardly lends itself to exact mathematical study. Rigorous results referring to discrete percolation theory which is its mostly developed direction have been summarized in the monograph [3]. Later results and also results referring to continuous theory have been summarized in the excellent review [4]. Physical literature dealing with different nonrigorous heuristic approaches to the investigation of the percolation phenomenon, computer experiments and special applications of the theory in theoretical physics is giant and we shall not pay attention to it in this short introduction to the problem.

Despite of the great flow of publications at 80-th in physical literature and simultaneously appearance of some reviews in which mathematical results are summarized, main questions of the percolation theory considered as the object of mathematical physics remain without answers up to now. It is the situation even for simplest case being studied in the theory when random set is generated by Bernoulli’s field on \( \mathbb{Z}^2 \). Even for this case any algorithm of the percolation threshold calculation (see §2) and, more generally, any algorithm of percolation probability evaluation was not found for an arbitrary periodic graph [1]. Our communication is dealing with the revision of upper estimate of
percolation threshold as compared to what may be found in literature
[4, 5] for the periodic graph on \( \mathbb{Z}^2 \) which is called the square lattice.

2. Percolation theory problem on \( \mathbb{Z}^2 \)

Let us consider an infinite graph with the vertex set \( \mathbb{Z}^2 \). For simplicity of statements and arguments, we shall study it as one immersed into \( \mathbb{R}^2 \). The adjacency relation on the graph is defined by the set of pairs \( \{(x, y) \in \mathbb{Z}^2 : x \varphi y \} \) where \( x \varphi y \) if and only if \( y = x \pm e_1 \) or \( y = x \pm e_2 \), \( e_1 = (1, 0) \), \( e_2 = (0, 1) \). We shall follow the terminology of statistical physics and that is why we shall call such a graph the square lattice and denote it by the same symbol \( \mathbb{Z}^2 \).

Let \( \{\tilde{c}(x)\} \) is the Bernoulli random field with the parameter

\[
c = \Pr\{\tilde{c}(x) = 1\}
\]

which is said to be the concentration. Below, the tilde marks the randomness of used objects. The field \( \{\tilde{c}(x)\} \) induces the random set with realizations \( \{\tilde{M} : \tilde{M} \subset \mathbb{Z}^2\} \) where \( \tilde{M} = \{x : \tilde{c}(x) = 1\} \). Sometimes we shall call these realizations configurations of completed vertices or, simply, configurations. This probability distribution for possible realizations \( \tilde{M} \) is clearly determined completely by the following probability collection

\[
\Pr\{\tilde{M} : A \subset \tilde{M}\} = c^{|A|}, \quad A \subset \mathbb{Z}^2.
\]

Here and further \(| \cdot | = \text{Card}\{\cdot\}\).

Naturally, the adjacency relation \( \varphi \) induces the connectedness relation for vertices having included into any configuration \( \tilde{M} \). We shall call two vertices \( x \) and \( y \) linked in \( \tilde{M} \) if there exists a path \( (x_i; i = 0, 1, 2, ..., n) \), \( x_i \in \tilde{M} \), \( x_0 = x \), \( x_n = y \) and \( x_i \varphi x_{i+1}, i = 0, 1, 2, ..., n - 1 \). The connectedness of vertices of \( \tilde{M} \) is the equivalence relation. Therefore, each configuration \( \tilde{M} \) is uniquely decomposed on some disjoint equivalence classes \( \tilde{M} = \bigcup_{j \in \mathbb{N}} \tilde{W}_j \) generated by the connectedness relation of vertices. These classes we shall name clusters. The collection of clusters related to configurations \( \tilde{M} \) will be denoted by \( \mathcal{W}[\tilde{M}] = \{\tilde{W}_j : j \in \mathbb{N}\} \). If \( x \in \tilde{W}_j \) for a \( j \in \mathbb{N} \) in configuration \( \tilde{M} \), then we shall denote this cluster \( \tilde{W}_j \) by \( \tilde{W}(x) \) [3].

