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# Transparent Quantum Graphs

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### Transparent Quantum Graphs

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We consider quantum graphs with transparent branching points. To design such networks, the concept of transparent boundary conditions is applied to the derivation of the vertex boundary conditions for the linear Schrödinger equation on metric graphs. This allows to derive simple constraints, which use equivalent usual Kirchhoff-type boundary conditions at the vertex to the transparent ones. The approach is applied to quantum star and tree graphs. However, extension to more complicated graph topologies is rather straight forward.

#### I. INTRODUCTION

The problem of wave transport in branched structures and networks is of importance for many areas of contemporary physics, such as optics, fluid dynamics, condensed matter and polymers. Optical and quantum mechanical waves propagation in such systems appears e.g., in different branched waveguides [1–7]. Effective transfer of light, charge, heat, spin and signal in networks requires solving the problem of tunable wave dynamics. This can be achieved using the models, which provide realistic description of particle and wave transport in branched structures.

An important feature of particle and wave dynamics in networks is the transmission through the branching points, which is usually accompanied by the reflection (backscattering) of a wave at these points. Dominating of reflection compared to transmission implies large "resistivity" of a network with respect to the wave propagation. Therefore, it is important from the viewpoint of practical applications, to reduce such resistivity by providing a minimum of reflection, or by its absence. This task leads to the problem of tunable transport in branched structures, whose ideal result should be reflectionless transmission of the waves through the branching points of the structure. From the viewpoints of practical applications in condensed matter, such transmission implies ballistic transport of charge, spin, heat and other carriers in lowdimensional branched materials. The latter is of importance for the effective utilization of different functional materials.

Reflectionless transport of waves in optical fiber networks is one of the central tasks for the fiber optics, as many information-communication devices (e.g., computers, computer networks, telephones, etc.) use optical fiber networks for information (signal) transfer. Such networks are also used in different optoelectronic devices. High speed and lossless transfer of information in such devices require minimum of backscattering or its absence. Important areas, where the reflectionless, or ballistic transport in branched structures is required, are molecular electronics and conducting polymers. Both deal with the modeling of reflectionless wave transport in

networks and require revealing the conditions providing such regime. Different quantum wire networks appearing in solid state physics are also potential structures, where the wave transport can be tuned from diffusive to ballistic regime using the transparent boundary conditions.

In this paper we study the problem of reflectionless transport in quantum networks, which are modeled in terms of the linear Schrödinger equations on metric graphs. To describe the regime, when there is no backscattering at the network branching points, we use the concept of transparent boundary conditions for the time-dependent Schrödinger equation studied earlier in detail in the Refs. [8–23]. Combining transparent boundary conditions concept with that of vertex boundary conditions for the linear Schrödinger equation on metric graphs, we derive the constraints, providing the regime of reflectionless transmission of the waves through the graph branching points (vertices).

More precisely, we reveal the condition for the regime, at which Kirchhoff-type boundary conditions at the branching point become equivalent to the transparent boundary conditions. The condition is obtained in a simple form of the sum rule for the coefficients, which can characterize physical properties of the network branches. We note that the linear and nonlinear wave equations on metric graphs have been studied earlier in the context of quantum graphs [24–28] and soliton dynamics in networks [29, 30, 32–40]. It was found in the Refs. [29, 35, 39] that transmission of the waves through the network branching point can be reflectionless, when provided certain constraints are fulfilled. However, no strict explanation for such effect have been presented in those studies.

This paper can be considered as the first step in the way for the formulation of clear, physically reasonable, strict mathematical conditions for the reflectionless wave transmission in network branching points in quantum regime. The paper is organized as follows. In the next section we briefly recall the concept of transparent boundary conditions for the linear Schrödinger equation on a line. In Section III we recall the concept of quantum graphs. Section IV provides extension of the concept of transparent boundary conditions to quantum networks described by the linear Schrödinger equation on metric

graphs and presents some numerical results. Finally, Section V presents some concluding remarks.

