

On the Wilson loops in 2D tight-binding models

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In the following paper we are considering Hamiltonians with multiband structure. In this case the important quantities to characterize topological states are non-Abelian connection matrix, Berry curvature and Wilson loop. We calculated some of the Wilson loops and showed that their set has a group structure and is isomorphic to $\pi_1(T^2) = \mathbb{Z} \times \mathbb{Z}$. It is shown how to get the same results using the facts known in differential geometry.

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1. Introduction

We considered a tight-binding model defined by a matrix Hamiltonian over 2D Brillouin zone. When a system has multiple bands in its energy spectrum, one can introduce a Berry connection matrix - A , whose dimension is equal to the number of bands. For defining topological indices and assigning them to the topologically distinct states of the system, the Wilson loop appears to be a useful object [1], [3]. It is a matrix equal to the path-ordered exponential of the Berry connection transported along a loop. The difficulty in computing the Wilson loop for particular cases arises from its path-ordered nature. The evident analogy between the Berry connection and a gauge field gives us a foundation to define a curvature tensor - F , similar to the strength tensor in the quantum field theory. Under the local unitary transformation of the first-quantized Hamiltonian, A and F transform as the gauge field and the strength tensor do under a gauge transformation, respectively.

We showed that the application of the non-abelian Stokes theorem, with a behavior of curvature tensor in mind, significantly simplifies the process of computing the path-ordered exponential for the Wilson loop. Nontrivial results for the Wilson loop is expected to come only from the loops that surrounds the points in \mathcal{BZ} where the eigenvectors of the first-quantized Hamiltonian are singular. Although, surprisingly, we arrived to the result that in our case $W_{mn} = \delta_{mn}$, where W is the Wilson loop and $n, m = 1, 2$, when our path encircles a point of a certain type in the \mathcal{BZ} , even though F has singularities there.

Additionally we considered a set of all Wilson loops that start and end in the same point in \mathcal{BZ} and came to the result that it satisfies group axioms and is indeed isomorphic to the fundamental group of Torus: $\pi_1(T^2) = \mathbb{Z} \times \mathbb{Z}$. Finally, looking at Wilson loops as elements of the holonomy group and using the facts known in differential geometry, we came to the same group structure.

2. First-quantized Hamiltonian

We have considered an infinite 2-dimensional lattice with two types of fermions in its sites. For now we are not interested in the exact configuration of these sites. After requiring a translational invariance, a useful step is to go to the momentum space via the Fourier transformations. Momentum vector, \mathbf{k} , will be 2-dimensional as well, in particular, $\mathbf{k} = m\mathbf{i} + n\mathbf{j}$, where m, n are the site-labels and \mathbf{i}, \mathbf{j} are basis vectors. After expanding creation and annihilation operators in the momentum space and rewriting the second quantized Hamiltonian accordingly, we arrive at the following expression

$$\hat{H} = \frac{1}{2\pi} \int_{\mathcal{BZ}} \Psi^\dagger \mathcal{H} \Psi \, d\mathbf{k}. \quad (1)$$

The integration is over the first \mathcal{BZ} . $\Psi(\mathbf{k}) = (c \quad d)^T$, where c and d are fermion annihilation operators. For our model we took the first quantized Hamiltonian in the momentum space to be

$$\mathcal{H}(\mathbf{k}) = \mathbf{h}(\mathbf{k}) \cdot \boldsymbol{\sigma}, \quad (2)$$

where $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$, σ_i $i = 1, 2, 3$, are Pauli matrices and $\mathbf{h} = (h_1, h_2, h_3)$ is the vector containing the parameters for the system under consideration. $\mathbf{h}(\mathbf{k})$ possesses the periodicity: $\mathbf{h}(k_1, k_2) = \mathbf{h}(k_1 + 2\pi, k_2) = \mathbf{h}(k_1, k_2 + 2\pi)$.

