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Randomized quantum graphs

Alison A. Silva, Dionisio Bazeia and Fabiano M. Andrade

***Abstract*— Quantum graphs (QGs) provides a framework to study transport quantum systems modeled by networks. In this work, we extend the studies of scattering on quantum graphs by defining the scattering probabilities of the transport in a quantum network with a randomization parameter associated on them, which here we focus on associate it to the presence of edges. We propose approaches to defining the transport in QGs. The first one consists on evaluating the scattering probabilities of all of it spanning quantum subgraphs and weight them with probabilities associated with the number of edges in each subgraph. In order to improve computationally the evaluation in these systems, we also propose an approximated transmission coefficient, which consists in only taking a sample of the spanning subgraphs. Finally, to illustrate this method, we applied in some quantum graphs with large number of edges. We evaluate the exact and approximate transmission coefficients and compare the variation between the values in both methods. Our results shows the characteristics of the transport as a function of the number of edges and the randomness parameter, which helps to understand the resilience of the transport with edges removal in quantum networks.**

***Keywords*— Quantum graphs, randomization, transport.**

I. Introduction

Quantum graphs (QGs) [1, 2] are models used to study the transport in quantum networks. They have been used to describe different phenomena in several areas of science, having applications in chemistry, mathematics and physics. Among the studies on quantum graphs we can highlight their applications in quantum chaos [3, 4], Anderson localization [5], and chaotic and diffusive scattering [6, 7], to name just a few possibilities of current interest.

In this work, we focus on applying randomness inside these structures, introducing a randomization parameter p associated with parameter changes in the structure of the graph. Then, we analyze the quantum transport in these random networks and how it is affected by the randomness. In order to do that we propose two approaches concerning quantum graphs with random edges, one proposing an exact randomized scattering amplitude of quantum graphs, and an approximated form.

Random construction of quantum graphs has been applied on filamentary switching models [8], in which the connection between the transmission amplitudes in random quantum graphs and memristor models was shown through Landauer-Büttiker framework. We go further on and combine these techniques from both models to estimate the transmission in randomized quantum graphs as a function of the randomization parameter, which can be used to estimate the current in such systems.

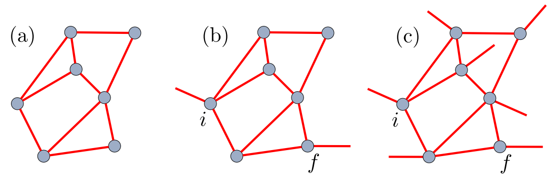

Fig. 1: Quantum graphs with 7 vertices and 10 edges with (a) no scattering channel (closed quantum graph, (b) Two scattering channels attached to the vertices i and f and (c) Seven scattering channels, from which a pair of them are chosen as i and f to the evaluation of the scattering between these channels.

II. Quantum graphs

A graph $G = (V, E)$ is defined as a pair consisting of a finite set of vertices $V = \{v_1, \ldots, v_n\}$ and a set of edges $E = \{e_1, \ldots, e_l\}$ [9]. A QG is a triple $\{\Gamma_G, H, \mathrm{BC}\}$ consisting of a metric graph Γ_G, a graph G with positive lengths $\ell_{e_{i,j}} \in (0, \infty)$ on each edge $\{i, j\}$, a differential operator H, and a set of boundary conditions (BCs) at the vertices, which define the individual scattering amplitudes at the vertices [2]. We consider the stationary free Schrödinger operator $H = -(\hbar^2/2m)d^2/dx^2$ on each edge. Then, to create an open QG with two scattering channels, Γ_G^2, we add two leads (semi-infinite edges) to two different vertices; see Fig. 1(b). The open QG Γ_G^2 is characterized by the global energy-dependent scattering matrix $\sigma^{(f,i)}_{\Gamma_G^2}(k)$, where, as usual, $k = \sqrt{2mE/\hbar^2}$ is the wave number, with i and f as the entrance and exit scattering channels, respectively. Thus, the global scattering amplitudes are intrinsically determined by the graph topology, its metric structure, the BCs at the vertices, and the energy of the incoming particle. This rich interplay of parameters provides a high degree of control over the scattering behavior, establishing quantum graphs as versatile and tunable platforms for investigating scattering phenomena.