# II. TRANSPARENT BOUNDARY CONDITIONS IN QUANTUM MECHANICS

The problem of transparent boundary conditions (TBC) for the wave equations has attracted much attention in different practically important contexts (see, e.g., papers [8–23] for review). Such boundary conditions describe the absorption or reflectionless transmission of particles (waves) at the boundary of two domains. Approximate TBCs for the linear Schrödinger equation were formulated by Shibata [41] and Kuska [42], where dispersion relations for the plane waves is approximated to derive TBCs. A strict mathematical analysis of TBC for different wave equations, including quantum mechanical Schrödinger equation can be found in the Refs. [11, 12, 15, 22, 23].

The explicit form of such boundary conditions are much more complicated than those of Dirichlet, Neumann and Robin conditions. Therefore, their discretization causes a serious accuracy loss in the numerical computations and also often reduce the stability range of the overall scheme. Here we briefly recall the formulation of TBCs on a line following the Refs. [9–12].

Let us consider the wave (particle) motion in a 1D domain  $(-\infty, +\infty)$  and described by the following time-dependent Schrödinger equation (with  $\hbar = m = 1$ ):

$$i\frac{\partial}{\partial t}\Psi = -\frac{1}{2}\frac{\partial^2}{\partial x^2}\Psi + V(x,t)\Psi,$$
 (1)

with the initial condition given as

$$\Psi(x,0) = \Psi^I(x),$$

where  $\Psi^I \in L^2(\mathbb{R})$ ,  $V(.,t) \in L^\infty(\mathbb{R})$  and V(x,t) is an external potential. Our purpose is to formulate the boundary conditions for Eq. (1), which provide reflectionless transmission of the wave via the given points, 0 and L. One of the prescriptions to design such boundary conditions was developed in the Refs. [9–11] and uses the following two basic assumptions: the initial data  $\Psi^I$  is compactly supported in the computational domain 0 < x < L, and the given external potential is constant outside this finite domain, i.e. V(x,t) = 0 for  $x \leq 0$ ,  $V(x,t) = V_L$  for  $x \geq L$ .

Then we can separate the whole problem into the socalled "interior" and "exterior" problems. The "interior" problem is given by

$$i\frac{\partial}{\partial t}\Psi = -\frac{1}{2}\frac{\partial^2}{\partial x^2}\Psi + V(x,t)\Psi, \ 0 < x < L, \ t > 0, \quad (2)$$

$$\Psi(x,0) = \Psi^I(x),$$

$$\frac{\partial}{\partial x}\Psi(0,t) = (T_0\Psi)(0,t),$$

$$\frac{\partial}{\partial x}\Psi(L,t) = (T_L\Psi)(L,t),$$

where  $T_{0,L}$  denotes the Dirichlet-to-Neumann (DtN) maps at the boundaries, which can be obtained by solving the two "exterior" problems given as

$$i\frac{\partial}{\partial t}v = -\frac{1}{2}\frac{\partial^2}{\partial x^2}v + V_L v, \ x > L, \ t > 0,$$

$$v(x,0) = 0,$$

$$v(L,t) = \Phi(t), \quad t > 0, \quad \Phi(0) = 0,$$

$$v(\infty,t) = 0,$$

$$(T_L \Phi)(t) = \frac{\partial}{\partial x}v(L,t),$$
(3)

and it can analogously be done for  $T_0$ . Using the Laplace transformation

$$\hat{v}(x,s) = \int_{0}^{\infty} v(x,t)e^{-st}dt,$$
(4)

the right "exterior" problem is transformed to

$$\frac{\partial^2}{\partial x^2}\hat{v} + 2i(s + iV_L)\hat{v} = 0, \quad x > L,$$

$$\hat{v}(L, s) = \hat{\Phi}(s).$$
(5)

The general solution for Eq. (5) can be written as

$$\hat{v}(x,s) = C_1 e^{\sqrt[t]{-2i(s+iV_L)}(x-L)} + C_2 e^{-\sqrt[t]{-2i(s+iV_L)}(x-L)}.$$

Since its solutions have to decrease as  $x \to +\infty$ , we obtain

$$\hat{v}(x,s) = e^{-\sqrt[4]{-2i(s+iV_L)}(x-L)}\hat{\Phi}(s), \tag{6}$$

where  $\sqrt{\phantom{a}}$  denotes the square root with nonnegative real part.