For the eigenvectors of $\mathcal{H}(\mathbf{k})$ we chose

$$\Psi_1 = \frac{1}{\sqrt{h(h-h_3)}} \begin{pmatrix} h_1 - ih_2 \\ h - h_3 \end{pmatrix}, \quad (3)$$

$$\Psi_2 = \frac{1}{\sqrt{h(h-h_3)}} \begin{pmatrix} -h + h_3 \\ h_1 + ih_2 \end{pmatrix}, \quad (4)$$

with energies $E_1 = |\mathbf{h}| \equiv h$, $E_2 = -h$, respectively. As we see, we have a gap in the energy spectrum. The gap closes if and only if $h = 0$, but this is a singularity of the eigenvectors; besides this singularity, they have an additional pole when $h = h_3 \neq 0$; we are assuming that this is the case only for isolated points in the \mathcal{BZ} .

3. Berry Connection Matrix and Curvature Tensor

In systems with multiband energy spectrum we construct a Berry connection matrix [6] via:

$$(A_\mu)_{mn} = i\psi_n \partial_\mu \psi_m, \quad (5)$$

where $\partial_\mu \equiv \frac{\partial}{\partial k_\mu}$ $\mu = 1, \dots, \dim(\text{The Momentum Space})$, ψ_i $i = 1, \dots, \#$ bands, are eigenvectors of the first-quantized Hamiltonian written in the momentum space, $n, m = 1, \dots, \#$ (different types of fermions).

In our case $\mu, m, n = 1, 2$. Using the chosen eigenvectors, we arrive to

$$(A_\mu)_{11} = \frac{h_1 \partial_\mu h_2 - h_2 \partial_\mu h_1}{2h(h-h_3)} = -(A_\mu)_{22}, \quad (6)$$

$$(A_\mu)_{21} = \frac{i \partial_\mu (h_1 + ih_2)}{2h} - \frac{i(h_1 + ih_2) \partial_\mu (h - h_3)}{2h(h-h_3)} = (A_\mu)_{12}^*. \quad (7)$$

Non-Abelian curvature tensor has the form

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + i[A_\mu, A_\nu].$$

The important feature of it that we made use of is the fact that after inserting the expression for A_μ (5) and having in mind the completeness and normalization conditions of the eigenvectors,

$$\sum_{i=1}^2 (\psi_m^\dagger)_i (\psi_n)_i = \delta_{mn}, \quad (8)$$

$$\sum_{i=1}^2 (\psi_i^\dagger)_m (\psi_i)_n = \delta_{mn}, \quad m, n = 1, 2, \quad (9)$$

led us to

$$\begin{aligned}
(F_{\mu\nu})_{mn} &= \partial_\mu(A_\nu)_{mn} - \partial_\nu(A_\mu)_{mn} + i[A_\mu, A_\nu]_{mn} = \\
&= i\partial_\mu [(\psi_n^\dagger)_k \partial_\nu(\psi_m)_k] - i\partial_\nu [(\psi_n^\dagger)_k \partial_\mu(\psi_m)_k] - \\
&- i [(\psi_q^\dagger)_k \partial_\mu(\psi_m)_k] [(\psi_n^\dagger)_p \partial_\nu(\psi_q)_p] + i [(\psi_q^\dagger)_k \partial_\nu(\psi_m)_k] [(\psi_n^\dagger)_p \partial_\mu(\psi_q)_p] = \\
&= i \left(\partial_\mu(\psi_n^\dagger)_k \right) (\partial_\nu(\psi_m)_k) + i(\psi_n^\dagger)_k \partial_\mu \partial_\nu(\psi_m)_k - i \left(\partial_\nu(\psi_n^\dagger)_k \right) (\partial_\mu(\psi_m)_k) - \\
&- i(\psi_n^\dagger)_k \partial_\nu \partial_\mu(\psi_m)_k + i\delta_{kp} \partial_\mu(\psi_m)_k \partial_\nu(\psi_n^\dagger)_p - i\delta_{kp} \partial_\nu(\psi_m)_k \partial_\mu(\psi_n^\dagger)_p.
\end{aligned}$$

So we came to the much more advantageous expression of the curvature tensor

$$(F_{\mu\nu})_{mn} = i(\psi_n^\dagger)_k (\partial_\mu \partial_\nu - \partial_\nu \partial_\mu) (\psi_m)_k. \quad (10)$$

This means that $F_{\mu\nu} \equiv \mathbb{O}_{2 \times 2}$ everywhere in the \mathcal{BZ} , unless eigenvectors have singularities within it.

