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In this paper, we discuss the concept of quantum graphs with transparent vertices by considering the case, where the graph interacts with an external time-independent field. In particular, we address the problem of transparent boundary conditions for quantum graphs, building on previous works on transparent boundary conditions for the stationary Schrödinger equation on a line.

Physically relevant constraints that make the vertex transparent under boundary conditions in the form of (weight) continuity and Kirchhoff rules are derived using two approaches, where transparent boundary conditions for the time-independent Schrödinger equation are found. The latter is derived by extending the transparent boundary condition concept to the time-independent Schrödinger equation on driven quantum graphs. For the constant potential, these constraints are also obtained using the scattering approach.

We also discuss how the eigenvalues and eigenfunctions of a quantum graph are influenced not only by its topology, but also by the shape/type of a potential when an external field is involved.

Keywords: quantum graphs; transparent boundary conditions; scattering approach; stationary Schrödinger equation

I. INTRODUCTION

The concept of quantum graphs appeared in the literature about two decades ago. The first studies of branched quantum wires described using the Schrödinger equation on metric graphs came from Exner, Seba and Stovicek [1]. Later, Kostrykin and Schrader [2] developed a more rigorous mathematical study of the problem by deriving general self-adjoint vertex boundary conditions. Various aspects of quantum graph theory have been considered in physical [3–12] and mathematical contexts [13–18]. The experimental realization of quantum graph spectra in microwave networks was presented in [19–23]. Such an experimental study is possible because such networks can "mimic" quantum graphs, since the waves there are described by the Helmholtz equation. Quantum graphs can be defined as a system of quantum wires connected according to a certain rule, called the *topology of a graph*.

Particles and waves in quantum graphs can be described by the stationary or time-dependent Schrödinger equation on metric graphs. In such an approach, the wave function is a multi-component vector, with each component associated with a particular bond, and the Schrödinger equation is defined on each bond of a graph. To solve this equation, boundary conditions (matching conditions) must hold at the nodes of the graph, i.e., at the vertices, as well as at the end of each bond.

In the case of the stationary Schrödinger equation, the vertex boundary conditions are used to obtain a secular equation to determine the eigenvalues of the problem. Depending on the topology of a graph, one obtains different eigenvalues, i.e., the eigenvalues and eigenfunctions of a quantum graph depend on its topology. When a quantum graph is subjected to the interaction of an external field, the solution of the problem depends not only on the topology but also on the shape/type of a potential.

In this paper, we address the problem of *transparent boundary conditions* for quantum graphs by considering these latter as interacting with an external time-independent potential, i.e. driven quantum graphs. To formulate and solve the problem, we use the concept of transparent boundary conditions for the time-independent Schrödinger equation, which was previously considered in [24–33]. In [27] the extension of absorbing boundary conditions in the time domain to the computation of steady states is studied. In recent works [32, 33] a general approach for the derivation of transparent boundary conditions for the stationary Schrödinger equation with arbitrary potential is proposed using the Weyl-Titchmarsh theory. The concept of transparent boundary conditions for the time-independent Schrödinger equation implies that its solutions (in the presence of an external time-independent potential) in the finite interval are equivalent to those in the whole space.

We note that driven quantum graphs are less studied topic in the context of quantum graph theory, despite its importance for modeling quantum transport in interacting low-dimensional branched systems. In [34] the trace formula for driven quantum graphs has been studied. In [35, 36] two-particle quantum graphs, interacting via the delta-potential is studied. Ref. [37] considers optimal potentials for quantum graphs. Previously, quantum graphs driven by the Coulomb potential were used to model exciton transport in branched conducting polymers [38]. Quantum graphs confined in the harmonic oscillator potential were considered in [39].

This paper is organized as follows. In Section II, we recall the problem of transparent boundary conditions for the stationary Schrödinger equation on a line. Section III presents an extension of the problem for graphs. Section IV presents numerical experiments. Finally, concluding remarks are made in Section V.

II. TRANSPARENT BOUNDARY CONDITIONS FOR THE STATIONARY SCHRÖDINGER EQUATION ON A LINE

The problem of transparent boundary conditions (also referred to as absorbing boundary conditions in some literature, which, of course, are not the same from a physical point of view) for the one-dimensional stationary Schroödinger equation has been considered earlier in Refs. [26, 27]. In these papers a hierarchy of novel absorbing boundary conditions for the one-dimensional stationary Schroödinger equation with general (linear and nonlinear) potential is proposed. Focusing on the results obtained in these works, we start with considering the one-dimensional *stationary Schrödinger equation*

$$\Big(-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+V\Big)\varphi = E\varphi, \quad x\in\mathbb{R}, \tag{1}$$

with a given potential $V := V(x)$. The solution of this problem is a pair (φ, E), namely the eigenvalues E and the corresponding eigenfunctions φ of the system. Let us now solve the Eq. (1) in an interval with some boundary conditions, so that its solution coincides with the solution of the problem for the whole space restricted to the considered interval. In the following, such boundary conditions are called *transparent boundary conditions (TBCs).*