In general, for an open QG with c scattering channels, as illustrated in Fig. 1 with (b) $c = 2$ and (c) $c = 7$, we can obtain the global scattering amplitudes $\sigma^{(f,i)}_{\Gamma_G^c}(k)$ by employing Green's function approach, which was developed in Refs. [10–12]. This approach is general and has been successfully used in several transport studies in QGs [13, 14]. The exact scattering Green's function for a quantum particle of fixed wave number k, with initial position x_i in the lead e_i and final position x_f in the lead e_f can be obtained by using the adjacency matrix of the underlying graph [11]. Thus, the Green's function is written as

$$G_\Gamma(x_f, x_i; k) = \frac{m}{i\hbar^2 k}\sigma^{(f,i)}_{\Gamma_G^i}(k)e^{ik(x_i+x_f)}, \tag{1}$$

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where

$$\sigma^{(f,i)}_{\Gamma^i_G}(k) = \sum_{j\in E_i} A_{ij} P_{ij}(k) t_i(k), \tag{2}$$

is the global transmission amplitude, with $P_{ij}(k)$ the family of paths between the vertices i and j, which are given by

$$P_{ij}(k) = z_{ij} P_{ji} r_j(k) + \sum_{l\in E_j^{j,n}} z_{ij} A_{jl} P_{jl} t_j(k) + z_{ij}\delta_{jn} t_n(k), \tag{3}$$

with $z_{ij} = e^{ik\ell_{\{i,j\}}}$ and $\ell_{\{i,j\}}$ the length of the edge between vertices i and j. The family $P_{ji}(k)$ is given by the same expression above, but with the swapping of indices i and j. Then, in each vertex i we associated one $P_{ij}(k)$ for every $j \in E_i$, where E_i is the set of adjacent vertices of i. In the above equation, $r_i(k)$ and $t_i(k)$ are the individual reflection and transmission amplitudes, respectively, associated with the boundary conditions imposed at the vertex i. For Neumann-Kirchhoff boundary conditions, these individual quantum amplitudes are independent of k, and are explicitly given by $r_i = (2/d_i) - 1$ and $t_i = 2/d_i$, where d_i is degree of the vertex i.

III. RANDOMIZED QUANTUM GRAPHS

We now introduce randomized quantum graphs (RQGs). A graph with a randomization parameter p_{e_j} associated to each edge has a probability

$$P_F = \binom{|E_G|}{|E_F|} p^{|E_F|}(1-p)^{|E_G\setminus E_F|}, \tag{4}$$

of obtaining any subgraph $F(V, E_F)$ edges from $G(V, E)$, with $E_F \subseteq E$. From that we now can define the global scattering coefficients of a randomized quantum graph (RQG) from its set of quantum spanning subgraphs in the following way.

Definition III.1 (Exact transmission coefficient of a RQG)**.** Let Γ^c_G be a quantum graph with c scattering channels. The exact transmission coefficient associated with the randomized quantum graph $R(\Gamma^c_G)$ is defined by

$$T^{(f,i)}_{R(\Gamma^c_G)}(k,p) = \sum_{\Gamma^c_F \text{ spans } \Gamma^c_G} p^{|E_{\Gamma^c_F}|}(1-p)^{|E_{\Gamma^c_G}\setminus E_{\Gamma^c_F}|} \left|\sigma^{(f,i)}_{\Gamma^c_F}(k)\right|^2, \tag{5}$$

in which p is the randomization parameter associated with the probability of the existence of an edge of the original quantum graph.

In the definition above, the number of quantum subgraphs will depend on the number of edges present in the original quantum graph. For instance, in the case of a complete quantum graph on n vertices, $\Gamma^c_{K_n}$, the number of quantum spanning subgraphs is $2^{\binom{n}{2}}$. Thus, the number of subgraphs scales exponentially with the number of vertices and the application of Eq. (5) can be hard to implement. To overcome this issue, we also propose a Monte Carlo method for calculating the scattering probabilities by taking an ensemble $S_{|E_{\Gamma^c_F}|}$ of size $|S_{|E_{\Gamma^c_F}|}|$ of different quantum subgraphs Γ^c_F, each one having exactly $|E_{\Gamma^c_F}|$ random edges, and calculate the scattering amplitude of each subgraph. Then, we calculate the average value of these scattering coefficients,

$$\left|\overline{\sigma}^{(f,i)}_{|E_{\Gamma^c_F}|}(k)\right|^2 = \frac{1}{|S_{|E_{\Gamma^c_F}|}|} \sum_{\Gamma^c_F \in S_{|E_{\Gamma^c_F}|}} \left|\sigma^{(f,i)}_{\Gamma^c_F}(k)\right|^2. \tag{6}$$