4. Wilson Loop and its Simplification

The Wilson loop is an important quantity for characterizing different states in multiband problems [1].

$$W(\mathbf{k}_0) = \mathcal{P} e^{-i \oint_{\mathbf{k}_0} A_\mu dk^\mu}, \quad \mu = 1, 2, \quad (11)$$

where " \mathcal{P} " denotes path-ordering and the integral is taken along a path encircling \mathbf{k}_0 . The integral is different from zero only if the path encloses at least one of the singular points of A_μ . Non-Abelian structure of A_μ complicates the computation of $W(\mathbf{k}_0)$. Our aim is to compute the Wilson loop even in the case of multiband energy spectrum.

For simplifying the computations we used the Non-Abelian Stokes theorem [5]

$$W = \mathcal{P} \exp \left(-i \oint_{\partial S} A_\mu dk^\mu \right) = \mathcal{P}_{k_2} \exp \left(-i \int_S T^{-1} F_{\mu\nu} T d\sigma^{\mu\nu} \right), \quad (12)$$

where $\sigma_{\mu\nu} = \frac{1}{2} dk_1 \wedge dk_2$, ($\mu, \nu = 1, 2$), is a surface element and T is a certain unitary matrix, its explicit form having no effect on the eigenvalues of $W(\mathbf{k}_0)$, as we will see.

Here we can use the previous result: $F_{\mu\nu}$ is everywhere zero, except for the isolated points. Assume that the loop encircles one of these points, \mathbf{k}_0 , which leaves us with only one term, so the path-ordering procedure becomes trivial

$$\begin{aligned}
W(\mathbf{k}_0) &= \mathcal{P}_{k_2} \exp \left(-i \int_S T^{-1} F_{\mu\nu} T d\sigma^{\mu\nu} \right) \\
&= \mathcal{P}_{k_2} \exp \left(-i \int_S T^{-1}(\mathbf{k}_0) F_{\mu\nu}(\mathbf{k}) T(\mathbf{k}_0) d\sigma^{\mu\nu} \right) \\
&= \exp \left(T^{-1}(\mathbf{k}_0) \left(-i \int_S F_{\mu\nu}(\mathbf{k}) d\sigma^{\mu\nu} \right) T(\mathbf{k}_0) \right), \\
&= T^{-1}(\mathbf{k}_0) \exp \left(-i \int_S F_{\mu\nu}(\mathbf{k}) d\sigma^{\mu\nu} \right) T(\mathbf{k}_0),
\end{aligned}$$

We can, as we have said, see that the existence of T matrix does not change the invariants of W . One of the important fact is that the non-zero term of F in (10) comes from its Abelian part. Now, if the area of integration goes to zero, then

$$W(\mathbf{k}_0) = \exp\left(-i \int_{S \rightarrow 0} F_{\mu\nu}(\mathbf{k}) dk^\mu dk^\nu\right) = \exp\left(-i \int_{S \rightarrow 0} (\partial_\mu A_\nu - \partial_\nu A_\mu) dk^\mu dk^\nu\right).$$

We can rewrite the last expression, using a Barry Phase

$$W(\mathbf{k}_0) = \exp\left(-i \int_{S \rightarrow 0} (\partial_\mu A_\nu - \partial_\nu A_\mu) dk^\mu dk^\nu\right) = e^{-i \oint A_\mu dk^\mu} = e^{-2\pi i \Phi(\mathbf{k}_0)}, \quad (13)$$

where

$$\Phi(\mathbf{k}_0) = \frac{1}{2\pi} \oint A_\mu dk^\mu,$$

is the Berry phase [2]. In this way, one sees that there indeed is a close connection between the Wilson loop and the Berry phase $\Phi(\mathbf{k}_0)$.

5. Results of Computations

We considered the gapped states ($h \neq 0$), in which the unit vector $\hat{\mathbf{h}} = \mathbf{h}/h$ is a map from T^2 to the unit sphere - S^2 with its center in the origin of the coordinate system. In this case the only singularities are of the form: $h = h_3 \neq 0$. The Hopf theorem states that the maps from an n -dimensional compact oriented manifold to S^n are completely characterized by their topological degree. From this we conclude that there is a topological number assigned to the states encountered in our problem and the states with different values of the topological number indicate different phases of the system.

