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Random Walks on Infinite $C_4C_8(S)$ Net, Nanotube and Nanotori

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Abstract

The movement of an excitation (or a vacancy) on a carbon nanotube can be regarded as a sequence of jumps between neighboring sites and described by a walk. In this paper, we give a mathematical model for the graph of $C_4C_8(S)$ net and using this model, we write a GAP program to calculate the adjacency matrix and the number of all k-step walks in the graph of infinite net of $C_4C_8(S)$ nanotube and nanotori.

1. Introduction

Walks can be used for characterization of molecular graphs for quantification of their complexity and for definition of various molecular descriptors. A walk in a graph is an alternating sequence of vertices and edges, such that each edge begins and ends with the vertices immediately preceding and following it. Note that repetition of vertices or edges is allowed in a walk.

Given a graph and starting point, we select a neighbor of it at random, and move to this neighbor; then we select a neighbor of this point at random, and move to it etc. The random sequence of this points selected this way is a *random walk* on the graph. A self-returning walk is a random walk starting and ending at the same vertex. Let $G=(V,E)$ be a connected graph

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with vertex set V and edge set E. Consider a random walk on G; we start at a vertex v_0; if at the t-th step we are at a vertex v_t, we move neighbor of v_t with probability $1/deg(v_t)$.

A random walk is a finite Markov chain that is time-reversible. In fact, there is not much different between the theory of random walks on graphs and the theory of finite Markov chains; every Markov chain can be viewed as random walk on a directed graph, if we allow weighted edges. Similarly, time-reversible Markov chains, as random walks on regular symmetric graphs[2].

Therefore, the sequence of random vertices is a Markov chain. Let $M=[m_{ij}]$ be the matrix of transition probabilities of this Markov chain that is called Markov matrix. Thus if $ij \in E$, then $m_{ij}=1/deg(i)$ and zero otherwise. Let A be the adjacency matrix of G and let D denote the diagonal degree matrix of G, then multiplication of inverse of degree matrix and adjacency matrix is Markov matrix i.e. $M=D^{-1}A$.

It is well known that the number of walks of length k beginning at vertex i, and ending at vertex j, is given by the ij-element of the k-th power of the vertex adjacency matrix A. Then the number of self-returning walks of length k is given by the ii-element of the k-th power of the adjacency matrix A.

It has been found that the total number of self-returning walks of length k that coincide with the trace of k-th power of A, can be applied to the theory of total π-electron energy, in as much as this gives moments of the eigenvalue distribution. Moreover, more recently, self-returning walk counts have been found to be applicable to systematic search of isocodal vertices in molecular graphs. Isocodal vertices in a graph are those vertices that have the same number of self-returning walks for each length of walk.

The atomic walk count of order k, denoted by $(awc)_k$, is the number of all possible walks of length k that start at a specified vertex i and end at any vertex j. The molecular walk count of order k, denoted by $(mwc)_k$ is obtained by summing up all atomic walks counts of order k. The total walk count, twc, is the sum of all $(mwc)_k$ for $k=1,..,N-1$, where N is the number of vertices of the graph. Finally, the probability that, starting at i, we reach j in k step is given by the ij-entry of the M^k. Therefore, that is enough to compute the adjacency matrix of the graph[6].

The theory of random walks is very closely related to a number of other branches of graph theory. Basic properties of a random walk are determined by the spectrum of the graph, and also by electrical resistance of the electric network naturally associated with graphs. There is a

number of other processes that can be defined on a graph, mostly describing some sort of diffusion (chip-firing, load-balancing in distributed networks etc.), whose basic parameters are closely tied with the above-mentioned parameters of random walks. All this connections are very fruitful and provide both tools for the study and opportunities for applications of random walks[2].

Much of the recent interest in random walks is motivated by important algorithmic applications. Random walks can be used to reach obscure parts of large sets, and also to generate random elements in large and complicated sets, such as the set of lattice points in a convex body or the set of perfect matching in a graph which, in turn, can be used to the asymptotic enumeration of these objects[2,6].

A C_4C_8 net is a trivalent decoration made by alternating squares C_4 and octagons C_8. It can cover either a cylinder or a torus. Such a covering can be derived from a square net by the leapfrog operation. In this paper, we introduce a mathematical model for the vertex set of infinite lattice of $C_4C_8(S)$ and define a distance function on this set and using these, we can give a mathematical model for the graph of this nano-structure.