For the derivation of TBCs for stationary Schrödinger equations, we refer to the work [27]. Here we first consider the time-dependent problem on the whole space given as

$$\begin{cases} \mathrm{i}\partial_t u + \partial_x^2 u + Vu = 0, & \forall (x,t)\in\mathbb{R}\times\mathbb{R}^+, \\ u(x,0) = u_0(x), & x\in\mathbb{R}. \end{cases} \tag{2}$$

We also consider a finite computational interval $\Omega = [x_l, x_r]$. The artificial boundary Σ is given by the two interval endpoints x_l and x_r and the outward unit normal vector to Ω is denoted by $\mathbf{n}$.

For this case derivation of TBCs for the time-dependent Schrödinger equation with a linear or nonlinear potential is referred to Ref.[24], where pseudo-differential operators theory was applied to obtain approximations of TBCs. The following second- and fourth-order TBCs (designated by ABC_2^2 and ABC_2^4 in [27]) on the boundary $\Sigma\times\mathbb{R}^+$

$$\mathrm{ABC}_2^2: \ \partial_{\mathbf{n}} u = \mathrm{iOp}\left(\sqrt{-\tau+V}\right)u, \tag{3}$$

$$\mathrm{ABC}_2^4: \ \partial_{\mathbf{n}} u = \mathrm{iOp}\left(\sqrt{-\tau+V}\right)u - \frac{1}{4}\mathrm{Op}\left(\frac{\partial_{\mathbf{n}} V}{-\tau+V}\right)u, \tag{4}$$

were derived (see Ref.[24] for more details). Here $P = \mathrm{Op}(p)$ means that P is the associated operator of symbol p, if a pseudo-differential operator $P(x,t,\partial t)$ is given by its symbol $p(x,t,\tau)$.

Now, using the transformation ('gauge transform') [29]

$$u(x,t) = \varphi(x)\, e^{-\mathrm{i}Et}, \tag{5}$$

we obtain the time derivative

$$\mathrm{i}\partial_t u = E\varphi(x)\, e^{-\mathrm{i}Et}.$$

Here the variable $-\tau$ can be identified with E and thus these considerations yield some stationary TBCs (designated by SABC^M in [27], where 'S' stands for stationary and M denotes the order of the boundary condition):

$$\mathrm{SABC}^2: \ \partial_{\mathbf{n}}\varphi = \mathrm{i}\sqrt{E-V}\,\varphi, \quad \text{on } \Sigma, \tag{6}$$

$$\mathrm{SABC}^4: \ \partial_{\mathbf{n}}\varphi = \mathrm{i}\sqrt{E-V}\,\varphi + \frac{1}{4}\frac{\partial_{\mathbf{n}} V}{E-V}\,\varphi, \quad \text{on } \Sigma. \tag{7}$$

In this way, the stationary TBCs were derived assuming that the solution of (2) can be written as a time-harmonic solution (5). It should be noted that the second- and fourth-order TBCs for the time-dependent Schrödinger equation (3), (4) were developed under a high frequency assumption $\tau \gg 1$ [24]. This relation can be translated to the stationary case in terms of links between E and V. This means that we require that $E_n - V_r \ll 0$ holds for a given

point x_r and for a fixed potential V. In the following, we will present an example of the use of TBCs for the case of the harmonic potential.

Alternatively, a general approach has been proposed in recent work [32, 33] for deriving transparent boundary conditions for the stationary Schrödinger equation with arbitrary potential. It was shown that the transparent boundary conditions can be written in terms of the Weyl-Titchmarsh coefficients. While the TBCs (6) and (7) are approximations, this approach determines exact transparent boundary conditions.

Theorem 1 ***([33], Theorem 3)*** *Let the differential expression $\mathcal{A} = -\frac{d^2}{dx^2} + V$ be in the limit point case at $\pm\infty$ and let the self-adjoint operator H, generated by the differential expression $\mathcal{A}$ in $L^2(\mathbb{R})$, has a discrete spectrum. Let (x_l, x_r) be a finite interval in $\mathbb{R}$, and let m_- and m_+ be the Weyl-Titchmarsh coefficients for operators $A_\pm$ associated in $L^2(I_\pm)$ (where $I_- = (-\infty, x_l]$ and $I_+ = [x_r, +\infty)$) with the differential expression $\mathcal{A}_\pm = -\frac{d^2}{dx^2} + V_\pm$. Then, the transparent boundary conditions for $\mathcal{A}$ on the interval $I = (x_l, x_r)$ can be chosen as*

$$\varphi'(E, x_l) + m_-(E)\varphi(E, x_l) = 0, \tag{8}$$
$$\varphi'(E, x_r) - m_+(E)\varphi(E, x_r) = 0. \tag{9}$$