Hence the Laplace-transformed Dirichlet-to-Neumann operator  $T_L$  reads

$$\widehat{T_L\Phi}(s) = \frac{\partial}{\partial x}\widehat{v}(L,s) = -\sqrt{2}e^{-i\pi/4} \sqrt[4]{s+iV_L}\widehat{\Phi}(s), \quad (7)$$

and  $T_0$  is calculated analogously.

An inverse Laplace transformation yields the right TBC at x = L:

$$\frac{\partial}{\partial x}\Psi(x=L,t) = -\sqrt{\frac{2}{\pi}}e^{-i\frac{\pi}{4}}e^{-iV_Lt}\frac{d}{dt}\int_0^t \frac{\Psi(L,\tau)e^{iV_L\tau}}{\sqrt{t-\tau}}d\tau.$$
(8)

Similarly, the left TBC at x = 0 is obtained as

$$\frac{\partial}{\partial x}\Psi(x=0,t) = \sqrt{\frac{2}{\pi}}e^{-i\frac{\pi}{4}}\frac{d}{dt}\int_{0}^{t}\frac{\Psi(0,\tau)}{\sqrt{t-\tau}}d\tau.$$
 (9)

In this paper we apply this procedure to quantum graphs. It should be noted that no practical applications of the TBCs in physical systems have been considered so far. Here we will do this for quantum networks, which appear in different branches of optics, condensed matter and polymer physics.

#### III. QUANTUM GRAPHS

The concept of quantum graphs has been introduced first by Exner, Seba and Stovicek to describe free quantum motion on branched wires [46]. However, the pioneering treatment of the quantum mechanical motion in branched structures dates back to the Refs. [43–45].

Later Kostrykin and Schrader derived the general boundary conditions providing self-adjointness of the Schrödinger operator on graphs [47]. Relativistic quantum mechanics described by Dirac [48] and Bogoliubovde Gennes operators [49] on graphs have been studied recently. Hul et al considered experimental realization of quantum graphs in optical microwave networks [25]. An important topic related to quantum graphs was studied in the context of quantum chaos theory and spectral statistics [24, 27, 48]. Spectral properties and band structure of periodic quantum graphs also attracted much interest [28, 52]. Different aspects of the Schrödinger operators on graphs have been studied in the Refs. [28, 51, 52]. Tunable directed transport in quantum driven graphs has been also studied in [53], where the reflection at the branching point has been discussed.

Nonlinear extensions of the quantum graph concept have been studied in the context of soliton transport in networks in the Refs. [29, 30, 32, 33, 35, 39, 40]. In [29] the nonlinear Schrödinger equation on metric graphs is studied and condition for integrability is derived in the form of a sum rule for nonlinearity coefficients. In [30] such study is extended to Ablowitz-Laddik equation. The stationary Schrödinger equation on metric graphs and standing wave solitons in networks are studied in [31, 34, 36]. In [54] the linear and nonlinear head equations on metric star graphs is studied in the context of thermal diffusion. The nonlinear Schrödinger equation with the subcritical power nonlinearity on a metric star graph generalized Kirchhoff boundary conditions in [37], where the stability of half-soliton solutions is also analyzed. Integrable sine-Gordon equation on metric graphs is studied in [32, 35, 38]. Linear and nonlinear systems of PDE on metric graphs are considered in [39, 48, 49].

Quantum graphs, which are the one- or quasi-one dimensional branched quantum wires, can be modeled in terms of quantum mechanical wave equations on metric graphs by imposing the boundary conditions at the branching points (vertices) and bond ends. The metric graphs are the set of bonds with assigned length and which are connected to each other at the vertices. The connection rule is called topology of a graph and given in terms of the adjacency matrix [24, 27]:

$$C_{ij} = C_{ji} = \begin{cases} 1 & \text{if } i \text{ and } j \text{ are connected,} \\ 0 & \text{otherwise,} \end{cases}$$
 (10)

for i, j = 1, 2, ..., N.