Since the lattice graphs of tube and tori are subgraphs of the infinite lattice, we can present mathematical models relating to graphs of these structures. By these models, we can write a simple GAP program, or in any mathematics software, for compute the all k-step walks between any two arbitrary vertices of the graphs (many other problem related to walks can be reduced to this important problem[1]). In addition, we can write a program to compute the very important adjacency matrix of these graphs. We know that there are some topological indices related to this matrix.

2. Describing the $C_4C_8(S)$ net with a mathematical model

Let us consider the vectors e_0, e_1, e_2 and e_3 as shown in Figure1. Put $a_1= e_0-e_1+e_3$ and $a_1= e_0+e_1-e_2$. The periodic set $\Gamma = \{n_1a_1 + n_2a_2 \,|(n_1, n_2) \in L\}$, where $L = \bigcup_{i=0}^{3} L^i$, $L^0=Z^2$, $L^1= Z^2+(\frac{1}{2+\sqrt{2}}, \frac{1}{2+\sqrt{2}})$, $L^2= Z^2+(\frac{-1}{2+\sqrt{2}}, \frac{1}{2+\sqrt{2}})$ and $L^3= Z^2+(0, \frac{-\sqrt{2}}{2+\sqrt{2}})$ is the $TUC_4C_8(S)$ lattice. Instead of the basis $\{a_1, a_2\}$ we have the possibility to use the vectors e_0, e_1, e_2 and e_3. Now we are ready to define a bijection that allow us to consider a subset of Z^4 as the set of all vertices of $C_4C_8(S)$ lattice as follows.

Theorem 1. There is a bijection $\psi : \ell \to \Gamma$, $(\alpha,\beta,\gamma,\delta) \mapsto \alpha e_0 + \beta e_1 + \gamma e_2 + \delta e_4$ from the set $\ell = \{(\alpha,\beta,\gamma,\delta) \in Z^4 \mid \beta+\gamma+\delta \in \{0,1\}, \alpha+\gamma-\delta \in \{0,1\}\}$ to the set Γ of all the vertices of a $C_4C_8(S)$ lattice.

Proof: It is clear that Ψ is well-defined. We prove that this map is one-to-one and onto. Let

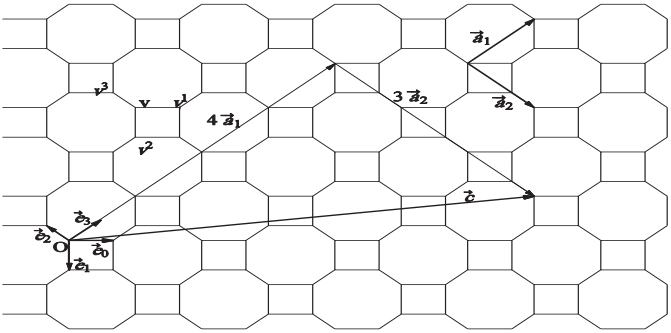

Figure1. $C_4C_8(S)$ net.

$v=(v_0,v_1,v_2,v_3)$ and $u=(u_0,u_1,u_2,u_3)$ be in ℓ and $\Psi(u)=\Psi(v)$. By considering the vectors e_0, e_1, e_2 and e_3, we have $\alpha e_0+\beta e_1+\gamma e_2+\delta e_3=(\alpha+\frac{\sqrt{2}}{2}(\delta-\gamma), -\beta+\frac{\sqrt{2}}{2}(\delta+\gamma))$. Thus from $\Psi(u)=\Psi(v)$ we have $v_0-u_0=\frac{\sqrt{2}}{2}((v_2-u_2)-(v_3-u_3))$ and $v_1-u_1=\frac{\sqrt{2}}{2}((v_3-u_3)+(v_2-u_2))$. However, the coordinates of v and u are integers, so $v_i=u_i$ for i=0, 1, 2, 3. Therefore, Ψ is one-to-one. By choosing an arbitrary point $P=n_1a_1+n_2a_2$ in Γ and considering four cases for $(n_1, n_2) \in \bigcup_{i=0}^{3} L^i$ we can give suitable $(\alpha, \beta, \gamma, \delta) \in \ell$ such that $\Psi(\alpha, \beta, \gamma, \delta)=P$, for example if $(n_1,n_2) \in L^0$ then $\Psi(n_1+n_2, n_2-n_1,-n_2,n_1)=P$. Thus, Ψ is onto and this completes the proof. ■