A. Example: Confined quantum harmonic oscillator

Here, we demonstrate practical applications of TBCs to realistic physical systems. Namely, we consider a quantum particle confined in a 1D box $[x_l, x_r]$ subjected to the interaction of a harmonic oscillator (parabolic) potential. Such a potential represents a parabolic well (caused by, e.g. an external constant uniform magnetic field) with the cut-off at the box walls. The Hamiltonian of the system can be written as (in the units $\hbar = m = 1$):

$$H = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2}\omega^2 x^2. \tag{10}$$

The complete solution of the stationary Schrödinger equation on the real line

$$H\phi = E\phi, \quad x \in \mathbb{R}, \tag{11}$$

can be written in terms of the confluent hypergeometric function of the first kind:

$$\phi(x) = \exp\Big(-\frac{1}{2}\omega x^2\Big)\Big[A\, M\Big(\frac{1}{4} - \frac{E}{2\omega}; \frac{1}{2}; \omega x^2\Big) + B\,\omega^{\frac{1}{2}} x M\Big(\frac{3}{4} - \frac{E}{2\omega}; \frac{3}{2}; \omega x^2\Big)\Big] \tag{12}$$

where A and B are constants and $M(\cdot;\cdot;\cdot)$ denotes the *Kummer's function* [44]. For asymptotic boundary conditions imposed as $\phi(|x| \to \infty) = 0$, the solutions are the Hermite functions and the corresponding eigenvalues can be written as

$$E_n = \omega\Big(n + \frac{1}{2}\Big). \tag{13}$$

Imposing the TBCs (6) results in a system of linear algebraic equations with respect to the coefficients A and B:

$$\mathbf{h}(E)\begin{pmatrix} A \\ B \end{pmatrix} = 0, \tag{14}$$

where the elements of the 2×2 matrix $\mathbf{h}$ are given as

$$h_{11} = -\Big(\omega x_l + \mathrm{i}\mathcal{E}_l\Big)M\Big(\frac{1}{4} - \frac{E}{2\omega}; \frac{1}{2}; \omega x_l^2\Big) + \Big(\frac{1}{2} - \frac{E}{\omega}\Big)M\Big(\frac{5}{4} - \frac{E}{2\omega}; \frac{3}{2}; \omega x_l^2\Big),$$
$$h_{12} = -\Big(\omega x_l^2 - 1 + \mathrm{i}x_l\mathcal{E}_l\Big)M\Big(\frac{3}{4} - \frac{E}{2\omega}; \frac{3}{2}; \omega x_l^2\Big) + x_l^2\Big(\frac{1}{2} - \frac{E}{3\omega}\Big)M\Big(\frac{7}{4} - \frac{E}{2\omega}; \frac{5}{2}; \omega x_l^2\Big),$$
$$h_{21} = -\Big(\omega x_r - \mathrm{i}\mathcal{E}_r\Big)M\Big(\frac{1}{4} - \frac{E}{2\omega}; \frac{1}{2}; \omega x_r^2\Big) + \Big(\frac{1}{2} - \frac{E}{\omega}\Big)M\Big(\frac{5}{4} - \frac{E}{2\omega}; \frac{3}{2}; \omega x_r^2\Big),$$
$$h_{22} = -\Big(\omega x_r^2 - 1 + \mathrm{i}x_r\mathcal{E}_r\Big)M\Big(\frac{3}{4} - \frac{E}{2\omega}; \frac{3}{2}; \omega x_r^2\Big) + x_r^2\Big(\frac{1}{2} - \frac{E}{3\omega}\Big)M\Big(\frac{7}{4} - \frac{E}{2\omega}; \frac{5}{2}; \omega x_r^2\Big),$$

TABLE I: The first five eigenvalues of the confined quantum harmonic oscillator (to be compared with those of unconfined one given by Eq. (13)) for which the transparent boundary conditions (6) are imposed at $x_l = -5$ and $x_r = 5$ ($\omega = 1$).

n	E_n
1	0.50000000005979
2	1.49999999734821
3	2.50000006391437
4	3.49999862590053
5	4.50000910443786

with $\mathcal{E}_{l,r} = \sqrt{E - \frac{1}{2}\omega^2 x_{l,r}^2}$.

The existence of non-trivial solutions of the above algebraic system (14) leads to the following secular equation with respect to E

$$\det\big(\mathbf{h}(E)\big) = 0. \tag{15}$$

The roots of Eq. (15) give the eigenvalues of the confined quantum harmonic oscillator with TBCs. These eigenvalues and corresponding eigenvectors must coincide with the solution of the whole-space problem restricted to $[x_l, x_r]$. To show this, the Table I shows the first five numerically computed eigenvalues (energies) of the considered system for $\omega = 1$ and interval $[-5, 5]$.