The subgraphs of the ensemble are chosen uniformly and randomly among all the possible subgraphs Γ^c_F having exactly $|E_{\Gamma^c_F}|$ edges, without repetition and taking into account all the isomorphic subgraphs. We proceed in this manner since determining whether two subgraphs are isomorphic is not an easy problem [15]. Based on this, we propose an approximated method for calculating the transmission coefficient for RQG.

Proposition 1 (Approximated transmission coefficient for RQG)**.** Let Γ^c_G be a quantum graph with c scattering channels and $\mathbb{S}_{|E_{\Gamma^c_F}|}$ the set of all subgraphs Γ^c_F of the quantum graph Γ^c_G with a given number of edges $|E_{\Gamma^c_F}|$. Take an ensemble $S_{|E_{\Gamma^c_F}|} \subset \mathbb{S}_{|E_{\Gamma^c_F}|}$, of size $|S_{|E_{\Gamma^c_F}|}|$ of quantum subgraphs Γ^c_F with a fixed number $|E_{\Gamma^c_F}|$ of edges and calculate the average scattering coefficient using Eq. (6). The approximated transmission coefficient associated with the randomized quantum graph $R(\Gamma^c_G)$ is

$$\mathcal{T}^{(f,i)}_{R(\Gamma^c_G)}(k,p) = \sum_{|E_{\Gamma^c_F}|=0}^{|E_{\Gamma^c_G}|} \binom{|E_{\Gamma^c_G}|}{|E_{\Gamma^c_F}|} p^{|E_{\Gamma^c_F}|}(1-p)^{|E_{\Gamma^c_G}\setminus E_{\Gamma^c_F}|} \left|\overline{\sigma}^{(f,i)}_{|E_{\Gamma^c_F}|}(k)\right|^2. \tag{7}$$

This approximation converges with the increasing of the ensemble size and reduces the computational cost.

The randomization method can be generalized by defining distinct probabilities p_{e_j} to obtain each edge e_j. Hence, a given set $\boldsymbol{P}$ of probabilities to obtain each edge, a set of subgraphs (F) from G is obtained, each one with a set of edges E_F. Thus, the probability to obtain each subgraph is now given from

$$p(F) = \prod_{e_j\in E_F} p_{e_j} \prod_{e_j\in E_G\setminus E_F} \left(1 - p_{e_j}\right). \tag{8}$$

In a special case where all the edges have the same probability p to occur, we recover the probability of obtaining a given subgraph from the previous case.

In this sense, a way to estimate the average scattering for an ensemble of many quantum graphs with random edges by a probability $p_{e_j} \in \boldsymbol{P}$ of formation is in the form

$$\mathcal{T}^{(f,i)}_{R(\Gamma^c_G)}(k,\boldsymbol{P}) = \sum_{F \text{ spans } G} \left[\prod_{e_j\in E_F} p_{e_j} \prod_{e_j\in E_G\setminus E_F} \left(1 - p_{e_j}\right) \left|\sigma^{(f,i)}_{\Gamma^c_F}(k)\right|^2\right]. \tag{9}$$

In [8] several random graphs are generated and the scattering transmission probability in them are used to obtain the current in the system. Then, the average current in each cycle is evaluated to obtain the statistics of many cycles. This method can be applied to that case by setting a graph that corresponds to all possible graphs in the space defined there, and then setting the corresponding probability of each edge being formed in the filament.

