Quantum graphs proposal for quantum devices

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The control of quantum information is an issue of current interest for the construction of quantum machines. In this work, we investigate this possibility in the realm of quantum graphs. The study allows the identification of two distinct effects which are related to quantum complexity, one being the Braess paradox and the other the presence of quantum interference in some elementary arrangements of graphs. Motivated by the power of quantum graphs, we elaborate on the construction of simple devices, based on microwave and optical fibers networks, and also on quantum dots, nanowires and nanorings. The elementary devices can be used to construct composed structures with important quantum properties, which may be used to manipulate quantum information.

Since the pioneering work of Linus Pauling [1] in the context of free electrons in organic molecules, quantum graphs have been used to describe the behavior of quantum particles in idealized physical networks [2, 3]. In the last twenty years or so, the interest in quantum graphs has increased importantly, mainly because of the richness of the subject, which is related to a variety of issues in physical and mathematical sciences. For instance, quantum graphs have been simulated experimentally in microwave networks [4] and it is also possible to synthesize quantum nanowires networks with sequential seeding of branching structures [5] and also, using conventional microfabrication facilities [6]. Many properties and techniques related to the study of graphs and their applications can be found in [7]. Moreover, in the recent literature we noted the interesting investigations [8–10], in which the authors deal with issues on graphs and simulations via microwave networks [8], in a way similar to Ref. [4].

The case of networks of fibers and splitters adds another perspective that consists in the construction of a lasing network (LANER) [9], a complex active optical network of fibers and splitters, which is further explored in [10] and may be nicely modelled by graphs.

Among the several possibilities to describe physical properties of quantum graphs, an interesting procedure concerns the Green’s function approach, which was proposed in [11] and further explored in [12, 13]. In this Letter we shall rely on the Green’s function approach to investigate specific scattering properties of quantum graphs. The graphs to be studied below have two leads attached to two distinct vertices that are further connected with two distinct edges. The details of the calculations and the use of graphs with the focus on the global transmission coefficients are all given in a companion work [14], in which we explain and explore carefully the concepts and techniques used to implement the calculations that ended up with the current study. In Ref. [14], in particular, we concentrated mainly on hexagonal graphs with vertices of degree 3, with ideal leads and edges. We did this to focus mainly on the transmission features of simple ideal graphs described by vertices of degree 3, in this way circumventing the appearance of effects related with the presence of vertices of distinct degrees. In this Letter we deal with the two simplest graphs, which contain only two vertices of degree 3. We investigate these graphs concentrating on the possibility to develop simple devices that engender interesting quantum effects.

The study starts with the calculation of global transmission amplitudes of quantum graphs as a function of the wave number of the incident signal, using the Green’s function approach developed in [12, 13]. The focus is on the Braess paradox [15] and the possibility to identify very narrow peaks of wave numbers in which the transmission coefficient increases significantly due to the quantum interference.

The Braess paradox was discussed by Dietrich Braess in 1968 [15]; see also Refs. [16–19]. The original observation is that, under the addition of extra road to a congested road traffic network to improve traffic flow, sometimes it may happen that the reverse occurs. An interesting interpretation is that the addition of a new road may under specific conditions enlarge the complexity of the system, opening new possibilities that may include surprisingly unexpected responses. The paradox may appear at the classical or quantum level, and it was discussed at the quantum level in Refs. [20–23]. In particular in [20], simulations of quantum transport in mesoscopic networks reveal the transport inefficiency, which is further confirmed by a scanning-probe experiment using a biased tip that measures the conductance variation in terms of the tip voltage and position. The effect also appeared in [21], in a numerical simulation in a quantum ring with the addition of a central horizontal branch at the nanometric scale. It also appeared in [22], in the context of matter transport in quantum dots (QDs) that are coupled together, and in [23] in the case of a phase-coherent quantum transport through a simple metallic fork. As we shall show, the Braess paradox also appears related to the global transmission of the quantum graphs that we examine in the current work.

We also examine other effects, in particular, very narrow peaks of full transmission that remind us of Feshbach resonances [24, 25]. In the context of quantum graphs, the presence of Feshbach resonances was investigated before in Ref. [26]. Here, however, we concentrate on the search of peaks of full transmission that we call peaks of constructive quantum interference, which appear inside regions of suppression of transmission. Evidently, the identification of those peaks
allows for a diversity of applications, since quantum interference is a fundamental phenomenon with a wide range of applications, including quantum state engineering with Josephson junction devices for quantum computation and communication [27], electronic transport in photosynthetic processes that seem to offer a biological advantage [28, 29], and single-molecule quantum transport in break junctions [30], among other possibilities.