With the unit vector $\hat{\mathbf{h}}$ we constructed the Pontryagin number that counts how many times $\hat{\mathbf{h}}$ wraps around S^2 ,

$$\frac{1}{4\pi} \int_{\mathcal{BZ}} \hat{\mathbf{h}} \left[\partial_\mu \hat{\mathbf{h}} \times \partial_\nu \hat{\mathbf{h}} \right] dk^\mu \wedge dk^\nu = \frac{\epsilon_{\mu\nu}}{8\pi} \int_{\mathcal{BZ}} \hat{\mathbf{h}} \left[\partial_\mu \hat{\mathbf{h}} \times \partial_\nu \hat{\mathbf{h}} \right] dk^\mu dk^\nu.$$

Using the expression $\hat{\mathbf{h}} = \psi_1^\dagger \boldsymbol{\sigma} \psi_1$, after some computations we have arrived at:

$$P = \frac{i}{2\pi} \int_{\mathcal{BZ}} \psi_+^\dagger (\partial_\mu \partial_\nu - \partial_\nu \partial_\mu) \psi_+ dk^\mu dk^\nu.$$

When we take the integration area and shrink it to zero, we get

$$P = \frac{1}{2\pi} \int_S (F_{12})_{11} dk^1 dk^2 = \frac{1}{2\pi} \int_{S \rightarrow 0} (\partial_1 A_2 - \partial_2 A_1)_{11} dk^1 dk^2, \quad (14)$$

which we can rewrite as

$$\frac{1}{2\pi} \int_{S \rightarrow 0} (\partial_1 A_2 - \partial_2 A_1)_{11} dk^1 dk^2 = \frac{1}{2\pi} \oint_{\mathbf{k}_0} (A_\mu)_{11} dk^\mu = \frac{1}{2\pi} \Phi_{11}(\mathbf{k}_0),$$

where, $h(\mathbf{k}_0) = h_3((\mathbf{k}_0)) \neq 0$. In fact, we have deduced that:

$$\Phi_{11}(\mathbf{k}_0) = -\Phi_{11}(\mathbf{k}_0) = \frac{1}{2\pi} \oint_{\mathbf{k}_0} \partial_\mu \phi dk^\mu \in \mathbb{Z},$$

where $\phi(\mathbf{k})$ is the polar angle of $\hat{\mathbf{h}} = (\sin \theta(\mathbf{k}) \cos \phi(\mathbf{k}), \sin \theta(\mathbf{k}) \sin \phi(\mathbf{k}), \cos \theta(\mathbf{k}))$. Since the other components of the Φ matrix are identically zero, we are left with $\Phi \in \mathbb{Z}\sigma_3 = \{n\sigma_3 | n \in \mathbb{Z}\}$, so, surprisingly, the Wilson loop in this case is

$$W(\mathbf{k}_0) = e^{-2\pi i \Phi(\mathbf{k}_0)} = e^{-2\pi i n \sigma_3} = \mathbb{1}. \quad (15)$$

This will be true for any number of this kind of singular points inside a loop; also, we can include T matrices and the result will not be affected.

6. Group Structure of Wilson loops

Consider a set of Wilson loops - $\mathcal{W}(\mathbf{k}_{01})$, with \mathbf{k}_{01} as a starting and ending point. It can be showed that this set satisfies group axioms. For example: for each element $W(\mathbf{k}_{01})$ of this group we have an inverse, which is Hermitian conjugate of this loop: $W^{-1}(\mathbf{k}_{01}) = W^\dagger(\mathbf{k}_{01})$. Moreover, we can characterize each element of this group with the loop labels (m, n) , where m counts a winding number around a big principal circle of torus and n – around a small principal circle. This kind of labeling comes from the fact that the fundamental group of torus is $\pi_1(T^2) = \mathbb{Z} \times \mathbb{Z}$.

To see this, we considered the Wilson loop shown in the picture below:

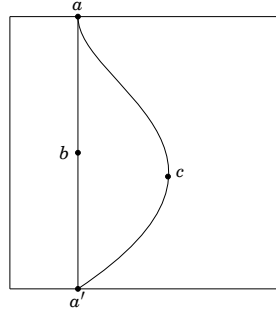


Figure 1

Since $W_{aba'ca} = \mathbb{1}$, because it does not contain any singular point and if it does, we assume that the gap is still open in the energy spectrum, we have $W_{aba'} = W_{aca'}$; this means that they are represented in the set by the same element and that we can assign to it the loop label $(0, 1)$ in this case.