IV. RESULTS

To study the behavior of the scattering in RQG, we focus on the family of complete graphs on n vertices, K_n, but with the removal of the edge $e = \{i, f\}$, as illustrated in Fig. 2. The complete graph on n vertices with the edge e removed is denoted by $K^e_n = K_n \setminus e$. Moreover, to transform this graph into an open quantum graph with 2 scattering channels, defined

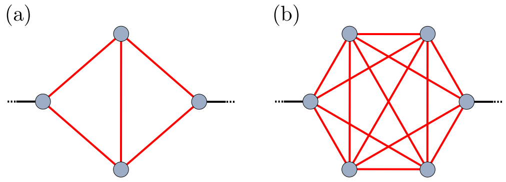


Fig. 2: The open quantum graphs $\Gamma^2_{K_n^e}$ with (a) $n = 4$ vertices, (b) $n = 6$ vertices.

as $\Gamma^2_{K_n^e}$, we have to associate lengths, and here we assign the same length ℓ on all edges. Also, we use Neumann-Kirchhoff boundary condition on all vertices and add two leads to the vertices i and f, the same vertices where we removed the connecting edge e; see Fig. 2. This procedure ensures that all vertices have the same degree $n-1$, then the individual reflection and transmission amplitudes are $r = 2/(n-1) - 1$ and $t = 2/(n-1)$, respectively. In Fig. 2, we show some examples of the quantum graphs $\Gamma^2_{K_n^e}$ with $n = 4$ and 6.

Taking the quantum graph $\Gamma^2_{K_4^e}$ displayed in Fig. 2(a) as an example and as the number of quantum subgraphs are not so high, we can calculate the exact transmission for the randomized quantum graph $R(\Gamma^2_{K_4^e})$ by evaluating the scattering transmission for all its quantum subgraphs, Eq. (5). We identified 14 non-isomorphic quantum subgraphs. Then, we evaluated their number of isomorphisms and transmission amplitudes, from which 7 of them had transmission amplitudes different of zero. The individual results are shown in Table I. These transmissions can be computed as a function of the number of edges. By grouping the graphs with the same number of edges and taking the average value of the scattering transmission, as defined in Eq. (6), we obtain the results presented in Fig. 3.

Thus, following Definition III.1 the scattering transmission for the randomized quantum graph $R(\Gamma^2_{K_4^e})$ can be expressed as the summation of all possible subgraphs weighted by their probabilities as

$$T_{R(\Gamma^2_{})}(k,p) = p^5\left|\sigma^{(f,i)}_{\Gamma^2_{}}(k)\right|^2 + p^4(1-p)\left(4\left|\sigma^{(f,i)}_{\Gamma^2_{}}(k)\right|^2 + \left|\sigma^{(f,i)}_{\Gamma^2_{}}(k)\right|^2\right) + p^3(1-p)^2\left(2\left|\sigma^{(f,i)}_{\Gamma^2_{}}(k)\right|^2 + 4\left|\sigma^{(f,i)}_{\Gamma^2_{}}(k)\right|^2\right) + p^3(1-p)^2\left(2\left|\sigma^{(f,i)}_{\Gamma^2_{}}(k)\right|^2\right) + p^2(1-p)^3\left(2\left|\sigma^{(f,i)}_{\Gamma^2_{}}(k)\right|^2\right) \quad (10)$$

The corresponding expressions for the transmission amplitudes are presented in Table I. This allows us to evaluate the exact transmission probability for the RQG as a function of $k\ell$, the wavenumber × edge length, and the randomization parameter p, as illustrated in Fig. 4.

To compare the exact and approximated transmission coefficients, we now consider a more complex case, the complete quantum graph minus an edge with $n = 6$, K_6^e. For K_6^e, there are $2^{14} = 16384$ possible subgraphs, which must be considered for the exact calculation. In Fig. 5, the background plots (blue curves) represent all the 16384 transmission probabilities for the quantum subgraphs of $\Gamma^2_{K_6^e}$. The red curves represent the average values of the transmission for a given number of edges [Eq. (7)], and the thin black curves represent the approximate average values of the transmission by considering ensembles with the same number of edges with up to 250 quantum

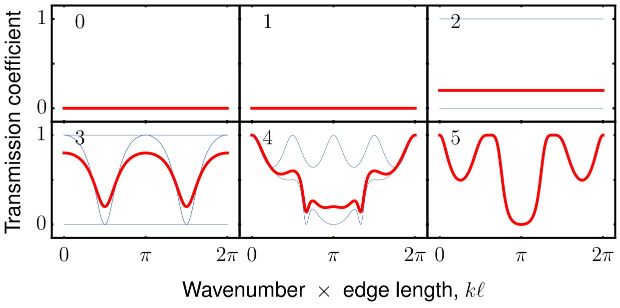
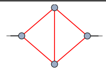
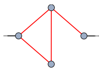
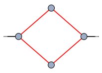
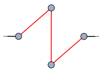
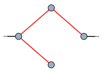
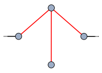
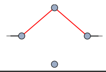


Fig. 3: Transmission coefficients of quantum subgraphs ensembles with 0 to 5 edges. The blue curves show the individual transmission coefficients of the subgraphs with a given number of edges, while the red curves represent the average transmission of the ensemble.