The two simple quantum graphs of interest in this Letter are depicted in Fig. 1. They are constructed owing to simplicity, that is, one considers ideal leads, edges and vertices. Also, one takes edges with the same length and uses the simplest boundary conditions at the vertices, the Neumann boundary conditions. The two graphs have only two vertices of degree 3, and they conform with the two simplest regular geometric forms, the equilateral triangle and the square, and we refer to them by $C_3$ and $C_4$, and highlight that they have three and four equal edges, respectively. The global transmissions properties of them are described by $|T_{C_3}(k)|^2$ and $|T_{C_4}(k)|^2$, and are calculated following the lines of the companion work [14]. The results are displayed in Fig. 2, and there one notices that although $|T_{C_3}(k)|^2$ (violet dotted curve) has a simpler undulating behavior, the $|T_{C_4}(k)|^2$ (blue solid curve) on the contrary shows a richer structure. This is an unexpected result and shows that, despite its geometric simplicity, the triangular arrangement leads to a complex behavior that may induce transport inefficiency.

To see how this appears in the present context, let us now focus on the Braess paradox. We recall that the paradox has been studied at the classical [15–19] and quantum [20–23] levels, and the investigations are in general based on, say, the addition of an extra path and the search for suppression of transmission. In the present work we innovate and show for the first time that it also appear in the simplest possible situation, in which we have only two simple distinct internal paths. This is of practical interest, since it will ultimately simplify the proposal, and experimentalists would certainly benefit from this simplicity. To understand this issue more accurately, we introduce the difference $|T_{C_3}(k)|^2 - |T_{C_4}(k)|^2$ and depict it in Fig. 3. The result shows that it can be positive or negative, depending on the wave number of the signal entering the graph, showing that the transmission through the triangle is not always higher than the one of the square. To add quantitative information on this, let us think of the calculation in terms of the hitting time, which we interpret here as the expected number of steps the signal has to give before leaving the graph at the right or left side, after entering it from the left or right side. The calculation is easier at the classical level, but since we are interested in quantum effects, one implement it at quantum level. This is fully discussed in [14], and the numerical results are based on random walks on graphs with extensions to the context of quantum walks [31, 32], and on results of Ref. [33]. The hitting time corresponding to the two graphs under consideration are $h_{C_3} = 1.91612$ and $h_{C_4} = 155/72 = 2.15278$, showing that the triangle is expected to be in general more efficient to transmit information. However, the effects that are captured by the transmission coefficients of the quantum graphs make the problem more complex, inducing the transmission of information through the triangular graph to follow the unexpected pattern that appear in Fig. 2, giving rise to transport inefficiency in a large region of wave number, which is clearly shown in Fig. 3.

The complexity of the transmission coefficient of the triangular graph suggests that we further explore other possibili-
ties. An interesting direction is to see the two quantum graphs as two independent devices that can be used to the construction of other structures. A simple possibility is to arrange the two graphs in series and in parallel. This is investigated in details in [14] for hexagonal graphs, and here we report on the interesting cases in which one adds together the compositions triangle-triangle ($C_3C_3$), square-square ($C_4C_4$), and triangle-square-triangle ($C_3C_4C_3$); see Fig. 4 for an illustration of the $C_3C_4C_3$ combination. They are series compositions of two and three elements and, in fact, there are several parallel and series arrangements. Here, however, we focus only on the above mentioned three cases, because they unveil the important effects that we are searching for, in particular, the appearance of very narrow peaks of full transmission inside regions of complete suppression. The transmission coefficients of the triangle-triangle, square-square, and triangle-square-triangle compositions are described by $|T_{C_3C_3}(k)|^2$, $|T_{C_4C_4}(k)|^2$, and $|T_{C_3C_4C_3}(k)|^2$, and they are displayed in Fig. 5. We see from these results that the series compositions with two triangles and two squares present bands of full suppression and narrow peaks of full transmission. Similarly, the transmission coefficient of the triple composition triangle-square-triangle has a larger band of full suppression and four narrow peaks of full transmission. We have studied these peaks of constructive quantum interference carefully and found that the two at the top panel are located at $\pi \pm 0.91393$, and they have the same width 0.02091. The four at the middle panel are located at $\pi \pm 1.76182$ and at $\pi \pm 1.37977$ and have the same width 0.00600. The other four peaks at the bottom panel of Fig. 5 are located at $\pi \pm 1.12611$, with width 0.00804, and at $\pi \pm 0.43440$, with width 0.00812. The presence of these peaks of full transmission inside regions of full suppression is another unexpected effect, which is due to the quantum complexity of the problem under investigation. This is another interesting effect that can be used to manipulate quantum information.

It is of interest to remark that there are other possible studies to be done. In particular, if one thinks of the square, for instance, we can connect the second lead to the second neighbor vertex. Also, we can consider the next polygon, the regular pentagon, and now we can connect the second lead to the first or the second neighbor vertex. Moreover, we can think of the regular hexagon, and here connect the second lead to the first, second or third neighbour vertex, and so on and so forth. We have examined some distinct cases, and found no qualitative difference with the results depicted in Fig. 5. Another remark of interest is that all the transmission coefficients described in this work obey $|T(\pi + k\ell)|^2 = |T(\pi - k\ell)|^2$, for $k\ell \in [0, \pi]$. This appears due to the time reversal symmetry of the quantum graphs that we are examining in this Letter, and they do not distinguish the signal entering from the left or right and leaving to the right or left.