The graph with the simplest topology is called star graph. It has one branching point, which connects three or more bonds (see, Fig. 1). The particle (wave) dynam-

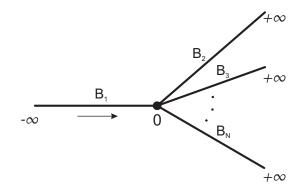


FIG. 1: Sketch of a star graph with N semi-infinite bonds.

ics in a quantum graph is described in terms of the linear Schrödinger equation (with  $\hbar=m=1$ ), which can be written for each bond of a star graph with N bonds as

$$i\frac{\partial \Psi_j}{\partial t} = \left[ -\frac{1}{2}\frac{d^2}{dx^2} + V_j(x,t) \right] \Psi_j, \ \ j = 1, 2, \dots, N, \ \ (11)$$

where  $\Psi_j = \Psi_j(x,t)$  is the wave function of jth bond,  $V_j(x,t)$  is the potential acting on jth bond and j is the bond number. In the following, for simplicity we assume that  $V_j = 0$ . To solve Eq. (11) one needs to impose initial condition and boundary conditions at the branching point and bond ends. Most general boundary conditions providing self-adjointness of the Schrödinger operator on graphs have been derived in [47]. Physically reasonable vertex boundary conditions, which are consistent with these general ones can be chosen as the continuity of the wave function at the vertex and Kirchhoff's rule [24, 27]:

$$\Psi_1(0,t) = \Psi_2(0,t) = \dots = \Psi_N(0,t), \tag{12}$$

$$\frac{\partial}{\partial x}\Psi_1(x=0,t) - \sum_{j=2}^N \frac{\partial}{\partial x}\Psi_j(x=0,t) = 0.$$
 (13)

According to the scattering approach [24] this "natural" boundary conditions, given at a vertex i, cause reflection of a wave packet with back-scattering amplitude  $s_j = -1 + 2/N$  and the reflection probability  $|s_j|^2$  approaches 1 as the number of bonds increases. Other details of the solution of the stationary version of Eq. (11) can be found elsewhere (see, e.g. [24, 27]). Here we will focus on the dynamical problem, which is described in terms of the time-dependent Schrödinger equation, by considering the wave transport in quantum graphs.

#### IV. TRANSPARENT QUANTUM GRAPHS

Here we combine the above concepts of transparent boundary conditions and quantum graphs to design the vertex boundary conditions providing reflectionless transmission of waves through the graph branching points. In the following such graphs will be called "transparent quantum graphs". Using such approach, below we show that Kirchhoff-type boundary conditions (weight continuity and current conservation) can become equivalent to transparent vertex boundary conditions under constraints in the form of a simple sum rule that is fulfilled for the weight coefficients. For simplicity (without losing generality) we consider first a star graph with three bonds. We assign to each bond  $B_i$  a coordinate  $x_i$ , which indicates the position along the bond: for bond  $B_1$  it is  $x_1 \in (-\infty, 0]$  and for  $B_{1,2}$  they are  $x_{2,3} \in [0, +\infty)$ . In the following we use the shorthand notation  $\Psi_i(x)$  for  $\Psi_j(x_j)$  and it is understood that x is the coordinate on the bond j to which the component  $\Psi_j$  refers. Then for the wave dynamics in such graph one can write the timedependent Schrödinger equation given by (in the units  $\hbar = m = 1$ 

$$i\frac{\partial}{\partial t}\Psi_j(x,t) = -\frac{1}{2}\frac{\partial^2}{\partial x^2}\Psi_j(x,t), \quad j = 1,2,3$$
 (14)

At the branching point (vertex) we impose the boundary conditions in the form of the wave function weight continuity given by

$$\alpha_1 \Psi_1(0, t) = \alpha_2 \Psi_2(0, t) = \alpha_3 \Psi_3(0, t), \tag{15}$$

and Kirchhoff type conditions, which is given as

$$\frac{1}{\alpha_1} \frac{\partial}{\partial x} \Psi_1(x=0,t) = \frac{1}{\alpha_2} \frac{\partial}{\partial x} \Psi_2(x=0,t) + \frac{1}{\alpha_2} \frac{\partial}{\partial x} \Psi_3(x=0,t).$$
(16)