We note that more detailed analysis of this example is done in the Ref. [27] by performing a numerical test which consists in presenting the error on both the energy and eigenfunctions depending on the computational domain size. Furthermore, another case of the Pöschl-Teller potential is also considered in that work. In [25, 28], the case of the Morse potential as well as the Woods-Saxon potential is also studied. These examples extend the conclusions on TBCs (6) and (7).

In a general approach, if we use Weyl-Titchmarsh theory, the TBCs (8)–(9) for this example can be derived explicitly [33], where Weyl-Titchmarsh functions are written in terms of Weber parabolic cylinder functions $U(-E, x)$ [44] as

$$m_+ = \frac{U'(-E, x_r)}{U(-E, x_r)}, \quad m_- = \frac{U'(-E, -x_l)}{U(-E, -x_l)}. \tag{16}$$

Imposing these boundary conditions to (10)-(11) (with $\omega = 1/2$) at the boundaries of the interval $[x_l, x_r]$ results the eigenvalues $2E_n = n + 1/2$, $n \in \mathbb{N}_0$ (for the proof see section "Examples" in [33]). This implies, that the boundary conditions determined by (16) are transparent.

III. QUANTUM GRAPHS WITH TRANSPARENT VERTICES

The concept of transparent boundary conditions has recently been extended to the case of evolution equations on graphs, by considering linear [40] and nonlinear [41] Schrödinger equations on graphs and the Dirac equation on quantum graphs [42]. In all cases the focus was on time-dependent equations.

Here we consider the Schrödinger equation in presence of some potential $V_j(x)$ on the star graph given on each of its bonds as

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Psi_j(x) + V_j(x)\Psi_j(x) = k^2\Psi_j(x), \quad j = 1, 2, \ldots, N, \tag{17}$$

where N is the number of bonds. Now we focus on j-th bond The coordinates x take the value 0 at the vertex and go to infinity at the unbounded ends.

The wave function must satisfy certain boundary conditions at the vertices, the imposition of which guarantees that the resulting Schrödinger operator is self-adjoint. One of these boundary conditions at the vertex can be written as a generalized form of the continuity condition

$$\alpha_1\Psi_1(0) = \alpha_2\Psi_2(0) = \ldots = \alpha_N\Psi_N(0), \tag{18}$$

and the current conservation

$$\sum_{j=1}^{N} \frac{1}{\alpha_j}\frac{\mathrm{d}}{\mathrm{d}x}\Psi_j(0) = 0, \tag{19}$$

where $\alpha_j \in \mathbb{R}$ are some non-zero coefficients.

A. Transparent boundary conditions for driven quantum graphs

Here we use the concept of transparent boundary conditions (TBCs) introduced in Section II, to derive the conditions for the vertex transparency. In particular, we focus on the solution of Eq. (17) with boundary conditions (18) and (19) imposed on the vertex.

Assuming that the solution of the time-dependent version of Eq. (17) can be written as a time-harmonic solution

$$\Psi_j(x,t) = \varphi_j(x)\, e^{-\mathrm{i}Et}, \quad j = 1, 2, \ldots, N, \tag{20}$$

we can write the stationary transparent boundary conditions for all the bonds as

$$\partial_{\mathbf{n}}\varphi_j = \mathrm{i}\sqrt{E - V_j}\,\varphi_j, \tag{21}$$

for the second-order approximation and

$$\partial_{\mathbf{n}}\varphi_j = \mathrm{i}\sqrt{E - V_j}\,\varphi_j + \frac{1}{4}\frac{\partial_{\mathbf{n}} V_j}{E - V_j}\varphi_j, \tag{22}$$

for the fourth-order approximation at the vertex ($x = 0$).

We now assume that the ith bond number is the computational domain and the other bonds are external bonds. Considering the higher order of the given approximations, i.e., the Eq. (22) and using the current conservation conditions (19), we obtain

$$\frac{1}{\alpha_i}\frac{\mathrm{d}}{\mathrm{d}x}\varphi_i + \sum_{\substack{j=1\\ j\neq i}}^{N} \frac{1}{\alpha_j}\Big(\mathrm{i}\sqrt{E - V_j}\,\varphi_j + \frac{1}{4}\frac{V_j'}{E - V_j}\varphi_j\Big) = 0, \tag{23}$$

where $V_j = V_j(0)$ and $V_j' = \frac{\mathrm{d}}{\mathrm{d}x}V_j(x)|_{x=0}$. Using the continuity condition (18) and taking into account that for the ith bond we have $\partial_{\mathbf{n}}\varphi_i = -\frac{\mathrm{d}}{\mathrm{d}x}\varphi_i$, we can write Eq. (23) in terms of φ_i as

$$-\frac{1}{\alpha_i}\partial_{\mathbf{n}}\varphi_i + \sum_{\substack{j=1\\ j\neq i}}^{N} \frac{\alpha_i}{\alpha_j^2}\Big(\mathrm{i}\sqrt{E - V_j}\,\varphi_i + \frac{1}{4}\frac{V_j'}{E - V_j}\varphi_i\Big) = 0. \tag{24}$$