Let us introduce the random field \( \{\tilde{a}(x) ; x \in \mathbb{Z}^2\} \) on the base of the set \( \tilde{M} \),

\[
\tilde{a}(x) = \begin{cases} 1 & \text{if } x \in \tilde{W} \subset \tilde{M}, \ |\tilde{W}(x)| < \infty, \\ 0 & \text{otherwise}. \end{cases}
\]

In view that \( \{\tilde{c}(x)\} \) is the uniform field (i.e. the probability measure is invariant relative to translations on vectors \( (n_1 e_1 + n_2 e_2), n_1, n_2 \in \mathbb{Z} \)), the random field \( \{\tilde{a}(x)\} \) is uniform too. Therefore, the probability

\[
Q(c) = \Pr\{\tilde{a}(x) = 1\}
\]
does not depend on \( x \in \mathbb{Z}^2 \). This probability is a nondecreasing function of \( c \) [3]. If \( Q(c) > 0 \), then the percolation on the \( \{c(x)\} \) is said to exist. In connection with this fact, the following characteristic value is introduced

\[
c^* = \sup\{c : Q(c) = 0\}.
\]

\( c^* \) is called the percolation threshold.

3. Finite clusters on \( \mathbb{Z}^2 \)

At construction of some upper estimates of the probability \( Q(c) \), it is necessary to enumerate all finite clusters \( W(x) \) including the fixed vertex \( x \). We perform the enumeration by using the concept of the external boundary for each finite cluster. To this end, let us introduce on \( \mathbb{Z}^2 \) the following new concept of the adjacency relation \( \bar{\varphi} \) side by side with the adjacency relation \( \varphi \) [3,4]. We denote \( \bar{\mathbb{Z}}^2 \) the corresponding graph having the same vertex set but with the adjacency relation \( \bar{\varphi} \).

Vertices \( x \) and \( y \) are named the \( \varphi \)-adjacent ones if one of two cases takes place: 1) \( x \varphi y \), 2) either \( y = x + e_1 \pm e_2 \) or \( y = x - e_1 \pm e_2 \).

The relation \( \bar{\varphi} \) induces the new relation of vertex connectedness on each configuration \( \bar{\mathcal{M}} \). This connectedness relation is the equivalence relation too and it leads to a decomposition of \( \bar{\mathcal{M}} \) on some connected sets of vertices relative to \( \bar{\varphi} \).

Let us introduce the external boundary concept of a finite cluster on \( \mathbb{Z}^2 \).

Definition 1. The set \( \partial W \) is named the boundary of the cluster \( W \) if it consists of those vertices \( y \) which are \( \varphi \)-adjacent to vertex \( x \) in the cluster \( W \) but do not belong to it.

Definition 2. The external boundary \( \bar{\partial} W \) of the cluster \( W \) is the set of vertices \( u \in \partial W \) such that for each of them there exists an infinite \( \varphi \)-path \( \alpha(u) \) on completed vertices of \( \mathbb{Z}^2 \) and, moreover, \( u \) is the unique vertex in \( \alpha(u) \) belonging to the union \( W \cup \partial W \).

Further classification of finite clusters \( W(x) \) is performed by the enumeration of all possible external boundaries \( \bar{\partial} W(x) \). Following statement is the key for such enumeration. It repeats the corresponding statement in the monograph [3] with the exception of the last item.

Theorem 1. Let \( W(x) \) be a finite cluster for a fixed vertex \( x \), \( |W(x)| < \infty \). Then \( W(x) \) has a nonempty finite external boundary \( \bar{\partial} W(x) \) having following properties.

1. \( \bar{\partial} W(x) \) is the \( \bar{\varphi} \)-connected vertex set in \( \bar{\mathbb{Z}}^2 \) which presents the cycle i.e. \( \bar{\partial} W(x) = (x_1, x_2, ..., x_n) \) where \( x_i \neq x_j, i \neq j, n = |\bar{\partial} W(x)|, x_i \bar{\varphi} x_{i+1}, i = 1, 2, ..., n, x_{n+1} = x_0 \) and each vertex has only two \( \bar{\varphi} \)-adjacent vertices in the \( \gamma \). It is possible to introduce the definite orientation on \( \bar{\partial} W(x) \). (it will be used the counter-clockwise orientation in further arguments.)
2. The vertex \( x \) is contained in the finite set \( \text{Int}[\partial W(x)] \) defined by
\[
\text{Int}[\partial W(x)] \equiv \{ u \not\in \partial W(x) : \forall (\alpha(u) : |\alpha(u)| = \infty) (\alpha(u) \cap \partial W(x) \neq \emptyset) \};
\]