TABELA I: Non-isomorphic quantum subgraphs from $\Gamma^2_{K_4^e}$, its number of edges l, its number of isomorphic subgraphs (NIS) in the ensemble, and the probability associated with the number of edges and the corresponding transmission amplitudes. In the transmission $z = e^{ik\ell}$.

Subgraph	l	NIS	Probability	Transmission Amplitude $\sigma^{(f,i)}_{\Gamma^2_F}(k)$
	5	1	p^5	$\frac{16(1+z)z^2}{27+9z+6z^2-6z^3-z^4-3z^5}$
	4	4	$p^4(1-p)$	$\frac{4\left(1+2z+2z^2+z^3\right)z^2}{9+9z+8z^2-z^4-z^5}$
	4	1	$p^4(1-p)$	$\frac{8z^2}{9-z^4}$
	3	2	$p^3(1-p)^2$	z^3
	3	4	$p^3(1-p)^2$	$\frac{2\left(1+z^2\right)z^2}{3+z^2}$
	3	2	$p^3(1-p)^2$	$\frac{2\left(1+z^2\right)z^2}{3+z^2}$
	2	2	$p^2(1-p)^3$	z^2

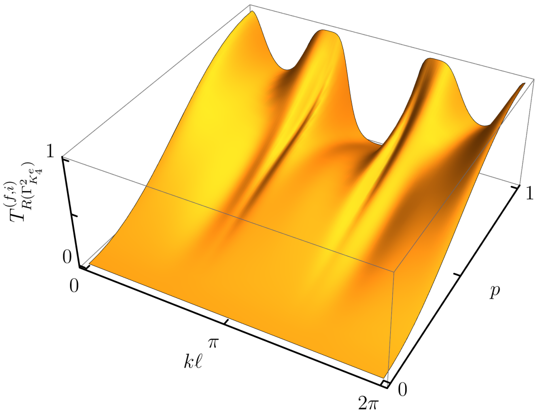


Fig. 4: The exact transmission coefficient for the RQG $R(\Gamma^2_{K_4^e})$ as function of the wavenumber × edge length $k\ell$ and randomization parameter p.

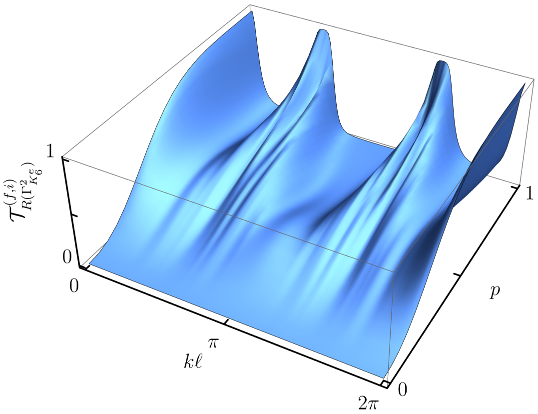


Fig. 6: Approximated transmission coefficient for the RQG $R(\Gamma^2_{K_6^e})$ as function of the wavenumber × edge length $k\ell$ and randomization parameter p.

subgraphs. Finally, the result obtained for the approximated scattering transmission probability considering these ensembles, which depend on the number of edges present in the quantum subgraph is shown in Fig. 6. Also, we calculated the exact transmission coefficient for this randomized quantum graph, and the results are almost indistinguishable from the approximated one, displaying a maximum error of 2.3%. This is an indication that our method is adequate.