At this point we assume that (i) $V_j(0) = V_i(0)$ and (ii) $V_j'(0) = -V_i'(0)$ for all bonds. This assumptions lead us to

$$\partial_{\mathbf{n}}\varphi_i = \Big(\mathrm{i}\sqrt{E - V_i}\,\varphi_i + \frac{1}{4}\frac{\partial_{\mathbf{n}} V_i}{E - V_i}\varphi_i\Big)\sum_{\substack{j=1\\ j\neq i}}^{N} \frac{\alpha_i^2}{\alpha_j^2}. \tag{25}$$

It is easy to see that Eq. (25) is the TBC for the bond i, when the following sum rule is fulfilled, i.e. when

$$\sum_{\substack{j=1\\ j\neq i}}^{N} \frac{\alpha_i^2}{\alpha_j^2} = 1. \tag{26}$$

It should be noted here that this condition (26) was derived earlier by applying the transparent boundary conditions to the time-dependent Schrödinger equation on graphs [40]. Thus we obtain the TBC for the bond with number i. Note that assumption (i) on the bond potentials is sufficient for the second-order approximation to derive the sum rule, while the inclusion of the second term in the fourth-order approximation additionally requires assumption (ii).

Moreover, under the same assumptions (i) and (ii) above, the condition for transparent vertex boundary conditions (26) can be generalized for the case when there are $M < N$ incoming leads (e.g., bonds $j = 1, 2, \ldots, M$) and $N - M$ outgoing leads (bonds $j = M+1, M+2, \ldots, N$). For this case we can write

$$\begin{aligned}\partial_{\mathbf{n}}\varphi_i = &\Big(\mathrm{i}\sqrt{E - V_i}\,\varphi_i + \frac{1}{4}\frac{\partial_{\mathbf{n}} V_i}{E - V_i}\varphi_i\Big)\cdot \\ &\left(-\sum_{\substack{j=1\\ j\neq i}}^{M} \frac{\alpha_i^2}{\alpha_j^2} + \sum_{j=M+1}^{N} \frac{\alpha_i^2}{\alpha_j^2}\right), \text{ for } i = 1, 2, \ldots, M.\end{aligned} \tag{27}$$

Then, the general form of the constraint reads

$$\sum_{j=1}^{M} \frac{1}{\alpha_j^2} = \sum_{j=M+1}^{N} \frac{1}{\alpha_j^2}. \tag{28}$$

We note that extending the above treatment to the case of other graphs (e.g., tree, loop, triangle, etc.) can be done along the same lines as for the star graph.

B. Treatment within the Weyl-Titchmarsh theory

Following the approach in [33], expected transparent boundary conditions for $x = 0$ (the branching point) can be formally expressed as

$$\Psi_1'(E,0) - m_1(E)\Psi_1(E,0) = 0 \tag{29}$$

for the first bond and as

$$\Psi_j'(E,0) + m_j(E)\Psi_j(E,0) = 0, \quad j = 2,3,\ldots,N \tag{30}$$

for others. Here m_j are the Weyl-Titchmarsh coefficients, corresponding to each bond and explained in section 2 (Theorem 1).

As we have weight continuity (18)

$$\alpha_1\Psi_1(E,0) = \alpha_2\Psi_2(E,0) = \cdots = \alpha_N\Psi_N(E,0) \tag{31}$$

and current conservation (19)

$$\frac{1}{\alpha_1}\Psi_1'(E,0) = \sum_{j=2}^{N} \frac{1}{\alpha_j}\Psi_j'(E,0) \tag{32}$$

at the branching point, using (29)-(30) one can rewrite this equation as

$$\frac{1}{\alpha_1}m_1(E)\Psi_1(E,0) = \sum_{j=2}^{N} \frac{\alpha_1}{\alpha_j^2}m_j(E)\Psi_1(E,0). \tag{33}$$

Then, it follows that

$$\frac{m_1(E)}{\alpha_1^2} = \sum_{j=2}^{N} \frac{m_j(E)}{\alpha_j^2}. \tag{34}$$

When $m_1(E) = m_2(E) = \cdots = m_N(E)$, Eq. (34) reduces to Eq. (26) (for $i = 1$). For instance, in the case of the harmonic oscillator potential, this condition holds, implying that the sum rule in Eq. (26) is equivalent to the transparent boundary conditions.

C. Derivation of the sum rule using the scattering approach

Now, let us consider the Schrödinger equation on the star graph with N bonds given as

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Psi_j(x) = k^2\Psi_j(x), \quad j = 1,2,\ldots,N, \tag{35}$$

with boundary conditions (18) and (19).