We have a group isomorphism: $\pi_1(T^2) = \mathbb{Z} \times \mathbb{Z} \rightarrow \mathcal{W}(\mathbf{k}_{01})$, so a group of Wilson loops is an Abelian group with two group generators corresponding to the loops $(1, 0)$ and $(0, 1)$. Hence, any element of the group can be written as

$$W_{(m,n)} = W_{(1,0)}^m \cdot W_{(0,1)}^n. \quad (16)$$

This can be seen if we consider Wilson loop along the loop that goes twice around a small principal circle of torus, as shown in the Fig.2

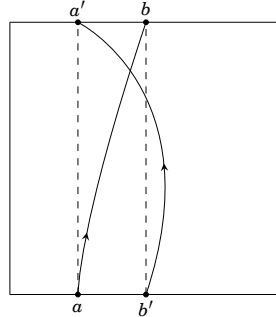


Figure 2

Now we can add to it the second \mathcal{BZ} :

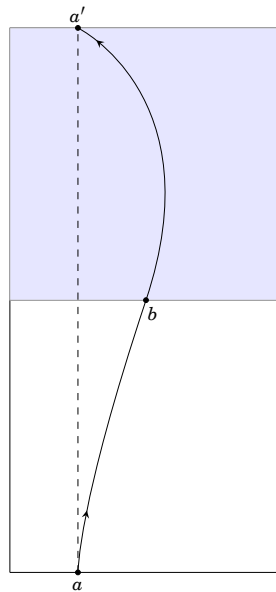


Figure 3

Using the previous result, we arrive to $W_{(0,2)} = W_{(0,1)}^2$.

The next step is to see what is the relation between two groups that differ with the starting and ending points. If we take two such groups, $\mathcal{W}(\mathbf{k})$ and $\mathcal{W}(\mathbf{k}')$, and consider one example shown in the Fig.4:

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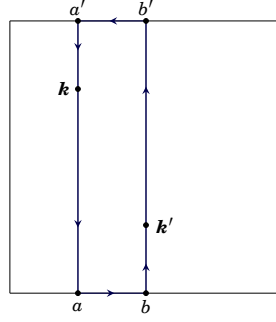


Figure 4

Again, since $W_{kabk'b'a'k} = \mathbb{1}$, the relation appears to have the following form

$$W_{k'b'b'k'} = U^\dagger W_{kaa'k} U, \quad (17)$$

where U is itself a unitary matrix, Wilson line, $U = W_{k'b'a'k}$. This means that every quantity that we are interested in remains the same, while having different starting and ending points.

7. A Different View of the Problem

We can look at the structure of the set of Wilson loops through a differential geometry viewpoint. Firstly, let us remind ourselves some of the core definitions [4].

Definition 7.1 (Horizontal curve). *Let M be a manifold, P a principal bundle over M , with fiber G , and D a connection in P . Let $\gamma : [0, 1] \rightarrow P$ be a smooth curve in P . Then $\dot{\gamma}(t) \in T_{\gamma(t)}P$ is tangent to $\gamma([0, 1])$ for each $t \in [0, 1]$. We call γ a horizontal curve if its tangent vectors are horizontal, that is, $\dot{\gamma}(t) \in D_{\gamma(t)}$ for each $t \in [0, 1]$. Similarly, if $\gamma : [0, 1] \rightarrow P$ is piecewise-smooth, we say that γ is horizontal if $\dot{\gamma}(t) \in D_{\gamma(t)}$ for t in the open, dense subset of $[0, 1]$ where $\dot{\gamma}(t)$ is well-defined.*