The mapping $d: \ell \times \ell \to N$ with $d(u,v)=|u_0-v_0|+|u_1-v_1|+|u_2-v_2|+|u_3-v_3|$ is a distance on ℓ. Note that this distance function gives us the length of a shortest path between any two arbitrary vertices of $C_4C_8(S)$ infinite lattice. Moreover u is a neighbor of order k of v if $d(u,v)=k$ and u is adjacent vertex of v if $d(u,v)=1$. By this fact one can easily see that the nearest neighbors of $v=(\alpha, \beta, \gamma, \delta) \in \ell$ are

$$v^1=(\alpha+\varepsilon_1(v), \beta, \gamma, \delta) \qquad v^2=(\alpha, \beta+\varepsilon_2(v), \gamma, \delta) \qquad v^3=(\alpha, \beta, \gamma+\varepsilon_{31}(v), \delta+\varepsilon_{32}(v))$$

where $\varepsilon_1(v)=(-1)^{\alpha+\gamma-\delta}$, $\varepsilon_2(v)=(-1)^{\beta+\gamma+\delta}$ and when $\alpha+\gamma-\delta=\beta+\gamma+\delta$, $\varepsilon_{31}(v)=\varepsilon_2(v)$ and 0 otherwise, also if $\alpha+\gamma-\delta \neq \beta+\gamma+\delta$ then $\varepsilon_{32}(v)=0$ and else $\varepsilon_{32}(v)=\varepsilon_2(v)$.

3. Random walks on infinite $C_4C_8(S)$ net, tube and nanotori

By the above theorem the graph of $C_4C_8(S)$ net is $G=(\ell,E)$, where $E=\{\{v,v^i\}|\ v\in\ell$, $i\in\{1,2,3\}\}$. A k-step walk on this graph with the starting point v has the form $\{v,v^{i_1}\},\{v^{i_1},v^{i_1i_2}\},...,\{v^{i_1i_2...i_{k-1}},v^{i_1i_2...i_{k-1}i_k}\}$ and will denoted by $(v,i_1i_2...i_k)$ [See Ref.3]. If we start with vertex v and after k-step walks be at vertex u then we write $u=v^{i_1i_2...i_k}$. The number N_k of all the k-step walks connecting the points (0, 0) and (n_1, n_2) on the Cartesian lattice graph Z^2 coincides to the coefficient of $x_1^{n_1}x_2^{n_2}$ in the expression $(x_1+x_1^{-1}+x_2+x_2^{-1})^k$ (for more details see Ref.1.). The description of the $C_4C_8(S)$ net presented in the above theorem allows us to compute the number $N_k(v,u)$ of all k-step walks from $v\in\ell$ to $u\in\ell$ using a simple GAP program. For this purpose, we write a function named *nbr* that its output is neighbors of any vertices of the net. At first we write a program to calculate the $N_k(v,u)$ in the infinite $C_4C_8(S)$ net as follows

```
nbr:=function(v,i)
if i=1 then return v+[(-1)^(v[1]+v[3]-v[4]),0,0,0];
elif i=2 then return v+[0,(-1)^(v[2]+v[3]+v[4]),0,0];
elif i=3 and v[1]+v[3]-v[4]=v[2]+v[3]+v[4] then
return v+[0,0,(-1)^(v[2]+v[3]+v[4]),0];
elif i=3 and v[1]+v[3]-v[4]<>v[2]+v[3]+v[4] then
return v+[0,0,0,(-1)^(v[2]+v[3]+v[4])];
fi;end;
v:=[5,-4,0,4];#(for example)
w:=v;
u:=[1,1,0,0]; k:=13#(for example)
A:=[];;
T:=Tuples([1,2,3],k);;
for x in T do
for i in [1..k] do
v:=nbr(v,x[i]);
od;
Add(A,v);
v:=w;;
od;
Nk:=Size(Filtered(A,x->x=u));
```

Now we are ready to calculate $N_k(v,u)$ in $C_4C_8(S)$ tube and tori. Let $T=TUC_4C_8(S)[p,q]$ be the lattice of $C_4C_8(S)$ tube in which p and q are the number of octagons in vertical and horizontal directions, respectively, Fig. 2.