Using the scattering approach [3], the total wave function $\mathbf{\Psi}$ can be written as a linear combination of functions Ψ_i, which are solutions for the case where an incoming wave enters the vertex from bond i and outgoing waves from

the vertex to all bonds j (including $j = i$ corresponding to the reflected part). Ψ_i is an N-dimensional vector with components $\Psi_{i,j}(x)$ for all $1 \le j \le N$,

$$\Psi_{i,j}(x) = \delta_{j,i}\, e^{-\mathrm{i}kx} + \sigma_{i,j}\, e^{\mathrm{i}kx}. \tag{36}$$

Here σ is the $N \times N$ scattering matrix, which provides a transformation between the incoming and the outgoing waves at the vertex. The continuity condition (18) together with (36) results in

$$\sigma_{i,j} = \frac{\alpha_i}{\alpha_j}(1 + \sigma_{i,i}), \quad \forall j \ (j \neq i). \tag{37}$$

Now, the current conservation condition (19) together with (36) leads to

$$1 - \sigma_{i,i} = \sum_{\substack{j=1 \\ j\neq i}}^{N} \frac{\alpha_i}{\alpha_j}\, \sigma_{i,j}. \tag{38}$$

Then, using (37) we can determine $\sigma_{i,i}$

$$\sigma_{i,i} = \Big(1 - \sum_{\substack{j=1 \\ j\neq i}}^{N} \frac{\alpha_i^2}{\alpha_j^2}\Big) \Big/ \Big(1 + \sum_{\substack{j=1 \\ j\neq i}}^{N} \frac{\alpha_i^2}{\alpha_j^2}\Big). \tag{39}$$

Since we are interested in non-reflecting waves, we need to make the reflection probability $|\sigma_{i,i}|^2$ vanish. Obviously, this can be achieved for the (39) by satisfying the following conditions on the coefficients α_j, $(j = 1, 2, \ldots, N)$, in the form of a sum rule

$$\frac{1}{\alpha_i^2} = \sum_{\substack{j=1 \\ j\neq i}}^{N} \frac{1}{\alpha_j^2}. \tag{40}$$

The satisfaction of (40) corresponds to the case where an incoming wave from bond i enters the vertex without reflection and outgoing waves from the vertex to all other bonds j.

Now, let us consider the same problem in presence of some constant potential V_j given for each bond j :

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Psi_j(x) + V_j \Psi_j(x) = k^2 \Psi_j(x), \quad j = 1, 2, \ldots, N, \tag{41}$$

with the same boundary conditions (18) and (19). In this case, the components $\Psi_{i,j}(x)$ of the total wave function can be written as

$$\Psi_{i,j}(x) = \delta_{j,i}\, e^{-\mathrm{i}\sqrt{k^2 - V_j}\,x} + \sigma_{i,j}\, e^{\mathrm{i}\sqrt{k^2 - V_j}\,x}. \tag{42}$$

The boundary conditions (18) and (19) at the vertex together with (42) can be used to determine $\sigma_{i,i}$

$$\sigma_{i,i} = \frac{1 - \sum\limits_{\substack{j=1 \\ j\neq i}}^{N} \frac{\alpha_i^2}{\alpha_j^2} \sqrt{\frac{k^2 - V_j}{k^2 - V_i}}}{1 + \sum\limits_{\substack{j=1 \\ j\neq i}}^{N} \frac{\alpha_i^2}{\alpha_j^2} \sqrt{\frac{k^2 - V_j}{k^2 - V_i}}}. \tag{43}$$

Again, by requiring the reflection probability to vanish we get the energy dependent expression

$$\frac{\sqrt{k^2 - V_i}}{\alpha_i^2} = \sum_{\substack{j=1 \\ j\neq i}}^{N} \frac{\sqrt{k^2 - V_j}}{\alpha_j^2}. \tag{44}$$

Under the condition that all the bond potentials are constant and have the same value, we can obtain the same constraint given by (40).

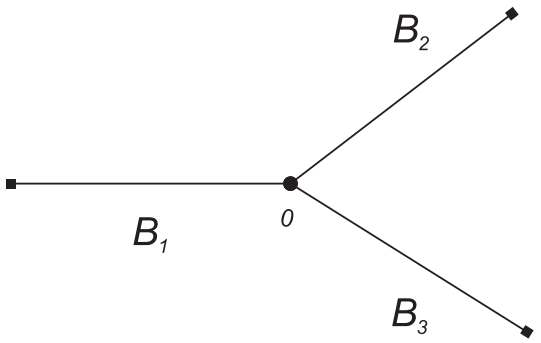

FIG. 1: Finite star graph with three bonds. The coordinates of the bonds B_j are $x \in [-L_1, 0]$ for B_1 and $x \in [0, L_j]$ for $j = 2, 3$.