3. Let \( u, v, w \in \partial W(x) \) be three \( \varphi \)-adjacent vertices following one after another according to the introduced orientation. Then if \( u \varphi v \), the vertex \( w \) belongs necessarily to one of the following collection:
   a) in the case \( u \varphi v \) the set of three elements \( \{2v - u, 2v - u \pm e\} \) where \( e \) is a unit basis vector that is orthogonal to the vector \( (v - u) \);
   b) in the case \( v = u + \varepsilon(e_1 - e_2) \) the set of five elements
      \[
      \{2v - u, 2v - u + \varepsilon e_1, 2v - u - \varepsilon e_2, 2v - u \pm e'/2\}
      \]
      where \( e' \) be an orthogonal vector to \( (v - u) \) and \( |e'| = \sqrt{2} \) and \( \varepsilon = \pm 1 \).

The proof of first and second statements of Theorem 1 is obvious (see [3]). What about the last statement, it is easy to verify its justification from the explaining figure 1(a, b). The full rigorous proof is found by us; it is quite tedious and goes beyond the scope of this communication. Unlike the proof of the analogous theorem in [3], our arguments are not used an application of Jordan’s theorem. Further we omit the proof and pass to the proof of the main statement in next paragraphs.

4. The cluster decomposition on \( \mathbb{Z}^2 \)

We shall consider the probability \( 1 - Q(c) = \Pr\{ \tilde{a}(0) = 0 \} \). Let \( \mathcal{A} = \{ W : W = W(0) \text{ is cluster}, |W| < \infty \} \) be the collection of all finite clusters including the vertex 0. We define the event
\[
A(W) = \{ \tilde{M} : \tilde{W} = W, 0 \in \tilde{M}, \tilde{W} \in \{ \tilde{W}_j : j \in \mathbb{N} \} \}
\]
for any cluster \( W \in \mathcal{A} \). This event has the definite probability
\[
\Pr\{ A(W) \} = c^{|W|}(1 - c)^{|\partial W|}.
\] (1)

According to statements in the previous section, any cluster of this collection \( \mathcal{A} \) is corresponded to a cycle \( \gamma \). Vertices of this cycle are \( \varphi \)-adjacent and such that \( 0 \in \text{Int}[\gamma] \). In this connection, let us introduce in consideration the collection \( \mathcal{B} \) of all \( \varphi \)-cycles having the last property. Let \( B(\gamma) \) be the event
\[
B(\gamma) = \{ \tilde{M} : 0 \in \tilde{M}, \tilde{W}(0) \in \mathcal{W}[\tilde{M}], \partial \tilde{W}(0) = \gamma \}
\] (2)
defined for any $\varphi$-cycle $\gamma \in \mathcal{B}$. It is represented by the finite union of mutually disjoint events

$$B(\gamma) = \bigcup_{W \in \mathcal{A} : \partial W = \gamma} A(W). \quad (3)$$

Hence, according to (1) and (3), such event has the definite probability

$$P(\gamma) = \Pr\{B(\gamma)\}.$$ 

It is equal

$$P(\gamma) = \sum_{W \in \mathcal{A} : \partial W = \gamma} \Pr\{A(W)\} = \sum_{W \in \mathcal{A} : \partial W = \gamma} c^{|W|}(1 - c)^{|\partial W|}.$$

Let us note that

$$\{\tilde{a}(0) = 0\} = \bigcup_{W \in \mathcal{A}} A(W). \quad (4)$$

The collection $\mathcal{A}$ is decomposed on some disjoint classes of clusters. Each class consists of those clusters $W \in \mathcal{A}$ which have the same external boundary. It is realized $\partial W = \gamma$ for them. Therefore, the following representation is correct

$$\bigcup_{W \in \mathcal{A}} ... = \bigcup_{\gamma \in \mathcal{B}} \bigcup_{W \in \mathcal{A} : \partial W = \gamma} ....$$