Note that the graph T has exactly $8pq$ vertices. We assume that a_{ij} denotes the (i,j)-entry of the two-dimensional lattice of T as shown in the Fig.2. We put the origin point O at the a_{41} and consider the vectors e_0, e_1, e_2 and e_3.

Consider the points $a=a_{11}$, $b=a_{21}$, $c=a_{31}$, $d=a_{41}=O$, $e=a_{12}$, $f=a_{22}$, $g=a_{32}$ and $h=a_{42}$. It is easy

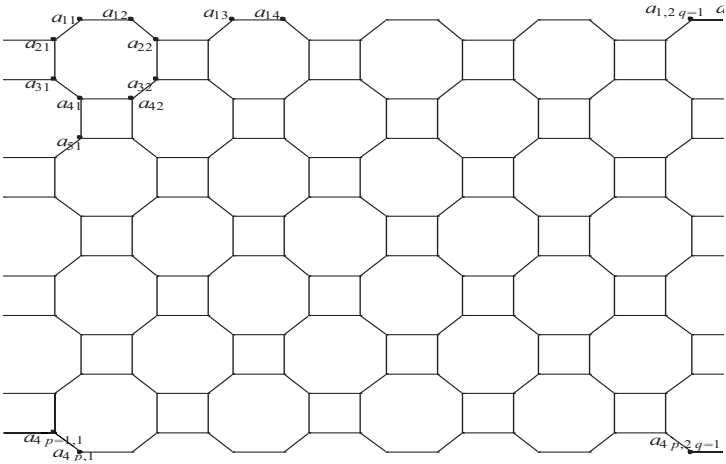

Figure2. The (i,j)-entry of $TUC_4C_8(S)[4,5]$ nanotube.

to see that every point of T can be constructed by a translation of these points in two directions $v=2e_0-e_2+e_3$ and $w=2e_1-e_2-e_3$. This is the content of lemma below.

Lemma 1. Assume that a_{ij}, $1\leq i\leq 4p$ and $1\leq j\leq 2q$, denotes the (i,j)-entry of the two-dimensional lattice of T, as shown in the Fig.2, in our model we have

$$a_{ij}=\begin{cases} a_{ij}^1 & i\equiv 1(\mathrm{mod}\,4),\ j \text{ odd or } i\equiv 3(\mathrm{mod}\,4),\ j \text{ even} \\ a_{ij}^2 & i\equiv 1(\mathrm{mod}\,4),\ j \text{ even or } i\equiv 3(\mathrm{mod}\,4),\ j \text{ odd} \\ a_{ij}^3 & i\equiv 2(\mathrm{mod}\,4),\ j \text{ odd or } i\equiv 0(\mathrm{mod}\,4),\ j \text{ even} \\ a_{ij}^4 & i\equiv 2(\mathrm{mod}\,4),\ j \text{ even or } i\equiv 0(\mathrm{mod}\,4),\ j \text{ odd} \end{cases} \quad (1)$$

where

$$a_{ij}^1=(j-1)\,e_0+(i-3)/2\,e_1+(7-i-2j)/4\,e_2+(3-i+2j)/4\,e_3,$$
$$a_{ij}^2=(j-1)\,e_0+(i-3)/2\,e_1+(9-i-2j)/4\,e_2+(1-i+2j)/4\,e_3,$$
$$a_{ij}^3=(j-1)\,e_0+(i-4)/2\,e_1+(8-i-2j)/4\,e_2+(-i+2j)/4\,e_3$$
$$a_{ij}^4=(j-1)\,e_0+(i-4)/2\,e_1+(6-i-2j)/4\,e_2+(2-i+2j)/4\,e_3.$$

Proof: It is enough to consider the coordinates of the points a, b, c, d, e, f, g, h and the vectors v, w. ■

