Transparent quantum graphs and nonlinear networks: Tunable transport in branched structures

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Motivation:
Why transparent quantum graphs

- Effective (lossless) signal transfer in optical fiber- and optoelectronic networks
- Tunable charge transport in branched nanostrctures
- Tunable charge transport in conducting polymers
- Effective spin, heat and quasiparticle transport in low-dimensional strctures arising in condensed matter

Network science

How networks are studied?

Statistical physics based approach
Statistical distributions of bonds and vertices and their dependence on graphs topology

Discrete, or tight binding approach:
Tight binding Hamiltonian on metric graphs

Continuum approach:
Evolution equations on metric graphs

What have been studied in the context of quantum graphs so far?

- **Mathematical formulation of the problem, boundary conditions:** Exner (1988), Kostrykin, Schrader (1999), Seba (2000)
- **Planar (fat) graphs:** Exner, Post (2006-2012), Dell Antonio (2006)
- **Quantum chaos in networks:** Kottos, Smilansky (1999), Gaspard (2004), Gnutzmann (2006)
- **Inverse problems:** Kurasov (2001), Smilansky (2004), Cheon (2010)
- **Casimir effect:** Kaplan (2005), Matrasulov (2006), Bellazini (2007)
- **Quantum hall effect :** Gaspard (2008)
- **PT-symmetric quantum graphs:** Matrasulov, et.al (2019)
- **Dirac Equation on graphs:** Bolte, Harrison (2005)
- **Periodic quantum graphs:** Berkolaiko, Band (2013)
- **Many particles in quantum graphs:** Bolte , Kerner (2013, 2017)
- **Microwave networks (networks of optical fibers):** Hull et.al (2007)

Metric graphs

A graph with the bonds which can be assigned length,

$$o < l_b : < D$$

is called metric graph

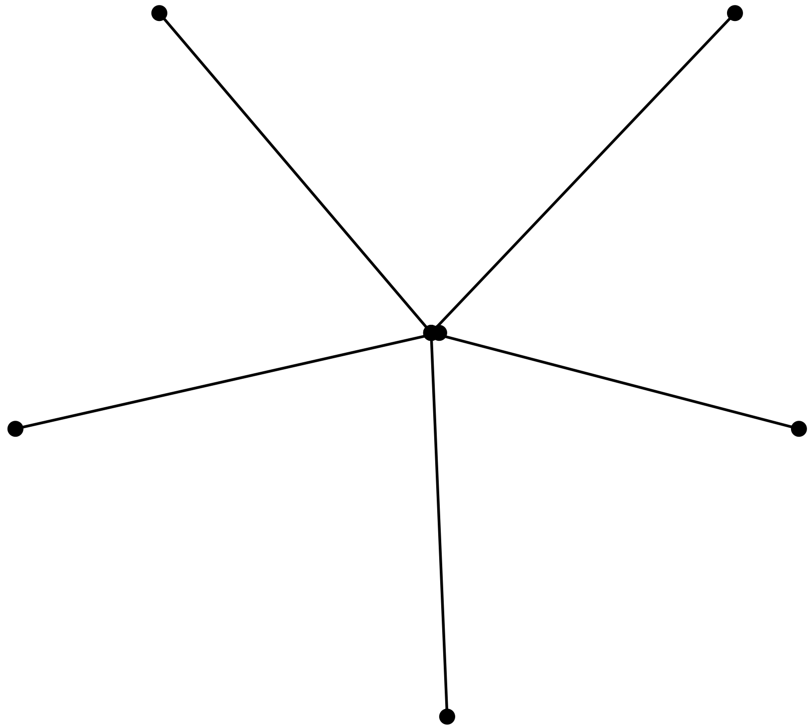
Graphs and their topology

The topology of the graph, that is, the way the vertices and bonds are connected is given in terms of the $V \times V$ connectivity matrix $C_{i,j}$ (sometimes referred to as the adjacency matrix) which is defined as:

$$C_{i,j} = C_{j,i} = \left\{ \begin{array}{l} 1 \text{ if } i,j \text{ are connected} \\ 0 \text{ otherwise} \end{array} \right\}, \quad i,j = 1, ..., V.$$

Constructing quantum graphs from finite interval (wires)

Metric graph as a collection of intervals glued to each other according to connectivity matrix



Evolution equation on graphs

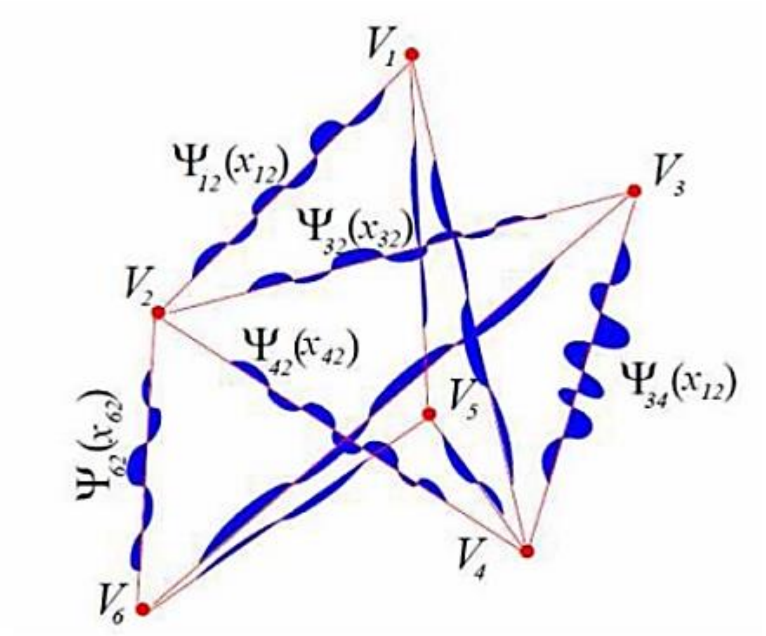
$$i\frac{\partial\psi}{\partial t} = H\psi$$