Then we obtain

$$\{\tilde{a}(x) = 0\} = \bigcup_{\gamma \in \mathcal{B}} B(\gamma)$$

using (3). Finally, we come to the statement

**Theorem 2.** The probability $1 - Q(c)$ is represented by the decomposition

$$1 - Q(c) = \sum_{\gamma \in \mathcal{B}} P(\gamma). \quad (5)$$

Usually, such decomposition is said to be the cluster one in the percolation theory [4].

5. The main theorem

The cluster decomposition (5) is represented by the sum of probabilities of some disjoint events. Therefore, definitely, the cluster decomposition is convergent. The function $Q(c)$ is not equal to zero only if $c > c^* > 0$. So, it is not an analytic function on the concentration $c$ and $c = c^*$ is its the singular point. Earlier [4], it was obtained that
$6/7 > 3 > 1/3$. We give the improvement of the upper estimate at the below-formulated statement.

**Theorem 3.** The inequality $c^* \leq c_0 = 3 - \sqrt{5}$ is correct for Bernoulli’s random field on $\mathbb{Z}^2$.

**Proof.** We use the elementary estimate

$$P(\gamma) \leq (1 - c)^{|\gamma|},$$

that follows from the Definition 2 and Eq.(2). Using it and Eq.(5), we come to the upper boundary

$$\sum_{\gamma \in \mathcal{B}} P(\gamma) \leq \sum_{\gamma \in \mathcal{B}} (1 - c)^{|\gamma|} = \sum_{\gamma \in \mathcal{B} : |\gamma| = 2k} (1 - c)^{2k} r_k \quad (6)$$

where $r_k = \text{Card}\{\gamma \in \mathcal{B} : |\gamma| = 2k\}, k \geq 2$.

Further, we shall find the upper estimate for the value $r_k$. Consider the infinite path $\alpha(0) = (je_1; j = 0, 1, 2...)$ with initial vertex 0. Then, according to Theorem 1 (2), each cycle $\gamma \in \mathcal{B}$ necessarily crosses the path in some vertices. Let us select the vertex in this set of all intersection vertices which is nearest to the vertex 0. Denote it by $z_\gamma$. All cycles of $\mathcal{B}$ is decomposed on disjoint classes $C_\gamma$, i.e. the cycles having the same vertex $z_\gamma$ belong to the same class. This class decomposition induces the decomposition of the cycle set $\{\gamma \in \mathcal{B} : |\gamma| = 2k\}$ on corresponding classes $C_i^{(k)}$ where $l$ is the distance from 0 to $z_\gamma$. In addition, $l < k$ and therefore,

$$\{\gamma \in \mathcal{B} : |\gamma| = 2k\} = \bigcup_{l=1}^{k-1} C_i^{(k)}, \quad r_k = \sum_{l=1}^{k-1} |C_i^{(k)}|.$$ 

Let $\gamma = (x_0, x_1, x_2, ..., x_{2k-1}, x_2k = z_\gamma)$. According to the earlier introduced orientation, the vertex $x_1$ that follows after $x_0$ in the cycle $\gamma$ may be one of the set only

$$\left(z_\gamma + e_1, z_\gamma + e_1 + e_2, z_\gamma + e_2, z_\gamma - e_1 + e_2\right). \quad (7)$$

Using this ordering, cycles belonging to the same class $C_i^{(k)}$ are distributed on disjoint collections $C_i^{(k,i)}$, $i = 1, 2, 3, 4$ independence of the selection of the vertex $x_1$ in the cycle $\gamma$. Hence,

$$C_i^{(k)} = \bigcup_{i=1,2,3,4} C_i^{(k,i)}, \quad \left|C_i^{(k)}\right| = \sum_{i=1,2,3,4} \left|C_i^{(k,i)}\right|.$$ 