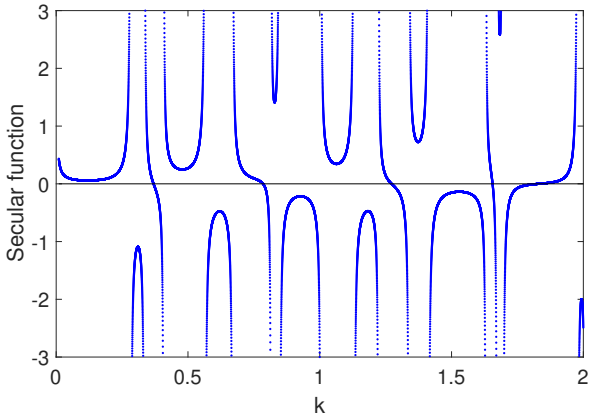

FIG. 2: The secular function (47) for the star graph is shown in Fig. 1 with $L_1 = 11.12$, $L_2 = 9.39$, $L_3 = 7.71$ and boundary condition parameters $\alpha_1 = 2.4$, $\alpha_2 = 3$, $\alpha_3 = 4$.

IV. THE ENERGY SPECTRUM OF A QUANTUM STAR GRAPH WITH TRANSPARENT VERTEX

Consider the Schrödinger equation (35) given on a star graph. Bonds of the graph have finite lengths and their coordinates are $x \in [-L_1, 0]$ for B_1 and $x \in [0, L_j]$ for $B_j (j = 2, 3, \ldots, N)$. The boundary conditions are given by the equations (18) and (19) at the central vertex and the Dirichlet boundary conditions at the edge vertices. These boundary conditions ensure that the Schrödinger equation is self-adjoint and thus that an unbounded discrete spectrum exists. For the given continuity (18) and Dirichlet conditions at each bond j $(j = 1, 2, \ldots, N)$, the wave function Ψ_j can be written as

$$\begin{aligned} \Psi_1(x) &= \frac{C_n}{\alpha_1 \sin kL_1} \sin k(L_1 + x), \\ \Psi_j(x) &= \frac{C_n}{\alpha_j \sin kL_j} \sin k(L_j - x), j = 2, 3, \ldots, N, \end{aligned} \tag{45}$$

where the normalization coefficients are found by requiring $\sum_j \int_{B_j} |\Psi_j(x)|^2 dx = 1$, which results in

$$C_n = \sqrt{2} \left(\sum_j \frac{2k_n L_j - \sin(2k_n L_j)}{2k_n \alpha_j^2 \sin^2(k_n L_j)} \right)^{-\frac{1}{2}}. \tag{46}$$

The current conservation condition (19) leads to equation

$$\frac{1}{\alpha_1^2 \tan kL_1} - \sum_{j=2}^{N} \frac{1}{\alpha_j^2 \tan kL_j} = 0. \tag{47}$$

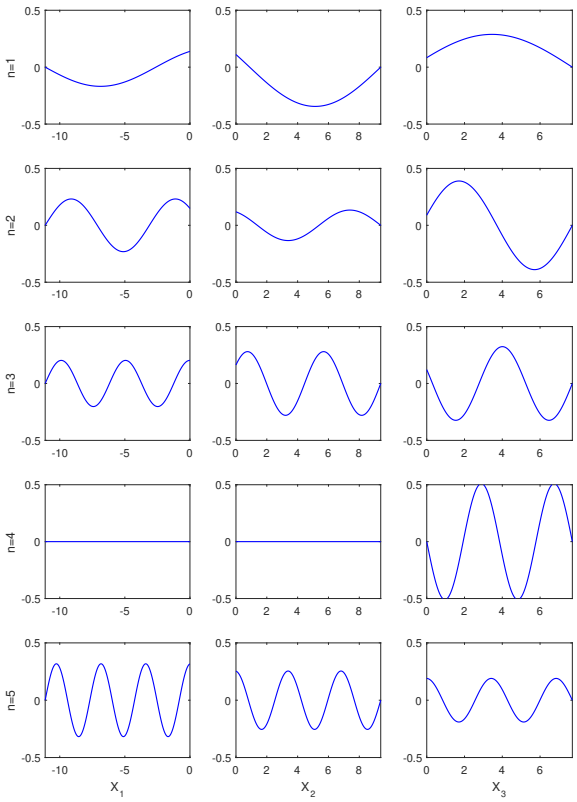

FIG. 3: Eigenfunctions corresponding to the first five energy eigenvalues.

Thus, the eigenvalues of the star graph are found by solving the secular equation (47).