The two quantum graphs depicted in Fig. 1 can be thought of as two elementary devices, so one can probe them following the lines of Ref. [4], in which experimental and theoretical results unveil how microwave networks can simulate quantum graphs. This is an interesting possibility, and is further connected to another very recent investigation [8] on graphs and simulations via microwave networks. Another perspective of current interest is to think of considering networks of fibers and splitters, in a way similar to the recent idea of a lasing network, a LANER [9] which is constructed as a complex active optical network of fibers and splitters, which is further

![FIG. 4. (Color online) Illustration of the series structure described by the triangle-square-triangle composition.](image_url)

![FIG. 5. (Color online) The transmission coefficients of the series arrangements triangle-triangle, square-square and triangle-square-triangle, displayed in the top, middle and bottom panels, respectively.](image_url)
explored in [10]. We think that the above results will foster further interest on microwave networks [4, 8, 34] and also, on the very recent proposal of networks of fibers and splitters [9, 10], in particular, on spatial arrangements of graphs, with the use of more complex topologies.

Another important line of research concerns the construction of quantum devices at the nanometric scale, simulating the two quantum graphs with QDs connected by leads. The use of QDs for quantum computing is not new [35], and the more recent works [36, 37] illustrate distinct possibilities of fabricating and evaluating compositions of two or more QDs in nanowires and in Josephson junctions. The idea here is to suppose that electrons in the incoming lead reach a QD from one side and leave the device through the QD at the outgoing lead on the other side, after interacting with the QDs via the edges that connect them. The flux of matter can be controlled by the chemical potentials of electronic sources that are attached to the left and right leads. A similar configuration was studied before in [22], and the weak localisation contribution due to the arrangement with two QDs connected by three edges also unveiled the Braess paradox. The QD composition suggested in [22] and the Braess paradox that appeared in the transmission results there obtained motivate us to suggest that structures composed of the two basic QDs will certainly display the presence of the peaks of full transmission that we found in the series composition described in the bottom panel in Fig. 5. Since QDs are mesoscopic devices, the current suggestion works to improve the fabrication of quantum devices at the mesoscopic level, in this sense directly contributing for the manipulation of information at the mesoscopic scale.

To implement the above suggestion experimentally, the fabrication of the two elementary devices, the two compositions that requires two QDs connected with two distinct edges is mandatory. They are double QDs and we call them DQDs, and we further require series arrangements of two and three of those DQDs. It can then be noted that the experimental realisation may be intricate, but we additionally observe that instead of QDs, we can use quantum wires or nanowires, which seem to be somehow easier to be implemented experimentally. An interesting line of investigation may follow the experimental implementation developed in [38], concerning the fabrication of single-crystal nanorings of zinc oxide, formed through spontaneous self-coiling process in the growth of polar nanobelts. Other possibilities were accomplished, for instance, in Refs. [39, 40]. Similar ideas were also considered in [20] and in [21], confirming the transport inefficiency in a ringlike disposition of wires of finite width with the addition of an extra central branch in the ring at the nanometric scale. The results provide another strong motivation for the study of the series compositions that we have investigated in this Letter. Since our graphs are very simple, the quantum devices are also very simple. The connection between quantum devices and quantum graphs is displayed in Fig. 6, with the identification of the two internal arms of the nanometric devices with the two internal edges of the quantum graphs shown in Fig. 1. Since we are dealing with Neumann vertices, there is no objection to think of the triangular and square graphs as ringlike structures, with the external leads being attached radially, in the first case forming an angle of $2\pi/3$, and in the second an angle of $\pi/2$, in this case reaching perhaps the simplest experimental realisation at the nanometric scale.

From the theoretical point of view, the current work motivates several distinct possibilities, an interesting one being the study of graphs with other topologies in the presence of more realistic edges and vertices; see Ref. [14] for more details on how to include different effects on edges and non-trivial boundary conditions on vertices. We can also add appropriate external magnetic field, which will break the time reversal symmetry and add novel effects in the important case of electronic transport of quantum information. Another perspective of current interest is to think of the elementary quantum graphs and their series and/or parallel arrangements as molecules. In this case, we can use them to describe quantum transport and interference with the help of mechanical and electrical break junctions, as recently reviewed in Ref. [30]. A particularly important realization may occur with the use of hexagonal arrangements of graphs, for instance, since they can model graphene and other ringlike configurations of current interest. This is now under examination, and we expect to report on the issue in the near future. We also hope the present study will attract interest toward the subject.

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