We obtain as the result

$$r_k = \sum_{i=1}^{k-1} \sum_{i=1,2,3,4} \left|C_i^{(k,i)}\right|.$$
We must find upper estimate of the value $|C_l^{(k,i)}|$. It is easy to see that $C_l^{(k,i)} \subset \mathcal{P}_l^{(2k-1,i)}$ where $\mathcal{P}_l^{(2k-1,i)}$ is the set of paths beginning at the vertex $z_\gamma$ and the distance from $z_\gamma$ to the vertex 0 along the path $\alpha(0)$ is equal to $l$. Besides, they have the length $2k - 1$ and the vertex $x_1$ is the $i$-th in the finite sequence (7). We sort out paths $\gamma$ with the length $2k$ but not with $2k$. It is connected with the fact that the last edge $x_{2k-1} \overline{\varphi} x_0$ of the cycle $(x_0, x_1, ..., x_{2k-1}, x_0)$ is fixed by the collection of vertices $x_0, x_1, ..., x_{2k-1}$. Therefore,

$$|C_l^{(k,i)}| \leq |\mathcal{P}_l^{(2k-1,i)}| = s_{2k-1}.$$

It is easy to see that $s_n$ does not depend on $l$ and $i$ due to our construction. Let us represent

$$s_n = s_n^+ + s_n^\times$$

where

$$s_n^+ = \text{Card}\{\gamma \in \mathcal{P}_l^{(n,i)} : x_{n-1} \varphi x_n\},$$

$$s_n^\times = \text{Card}\{\gamma \in \mathcal{P}_l^{(n,i)} : x_{n-1} \overline{\varphi} x_n, x_{n-1} \varphi x_n\}.$$

We introduce the two-component vector $[s_n^+, s_n^\times]$ (not distinguishing column-vectors and tuple-vectors). Then the following equation takes place

$$\begin{bmatrix} s_n^+ \\ s_n^\times \end{bmatrix} = T \begin{bmatrix} s_{n-1}^+ \\ s_{n-1}^\times \end{bmatrix}$$

with the transfer matrix

$$T = \begin{bmatrix} 1 & 2 \\ 2 & 3 \end{bmatrix},$$

according to Theorem 1 (3). Hence,

$$\begin{bmatrix} s_n^+ \\ s_n^\times \end{bmatrix} = T^{n-1} \begin{bmatrix} s_1^+ \\ s_1^\times \end{bmatrix}.$$  \hspace{1cm} (9)

Eigenvalues of the matrix $T$ is equal to $\lambda_+ = 2 + \sqrt{5}$, $\lambda_- = 2 - \sqrt{5}$ and corresponding eigenvectors (they are orthogonal but are not normalized) have the form

$$t_+ = \begin{bmatrix} 1 \\ 1+\sqrt{5} \end{bmatrix}, \quad t_- = \begin{bmatrix} 1 \\ 1-\sqrt{5} \end{bmatrix}.$$

Decomposing the vector $[s_1^+, s_1^\times] = [2, 2]$ on eigenvectors $t_+, t_-,$

$$[s_1^+, s_1^\times] = g_+ t_+ + g_- t_-,$$
we obtain \( g_+ = 1 + \sqrt{5}/5 \), \( g_- = 1 - \sqrt{5}/5 \). Therefore, \([s^+_n, s^-_n]\) = \(g_+ \lambda_{n-1} t_+ + g_- \lambda_{n-1} t_-\) and, according to (8), (9), we find

\[
s_n = (g_+ \lambda_{n-1}^{-1} + g_- \lambda_{n-1}^{-1}) + \frac{1}{2} \left( (g_+ \lambda_{n-1}^{-1} + (1 + \sqrt{5}) + g_- \lambda_{n-1}^{-1} (1 - \sqrt{5})) \right) \leq 4 \left( 2 + \sqrt{5} \right)^{n-1}.
\]

Since \( r_k < 4(k - 1) s_{2k-1} \), hence, putting \( n = 2k - 1 \) at the estimate having found, we obtain the majorant series from (6). It is summable at \( c > 3 - \sqrt{5} \). Then, if this condition is satisfied, we shall obtain

\[
\sum_{\gamma \in B} P(\gamma) \leq \infty.
\]