In the following we consider the wave going from the first to second and third bonds, i.e., the initial condition is compactly supported in the first bond. Then the "interior" problem for the first bond,  $B_1$  can be written as

$$i\frac{\partial}{\partial t}\Psi_{1} = -\frac{1}{2}\frac{\partial^{2}}{\partial x^{2}}\Psi_{1}, \quad x < 0, \quad t > 0,$$

$$\Psi_{1}(x,0) = \Psi^{I}(x),$$

$$\frac{\partial}{\partial x}\Psi_{1}(0,t) = (T_{0}\Psi_{1})(0,t).$$
(17)

Corresponding "exterior" problems for  $B_{2,3}$  are given by

$$i\frac{\partial}{\partial t}\Psi_{2,3} = -\frac{1}{2}\frac{\partial^{2}}{\partial x^{2}}\Psi_{2,3}, \quad x > 0, \quad t > 0, \qquad (18)$$

$$\Psi_{2,3}(x,0) = 0,$$

$$\Psi_{2,3}(0,t) = \Phi(t), \quad t > 0, \quad \Phi(0) = 0,$$

$$(T_{0}\Phi)(t) = \frac{\partial}{\partial x}\Psi_{2,3}(0,t).$$

Finally, using the Laplace transformation (4), the two

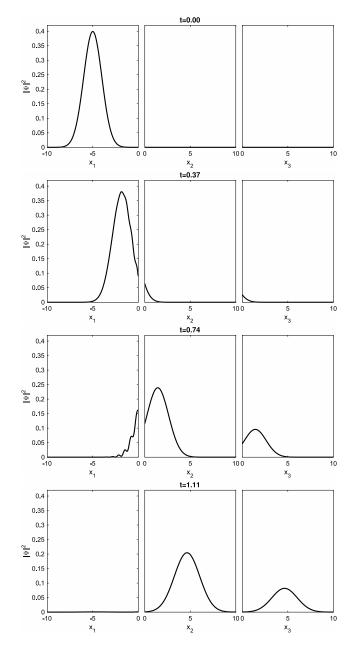


FIG. 2: The profile of the wave function plotted at different time moments for the regime when the sum rule is fulfilled (no reflection is occurred):  $\alpha_1 = 1/\sqrt{1/20 + 1/50}$ ,  $\alpha_2 = \sqrt{20}$  and  $\alpha_3 = \sqrt{50}$ . Each column number (from the left to the right) corresponds to a bond number.

"exterior" problems are transformed to

$$\frac{\partial^2}{\partial x^2} \hat{\Psi}_{2,3} + 2is\hat{\Psi}_{2,3} = 0, \quad x > 0,$$

$$\hat{\Psi}_{2,3}(0,s) = \hat{\Phi}(s).$$
(20)

The general solution of the exterior problems can be written as

$$\hat{\Psi}_{2,3}(x,s) = C_1 e^{\sqrt[t]{-2is}x} + C_2 e^{-\sqrt[t]{-2is}x}.$$
 (21)

Since we have  $\hat{\Psi}_{2,3} \in L^2(0,\infty)$ , we obtain

$$\hat{\Psi}_{2,3}(x,s) = e^{-\sqrt[4]{-2is}x} \hat{\Phi}(s). \tag{22}$$

Then

$$\frac{\partial}{\partial x}\hat{\Psi}_{2,3}(x,s) = -\sqrt[+]{-2is}\hat{\Psi}_{2,3}(x,s), \quad x \ge 0.$$
 (23)

At the vertex (x = 0) for bonds  $B_{2,3}$  ("input" from interior) using the continuity boundary conditions (15) we get

$$\frac{\partial}{\partial x}\hat{\Psi}_{2,3}(x=0,s) = -\sqrt[4]{-2is}\frac{\alpha_1}{\alpha_{2,3}}\hat{\Psi}_1(x=0,s). \quad (24)$$

The Laplace transformed current conservation (at x=0) takes the form

$$\begin{split} \frac{\partial}{\partial x} \hat{\Psi}_1 &= \frac{\alpha_1}{\alpha_2} \frac{\partial}{\partial x} \hat{\Psi}_2 + \frac{\alpha_1}{\alpha_3} \frac{\partial}{\partial x} \hat{\Psi}_3 \\ &= -\sqrt[4]{-2is} \ \alpha_1^2 \left( \frac{1}{\alpha_2^2} + \frac{1}{\alpha_3^2} \right) \hat{\Psi}_1. \end{split} \tag{25}$$

Using the inverse transform we have

$$\frac{\partial}{\partial x}\Psi_1(x=0,t) = A_1 \sqrt{\frac{2}{\pi}} e^{-i\frac{\pi}{4}} \frac{d}{dt} \int_0^t \frac{\Psi_1(0,\tau)}{\sqrt{t-\tau}} d\tau, \quad (26)$$

with 
$$A_1 = \alpha_1^2 \left( \alpha_2^{-2} + \alpha_3^{-2} \right)$$
.