Let us give an example. We consider the simple case of a star graph with three bonds of lengths $L_1 = 11.12$, $L_2 = 9.39$, $L_3 = 7.71$ (see Fig. 1). We will compute the spectrum of the quantum star graph with boundary conditions (18) and (19) in the central vertex and Dirichlet boundary conditions in the edge vertices. To make the central vertex transparent, we choose parameters such as $\alpha_1 = 2.4$, $\alpha_2 = 3$, $\alpha_3 = 4$ that satisfy the sum rule (40). The eigenvalues of this graph are found by computing the zeros of the secular function on the left side of Eq. (47). The graph of this function is shown in Fig. 2. The first five eigenvalues are listed in Table II. The corresponding eigenfunctions are plotted in Fig. 3. The case requiring attention here corresponds to the fourth level ($n = 4$), where eigenfunctions of the first and second bonds vanish, while for the third bond we have a non-zero eigenfunction. This happens due to the factor $C_n/\sin^2(L_j k_n)$ in Eqs. (45), which vanish for $j = 1, 2$ and is non-zero for $j = 3$. One can avoid such a case by choosing a non-commensurable length with the considered modes $k_n L_j \neq n\pi$.

TABLE II: Values of the first five eigenvalues of the considered quantum star graph.

n	k_n
1	0.369458684400225
2	0.785050383772513
3	1.272399270052320
4	1.629879457115328
5	1.829920221965212

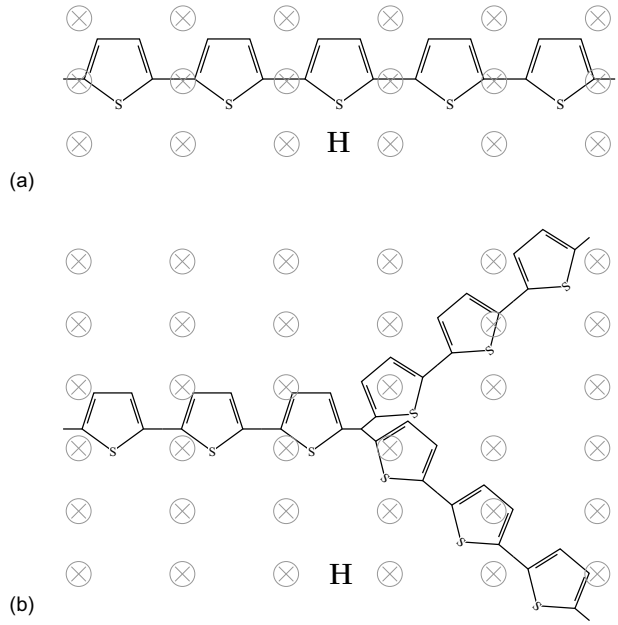

FIG. 4: Conducting polymer chains in a constant uniform magnetic field: Linear (unbranched) (a) and branched (b) configurations.

V. POSSIBLE EXPERIMENTAL REALIZATION OF THE MODEL

The above model can be applied to the so-called conjugated or conducting polymers. These are organic semiconductors based on conjugated polymers. Due to their flexibility and very low weight, they have attracted much attention in physics and chemistry [45–47] and have become basic materials for organic electronics [49]. Branched versions of such polymers can be synthesized [48] or formed into thin films organic solar cells [50]. Charge transport in such branched structures has recently been studied in [51]. The structure described by the above model can be realized experimentally and consists of a conducting polymer (linear or branched) that interacts with an external constant uniform magnetic field $\mathbf{H}$ (see, Fig. 4).

An important problem that can be studied in such a structure is the effect of the magnetic field on the electronic band structure. In other words, using our model one can reveal the conditions that ensure the equivalence of the electronic band spectrum of the unperturbed conducting polymer with that of the polymer interacting with the constant uniform magnetic field. Similarly, conducting polymers can also interact with a constant uniform electric field. Such a finding would make it possible to achieve stability of organic devices with respect to the influence of external electromagnetic fields, which occur in many cases. Such stability implies stable functionality of the organic electronic devices.

VI. CONCLUSIONS

We addressed the problem of a driven (interacting with an external field) quantum graph with transparent vertex by combining the concept of transparent boundary conditions with quantum graphs. The transparent vertex here implies the absence of backscattering at the branching points of the graph. Transparent vertex boundary conditions for the time-independent Schrödinger equation on the graph containing an external potential are derived by extending two different approaches to TBCs previously studied for systems on a line. The first approach uses pseudodifferential operator theory to approximate TBCs, while the second, more general method uses Weyl-Titchmarsh functions to derive exact TBCs. Both approaches lead to a "sum rule" that determines conditions for parameters of the vertex boundary conditions to make them transparent. It is shown that such conditions can also be derived using the scattering approach, when the external potential is constant.

A more rigorous mathematical study of quantum graphs has been carried out considering vertex boundary conditions leading to a self-adjoint Schrödinger equation. Although the above results are obtained for the case of a star-branched graph, the extension of the approach to other graph topologies is rather trivial.

The transparent quantum graph model presented in this study can be directly applied to describe reflectionless

quantum transport in various low-dimensional systems, such as branched molecular chains and conducting polymers, semiconductor quantum wire networks, and branched topological insulators, etc. The extension of the approach to other quantum mechanical wave equations, such as Dirac, Klein-Gordon, and Bogoliubov de Gennes equations, is important and is the subject of future research.

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