After rolling up the lattice and forming the nanotube we have $a^1_{i1} = a_{i,2q}$ and so $a^1_{i,2q} = a_{i1}$ when $i \equiv 2 \pmod 4$ or $i \equiv 3 \pmod 4$. By the previous lemma and above explanation we can write a neighbor-function program that is necessary to generating adjacency matrix of the nanotube molecular graph. For this purpose, we must generate the vertex set of the nanotube, which is easy according to the above lemma. Now we write a GAP program to compute the adjacency matrix of the nanotube molecular graph.

```
p:=4;q:=5;#(for example)
a:=[0,-1,1,1];b:=[0,-1,1,0];c:=[0,0,1,0];d:=[0,0,0,0];e:=[1,-1,1,1];f:=[1,-1,0,1];
g:=[1,0,0,1];h:=[1,0,0,0]; v:=[2,0,-1,1];w:=[0,2,-1,-1];V:=[];
for i in [1..4*p] do
for j in [1..2*q] do
if i mod 4=1 and j mod 2=1 then Add(V,a+(i-1)/4*w+(j-1)/2*v);
elif i mod 4=1 and j mod 2=0 then Add(V,e+(i-1)/4*w+(j/2-1)*v);
elif i mod 4=2 and j mod 2=1 then Add(V,b+(i-2)/4*w+(j-1)/2*v);
elif i mod 4=2 and j mod 2=0 then Add(V,f+(i-2)/4*w+(j/2-1)*v);
elif i mod 4=3 and j mod 2=1 then Add(V, c+(i-3)/4*w+(j-1)/2*v);
elif i mod 4=3 and j mod 2=0 then Add(V, g+(i-3)/4*w+(j/2-1)*v);
elif i mod 4=0 and j mod 2=1 then Add(V, d+(i/4-1)*w+(j-1)/2*v);
elif i mod 4=0 and j mod 2=0 then Add(V, h+(i/4-1)*w+(j/2-1)*v);
fi;
od;
od;
nbr:=function(v,i,p,q)
if i=1 and v[1]=0 and v[3]-v[4]=1 and (2*v[2]+4) mod 4=2 then
return v+[2*q-1,0,-1*q,q];
elif i=1 and v[1]=2*q-1 and v[3]-v[4]=1-2*q and (2*v[2]+4) mod 4=2 then
return v-[2*q-1,0,-1*q,q];
elif i=1 and v[1]=0 and v[3]-v[4]=1 and (2*v[2]) mod 4=0 then
return v+[2*q-1,0,-1*q,q];
elif i=1 and v[1]=2*q-1 and v[3]-v[4]=1-2*q and (2*v[2]) mod 4=0 then
return v-[2*q-1,0,-1*q,q];
elif i=1 then  return v+[(-1)^(v[1]+v[3]-v[4]),0,0,0];
elif i=2 and v[2]=-1 and v[3]+v[4]=2 then  return v;
elif i=2 and v[2]=2*(p-1) and v[3]+v[4]=2*(1-p) then return v;
elif i=2 then return v+[0,(-1)^(v[2]+v[3]+v[4]),0,0];
elif i=3 and v[1]+v[3]-v[4]=v[2]+v[3]+v[4] then
return v+[0,0,(-1)^(v[2]+v[3]+v[4]),0];
elif i=3 and v[1]+v[3]-v[4]<>v[2]+v[3]+v[4] then
return v+[0,0,0,(-1)^(v[2]+v[3]+v[4])];
fi;end;
dis:=function(u,v)
if v[1]=0 and v[3]-v[4]=1 and (2*v[2]+4) mod 4=2 and u[1]=2*q-1 and u[3]-u[4]=1-2*q
and (2*u[2]+4) mod 4=2 and u[2]=v[2] then return 1;
elif v[1]=0 and v[3]-v[4]=1 and (2*v[2]) mod 4=0 and u[1]=2*q-1 and u[3]-u[4]=1-2*q
```

```
and (2*u[2]) mod 4=0 and u[2]=v[2] then return 1;
else return AbsInt(u[1]-v[1])+AbsInt(u[2]-v[2])+AbsInt(u[3]-v[3])+AbsInt(u[4]-v[4]);
fi; end;
Dis:=function(u,v)
return dis(v,u); end;
A:=0*IdentityMat(8*p*q);;
for i in [1..8*p*q] do
for j in [1..8*p*q] do
if dis(V[i],V[j])=1 or Dis(V[i],V[j])=1 then A[i][j]:=1;A[j][i]:=1;
fi;
od;
od;
```