The boundary condition given by (26) coincides with that in Eq. (9) and thereby providing reflectionless transmission for the bond  $B_1$ , when  $A_1 = 1$ , i.e. the following sum rule is fulfilled:

$$\frac{1}{\alpha_1^2} = \frac{1}{\alpha_2^2} + \frac{1}{\alpha_3^2}. (27)$$

Hence, the vertex boundary conditions given by Eqs. (15) and (16) become equivalent to the transparent vertex boundary conditions, provided the sum rule in Eq. (27) is fulfilled.

The numerical example in Fig. 2 shows a simulation of a right traveling Gaussian wave packet

$$\Psi^{I}(x) = (2\pi)^{-1/4} \exp(5ix - (x+5)^2/4)$$

at four consecutive time steps. The Crank-Nicolson finite difference scheme with the space discretization  $\Delta x = 0.016$  and the time step  $\Delta t = 5 \cdot 10^{-5}$  has been used. It is clear from this figure that the wave completely transmits to the second and third bonds when time elapses. We note that the above boundary conditions provide conservation of the total norm, which is defined as the sum of partial norms for each bond. Detailed derivation of the norm conservation is provided in Appendix.

Fig. 3 presents plots of the partial and total norms for this case. In Fig. 4 the reflection coefficient determined

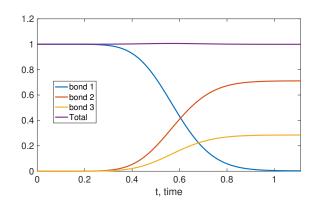


FIG. 3: (Color online). Time dependence of the partial and total norms for the case shown in Fig.2.

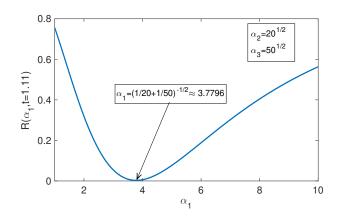


FIG. 4: Dependence of the vertex reflection coefficient R on the parameter  $\alpha_1$  when time elapses (t = 1.1).

as the ratio of the partial norm for the first bond to the total norm

$$R = \frac{N_1}{N_1 + N_2 + N_3}$$

is plotted as a function of  $\alpha_1$  for the fixed values of  $\alpha_2$  and  $\alpha_3$ . As this plot shows, at the value of  $\alpha_1$  that provides fulfilling of the sum rule (27) the reflection coefficient becomes zero. This confirms once more that the sum rule in Eq. (27) makes the vertex boundary conditions in Eqs. (15) and (16) equivalent to the transparent ones.

We note that the above approach can be extended for other network branching topologies, e.g., for tree graph presented in Fig. 5. The graph consists of three "layers"  $B_1$ ,  $(B_{1i})$ ,  $(B_{1ij})$ , where i,j run over the given bonds. On each bond  $B_1$ ,  $B_{1i}$ ,  $B_{1ij}$  we have the time-dependent Schrödinger equation given by (14), for which Kirchhoff-type boundary conditions are imposed at each vertex. Transparent boundary conditions can be imposed similarly to those for the star graph. Then, for all i, j, the  $\alpha_{1i}$  and  $\alpha_{1ij}$  have to be determined from the sum rule like (27) at each vertex. For instance, at the three vertices in

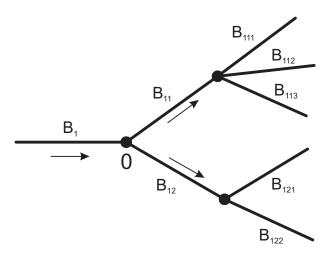


FIG. 5: Tree graph with three layers,  $B_1 \sim (-\infty, 0]$ ,  $B_{11}$ ,  $B_{12} \sim [0, L_k)$ , k = 1, 2, and  $B_{1ij} \sim [0, +\infty)$  with i, j = 1, 2, 3.