Definition 7.2 (Holonomy Group). *Let M be a manifold, P a principal bundle over M , with fiber G , and D a connection in P . for $p, q \in P$, write $p \sim q$ if there exists a piecewise-smooth horizontal curve in P joining p to q . Clearly, \sim is an equivalence relation. Fix a point $p \in P$, and define the holonomy group of (P, D) based at p to be*

$$\text{Hol}_p(P, D) = \{g \in G : p \sim g \cdot p\}.$$

It can be shown that it is indeed a group. Also, note that if the base space and total space are connected, then $\text{Hol}_p(\Delta^E) = g^{-1} \text{Hol}_q(\Delta^E) g$, where $g \in G$. So in this sense holonomy group is independent of the base point and from now on we can omit the subscript of it. We will need some features of holonomy groups for the future. For example, there is a special subgroup, called restricted holonomy group, denoted by $\text{Hol}_x^0(D, P)$ which is the set of $g \in G$ for which there exists a piecewise-smooth horizontal curve $\gamma : [0, 1] \rightarrow P$ such that $\gamma(0) = p$, $\gamma(1) = g \cdot p$, and $\pi \circ \gamma$ is null-homotopic in M .

Theorem 7.1. *Let M be a manifold, P a principal bundle over M with fiber G , and D a connection in P . Then $Hol^0(P, D)$ is a connected Lie subgroup of G . It is the connected component of $Hol(P, D)$ containing the identity, and is a normal subgroup of $Hol(P, D)$. Moreover There is a natural, surjective group homomorphism $\phi : \pi_1(M) \rightarrow Hol(P, D)/Hol^0(P, D)$. Thus, if M is simply-connected, then $Hol(P, D) = Hol^0(P, D)$.*

There is a fundamental relations between the holonomy group and the curvature of the connection. One of them that we will need states: connection is flat (i.e. has vanishing curvature) if and only if $Hol^0(P, D)$ is trivial.

Now we can go back to our question. There is an evident connection between holonomy group and group of Wilson loops. Indeed, firstly we can look at any loop γ on the base space and then horizontally lift it in the total space, so that γ_\uparrow is horizontal; the starting and the ending points in the total space generally will not coincide, although they will lay in the same fiber; group element of the fiber that is needed to get from the ending point to the starting point is essentially what makes up the holonomy group as well as the group of Wilson loops. This means that we can use the features that were listed above for Wilson loops. We can start by noting that in our case we have $T^2 \times SU(2)$ principal bundle, where $SU(2)$ comes from the solution space (3),(4).

Our base space is torus which is connected but not simply connected; that would mean $Hol(A) \neq Hol^0(A)$ which agrees with our results. Secondly on torus we have 2 types of loops, ones that are contractible and ones that are not: $\pi_1(T^2) = \mathbb{Z} \times \mathbb{Z}$. From our calculations we saw that if the path is contractible $W(\gamma) = \mathbb{1}$. Consequently $Hol^0(A)$ is trivial ($Hol^0(A) = \mathbb{1} \in SU(2)$). Now, using the relation between holonomy group and curvature, we can conclude that A is flat $\Rightarrow F_{\mu\nu} = 0$; again, it agrees with our results except the points that are problematic for the eigenvectors.

Loops that are not contractible can be characterized with 2 integers, they count winding around the 2 principal circles of torus. Wilson loops along them are nontrivial elements of the holonomy group. Using the feature of holonomy groups, we see that there exists a natural surjective group homomorphism:

$$\pi_1(T^2) = \mathbb{Z} \times \mathbb{Z} \rightarrow Hol(A) = Hol(A)/Hol^0(A),$$

where $Hol(A)$ in our case is a group of the Wilson loops. Moreover, we have a group isomorphism, since kernel of this map consists of only one element: $(0, 0)$. Next, we can use the fact that $T \times SU(2)$ is connected, so holonomy groups are same for different points up to the conjugation

$$\tilde{W}(m, n) = U^\dagger W(m, n)U, \quad U \in SU(2);$$

We came to this relation as well in the previous chapter (17).

8. Conclusion

Using the expression of non-Abelian connection matrix, we showed the useful feature of the curvature tensor (10): it is zero everywhere on T^2 except the singular points for eigenvectors. Using non-Abelian Stokes theorem, computations for Wilson loops can be simplified; using this saw that the Wilson loop was trivial, equal to identity, whenever a loop did not contain any singular point or contained only those that maintained a gap in the energy spectrum. Using the results we concluded that a set of Wilson loops with the same base point was isomorphic to the fundamental group of

torus. Lastly, the same results were achieved while looking at the problem through a different viewpoint.

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