Some characteristics of these results that can be highlighted are: i) the transmission is periodic, so we concentrate on the interval $0 \leq k\ell \leq 2\pi$; ii) the transmission vanishes for all $k\ell$ when the number of edges $|E_{\Gamma_F^2}|$ is less than or equal to 1, which is expected as in this case, there is no direct connection between the input and the output channels, so the graph requires at least two edges to induce transmission; iii) for $|E_{\Gamma_F^2}| = 2$, due to the Neumann-Kirchhoff boundary conditions, either the signal is fully transmitted or there is no transmission at all; iv) for $k\ell = \pi$, we notice that there is transmission only in the interval of $2 \leq |E_{\Gamma_F^2}| \leq 9$, where the maximum transmission of the ensemble is reached when 9 edges are removed; v) the transmission probability displays a band of full suppression in the region around $k\ell = \pi$, even when one removes up to 4 edges due to destructive interference in the transmission. This is a significant result, informing us about the resilience of the quantum graph at this region, which allows us to suggest that the graph can still be used as a filter even in the presence of some noise of imperfections, i.e., by edge removals. With these average values of transmission coefficients, we use Eq. (7) in Proposition 1. Working in this direction, we have obtained the results shown in Fig. 6.

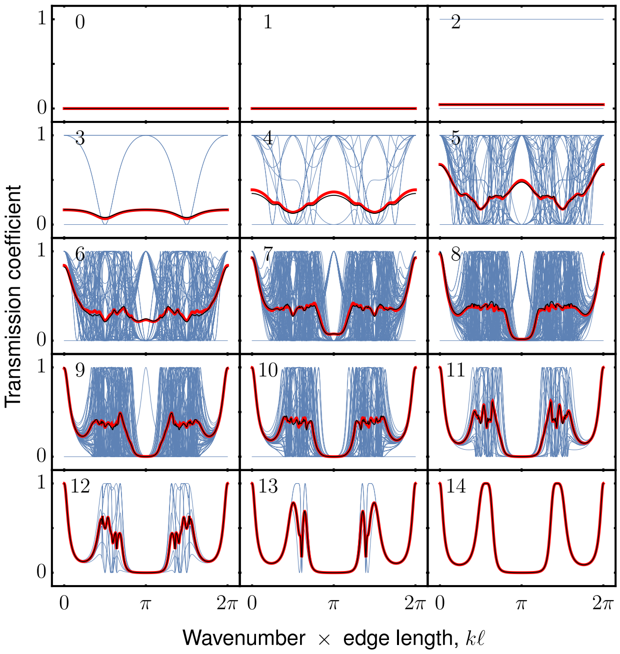


Fig. 5: Transmission coefficients of ensembles of quantum subgraphs Γ_F^2 of the quantum graph $\Gamma^2_{K_6^e}$ with $|E_{\Gamma_F^2}| = 0, 1, \ldots, 14$. The blue curves in the background show the transmissions coefficients of the corresponding subgraphs, while the red curves represent the average transmission of the corresponding ensembles and the thin black lines show the average value of transmission by taking up to 250 Monte Carlo samples of subgraphs from the ensemble.

V. Conclusions

In this work, we analyzed randomized quantum graphs (RQGs) as a model to understand the characteristics of the transport in quantum networks with probabilities associated to them. To achieve this, we developed two methods. The first one consists of an exact transmission coefficient, which considers all the possible quantum graphs. We also proposed another method that approximates the coefficient by using ensembles, reducing the computational cost.

To apply this method, we utilized a complete quantum graph with an edge removed, which has a large number of edges, while not being the trivial complete graph usually used in these studies. This allow us to show that our method, using spanning subgraphs is general for any aimed quantum graph. Our results allowed us to verify the behavior of the transport in the subgraphs comparing different number of edges on them and the randomization parameter.

These results showed some features as the suppression around $k\ell = \pi$, that is maintained even with some edges being removed. This indicates that quantum graphs can act as robust quantum filters, keeping some transport characteristics in the presence of imperfections.

The findings here can motivate research on other types of quantum graphs and the possibility of using different edge lengths or dressed quantum graphs. The way the randomization of quantum graphs is defined here also allows us to randomize a given set of edges of the graph instead of all edges of the graph, letting us study the introduction of defects in some parts of the graph, adding or removing some edges randomly, which enables the study of the impact of the presence of these random edges in the transmission probability. These and other generalizations will be reported in future works.

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DATA AVAILABILITY STATEMENT

No Data is associated with the manuscript

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