As you see in the first section, we have that the number of k-step walks from i to j is $N_k(i,j)=(A^k)_{ij}$. The number of self-returning walks of length k is $(A^k)_{ii}$,total number of self-returning walks of length k is $Tr(A^k)$, the atomic walk count of order k is $(amc)_k(i)=\sum_j (A^k)_{ij}$. Also the molecular walk count of order k is $(mwc)_k= \sum_i \sum_j (A^k)_{ij}$ and finally the total walk count is $twc=\sum_{k=1}^{N-1}(mwc)_k$. Therefore, we can easily add some lines to the above program and compute all of the above counting.

Also we have $D_{ii}=A^2_{ii}$, and we now that the Laplacian matrix of a graph is A-D where its eigenvalues are very important and have been used for calculating the some of topological indices as Quasi-Wiener index , Mohar indices TI_1, TI_2 and the number of spanning trees [4,5,8]. Of course, several topological indices are related to adjacency matrix of graph.

Now we describe the molecular graph of nanotori, and by this description, we write a program for generating the adjacency matrix of this graph.

Let V_1, V_2 be the set of all vertices of $C_4C_8(S)[p,q]$ tube and $C_4C_8(S)[p,q]$ torus, respectively, then $V_1=V_2$. Let E_1, E_2 be the set of all edges of $C_4C_8(S)[p,q]$ tube and $C_4C_8(S)[p,q]$ torus, respectively, then $E_1 \cap \{\{a_{1,j},a_{4p,j}\} \mid 1 \leq j \leq 2q\}=E_2$. Similarly, we can write a neighbor function and a simple program for generating the adjacency matrix of nanotori molecular graph. For this goal, we repeat first 26 lines of the last program and add these below lines to it.

```
elif i=2 and v[2]=-1 and v[3]+v[4]=2 then  return v+[0,2*p-1,-1*p,-1*p];
elif i=2 and v[2]=2*(p-1) and v[3]+v[4]=2*(1-p) then
return v-[0,2*p-1,-1*p,-1*p];
elif i=2 then return v+[0,(-1)^(v[2]+v[3]+v[4]),0,0];
elif i=3 and v[1]+v[3]-v[4]=v[2]+v[3]+v[4] then
return v+[0,0,(-1)^(v[2]+v[3]+v[4]),0];
```

```
elif i=3 and v[1]+v[3]-v[4]<>v[2]+v[3]+v[4] then
return v+[0,0,0,(-1)^(v[2]+v[3]+v[4])];
fi;end;
dis:=function(u,v)
if v[1]=0 and v[3]-v[4]=1 and (2*v[2]+4) mod 4=2 and u[1]=2*q-1 and u[3]-u[4]=1-2*q
and (2*u[2]+4) mod 4=2 and u[2]=v[2] then return 1;
elif v[1]=0 and v[3]-v[4]=1 and (2*v[2]) mod 4=0 and u[1]=2*q-1 and u[3]-u[4]=1-2*q
and (2*u[2]) mod 4=0 and u[2]=v[2] then return 1;
elif v[2]=-1 and v[3]+v[4]=2 and u[2]=2*(p-1) and u[3]+u[4]=2*(1-p) and u[1]=v[1] then
return 1;
else return AbsInt(u[1]-v[1])+AbsInt(u[2]-v[2])+AbsInt(u[3]-v[3])+AbsInt(u[4]-v[4]);
fi;end;
Dis:=function(u,v)
return dis(v,u); end;
A:=0*IdentityMat(8*p*q);;
for i in [1..8*p*q] do
for j in [1..8*p*q] do
if dis(V[i],V[j])=1 or Dis(V[i],V[j])=1 then A[i][j]:=1;A[j][i]:=1;
fi;
od;
od;
```

4. Conclusion

The mathematical models, introduced in this paper, are useful tools for computing some structural properties of nano-structures. For example, we can compute the full symmetry group and the irreducible representations of these graphs[7]. Also by defining suitable subsets of vertex set of nanotube and tori, for every fixed vertex v, we can compute the distance matrix and so some distance-based topological indices of these graphs. Moreover, using these definitions, we can compute the diameter of these graphs.

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