Fig. 5 we have

end of 
$$B_1$$
:  $\alpha_1^{-2} = \alpha_{11}^{-2} + \alpha_{12}^{-2}$ ,  
end of  $B_{11}$ :  $\alpha_{11}^{-2} = \alpha_{111}^{-2} + \alpha_{112}^{-2} + \alpha_{113}^{-2}$ , (28)  
end of  $B_{12}$ :  $\alpha_{12}^{-2} = \alpha_{121}^{-2} + \alpha_{122}^{-2}$ .

Fulfilling of these sum rules turns the Kirchhoff-type boundary conditions equivalent to the transparent ones at the each vertex of a tree graph. The constants  $\alpha_j$  in Eq. (27) characterize the physical properties of the material, which is used to construct the network and can have different meaning for each specific system under consideration.

#### V. CONCLUSIONS

In this paper we studied the problem of transparent quantum graphs by determining them as branched quantum wires providing reflectionless transmission of waves at the branching points. The boundary conditions for the time-dependent Schrödinger equation on graphs, providing such transmission, are formulated explicitly. A simple constraint that makes the usual Kirchhoff-type boundary conditions at the vertex equivalent to those of transparent ones is derived.

We have shown numerically for the star graph a reflectionless transmission of the Gaussian wave packet through the vertices, if these constraints are fulfilled. The approach can be extended straight forward for arbitrary graph topologies, which contain any subgraph connected to two or more outgoing, semi-infinite bonds. Stability analysis for the boundary conditions discretization scheme is not included into the above treatment and will be subject of forthcoming papers.

The motivation for the study of transparent quantum graphs comes from different practically important problems of optics, condensed matter and polymers. One of the problems allowing direct application the above model is charge carrier transport in conducting polymers, which are highly branched nanoscale structures. Reflectionless transmission of charge carriers in these structures causes high conductivity and optimal functioning of different organic electronic devices. One of such structures was discussed recently in the context of nonlinear charge carriers in branched conducting polymers [55]. More attractive applications are possible also in linear fiber networks, where the wave dynamics is described in terms of the Helmholtz equation.

Finally, we note that extension of the above approach of other linear wave equations, such as heat, diffusion, Dirac and Klein-Gordon equations should be rather straightforward. Moreover, the method can be modified and applied for the nonlinear partial differential equations widely used in physics.

#### VI. ACKNOWLEDGEMENTS

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#### Appendix A: Norm conservation

For quantum star graph with three bonds, the total norm is given as

$$N(t) = \sum_{j=1}^{3} \int_{B_j} |\Psi_j(x,t)|^2 dx,$$
 (A1)

where  $B_j$  is the domain of the bond j.

For Eq. (14) an easy calculation shows that the derivative of the norm with respect to t reads

$$\dot{N}(t) = \sum_{j=1}^{3} \int_{B_{j}} \left[ -\frac{i}{2} \frac{\partial^{2} \Psi_{j}^{*}}{\partial x^{2}} \Psi_{j} + \frac{i}{2} \frac{\partial^{2} \Psi_{j}}{\partial x^{2}} \Psi_{j}^{*} \right] dx \qquad (A2)$$

Taking into account that  $\Psi_1$  vanishes as  $x \to -\infty$  and  $\Psi_{2,3}$  vanish as  $x \to +\infty$  we obtain

$$\dot{N}(t) = \Im m \left[ \Psi_1 \frac{\partial \Psi_1^*}{\partial x} \right]_{x=0} \\
- \Im m \left[ \Psi_2 \frac{\partial \Psi_2^*}{\partial x} \right]_{x=0} - \Im m \left[ \Psi_3 \frac{\partial \Psi_3^*}{\partial x} \right]_{x=0}, \quad (A3)$$

and using boundary conditions (15) and (16) we get

$$\dot{N}(t) = 0, \tag{A4}$$

which means the preservation of the norm over time.

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