Completion of the proof is performed on the base of arguments which are standard in the percolation theory (see, for example, [5]). The inequality (11) permits to apply the Borel-Cantelli lemma (see, for example, [6]) to the event family \( B \). According to this statement, the probability of the event that consists in simultaneous realization of an infinite set of events belonging to the family, is equal to zero. Then, with the probability one, there exists a maximal cycle \( \gamma \in B \). For this cycle, there is a vertex \( z \) out of it and, besides, there is the infinite path \( a(z) \) without intersections and with the initial vertex \( z \). The path does not intersect the cycle. This means that the event \( \{ \tilde{M} : \exists (\tilde{W} \in \mathcal{W}[\tilde{M}] \ (|\tilde{W}| = \infty) \} \) of Bernoulli’s field \( \{ \tilde{c}(x) \} \) has the probability 1. On the other hand, the countable decomposition

\[
\{ \tilde{M} : \exists (\tilde{W} \in \mathcal{W}[\tilde{M}] \ (|\tilde{W}| = \infty) \} = \bigcup_{v \in \mathbb{Z}^2} \{ \tilde{M} : \tilde{W}(v) \in \mathcal{W}[\tilde{M}], |\tilde{W}(v)| = \infty \}
\]

(12)
takes place. In view of the random field \( \{ \tilde{a}(x) \} \) is uniform, the probability

\[
\Pr \{ \tilde{M} : \tilde{W}(v) \in \mathcal{W}[\tilde{M}], |\tilde{W}(v)| = \infty \} = Q(c)
\]
does not depend on \( v \). Therefore, it cannot be equal to zero, since the following inequality is correct according to (12)

\[
1 \leq \sum_{v \in \mathbb{Z}^2} \Pr \{ \tilde{M} : \tilde{W}(v) \in \mathcal{W}[\tilde{M}], |\tilde{W}(v)| = \infty \}. \quad \blacksquare
\]

**Consequence.** At \( c > c_0 \), the probability \( Q(c) \) may be represented with any preassigned accuracy by finite sum of series (5). It is defined by summands which correspond to cycles \( \gamma \) with the length not exceeding \( 2m \) with fixed \( m \in \mathbb{N} \). In this case, the following error estimate takes place

\[
\sum_{\gamma \in B : |\gamma| > 2m} P(\gamma) \leq \sum_{\gamma \in B : |\gamma| > 2m} (1 - c)^{|\gamma|} \leq \sum_{k > m} (1 - c)^{2k-1} s_{2k-1} =
\]
Thus, the decomposition (5) is the key for solving of the main percolation problem on $\mathbb{Z}^2$ that is to calculate the probability $Q(c)$ with any guaranteed accuracy. In addition, due to presence of the singular point $c^* = c^*$, the majorant series for the remainder must have a singularity in a point $a_0 > c^*$ for any initial finite sum of the cluster decomposition. Such a situation will take place in any way of upper estimation of the percolation threshold. Then, it follows that the solution of the main problem is impossible without building of a calculation algorithm for the percolation threshold $c^*$ with any preassigned accuracy.

6. Discussion

One can see on the base of the above proof that the singularity $c^*$ is possibly connected with the singularity of the generating function for the nonintersecting contours number. If it is true, so the regular method of sequential approximative calculation of this point may be based on the sequential exclusion of intersections in paths $(z_{\gamma}, x_1, ..., x_{2k-1})$ corresponding to cycles $\gamma$. Such an exclusion must be fulfilled with the increasing of approximation order. In this case the estimate given by Theorem 2 may be considered as the zero approximation.

Generally, the algorithm of approximations of the point $c^*$ should be consist in such a construction when estimates $c_n^- < c^* < c_n^+$, $c_{n+1}^- > c_n^-$, $c_{n+1}^+ < c_n^+$ are build sequentially step by step. They have the property $\lim_{n \to \infty} c_n^\pm = c^*$ and besides, for sure, $Q(c) = 0$ at $c < c_n^-$; $Q(c) > 0$ at $c > c_n^+$. 
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