where H is the Shrödinger, Dirac, or other differential operator

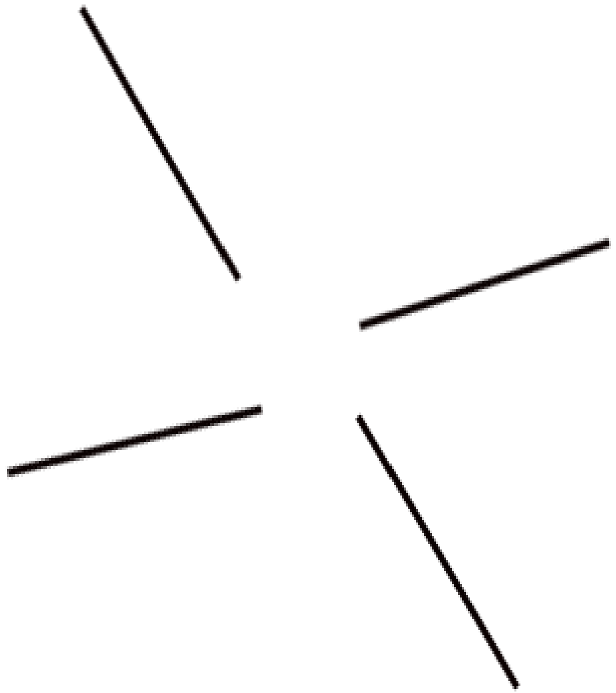
Wave equation on graphs: Wave function

Wave function Ψ is a B-component vector

$$\left(\Psi_{b_1}(x_{b_1}), \Psi_{b_2}(x_{b_2}), \dots, \Psi_{b_B}(x_{b_B})\right)^T$$



Wave equation on graphs:
Vertex Boundary conditions



Differential operators on graphs

For given self-adjoint differential operator on graph *D* skew-Hermitian form can be constructed as

$$\Omega(\varphi,\phi)=\langle D\varphi,\phi\rangle-\langle\varphi,D\phi\rangle$$

V.Kostrykin, R.Schrader, J. Phys. A. **32** 595 (1999)

Boundary conditions

$$\mathbf{A}\psi(0)+\mathbf{B}\psi'(0)=0$$

where A and B are two $n \times n$ matrices

V.Kostrykin, R.Schrader, J. Phys. A: Math. Gen. **32** (1999) 595–630.

The Schrödinger equation on graphs: Wave function

For each bond $b = (i, j)$ a coordinate $x_{i,j}$ which indicates the position along the bond is assigned. The variable $x_{i,j}$ takes the value 0 at the vertex i and the value $L_{i,j} \equiv L_{j,i}$ at the vertex j while $x_{j,i}$ is zero at j and $L_{i,j}$ at i.
We have thus defined the length matrix $L_{i,j}$ with matrix elements different from zero, whenever $C_{i,j} \neq 0$ and $L_{i,j} = L_{j,i}$ for $b = 1, \dots, B$.

The wavefunction Ψ is a $B-$component vector and can be written as

$$\left(\Psi_{b_1}(x_{b_1}), \Psi_{b_2}(x_{b_2}), \dots, \Psi_{b_B}(x_{b_B})\right)^T$$

where the set $\{b_i\}_{i=1}^{B}$ consists of B different bonds.

The Schrödinger equation on graphs: Boundary Conditions

The wave function must satisfy boundary conditions at the vertices, which ensure continuity (uniqueness) and current conservation. For every $i = 1, \ldots, V$:

- *Continuity*

$$\Psi_{i,j}(x)\Big|_{x=0} = \varphi_i, \qquad \Psi_{i,j}(x)\Big|_{x=L_{i,j}} = \varphi_j \qquad \text{For all } i < j \text{ and } C_{i,j} \neq 0$$

- *Current conservation*

$$-\sum_{j<i} C_{i,j} \left.\frac{d\Psi_{i,j}(x)}{dx}\right|_{x=L_{i,j}} + \sum_{j>i} C_{i,j} \left.\frac{d\Psi_{i,j}(x)}{dx}\right|_{x=0} = \lambda_i \varphi_i$$

The parameters λ_i are free parameters which determine the type of the boundary conditions.

The special case of zero λ_i's, corresponds to Neumann boundary conditions. Dirichlet boundary conditions are introduced when all the $\lambda_i = \infty$.

The Schrödinger equation on graphs: Solutions

At any bond $b = (i, j)$ the component b can be written in terms of its values on the vertices i and j as

$$\Psi_{i,j} = \frac{1}{\sin kL_{i,j}}\left(\varphi_i \sin\left[k\left(L_{i,j} - x\right)\right] + \varphi_j \sin kx\right) C_{i,j}, \qquad i < j.$$

The current conservation condition leads to

$$-\sum_{j<i} \frac{kC_{i,j}}{\sin(kL_{i,j})}(-\varphi_j + \varphi_i \cos(kL_{i,j})) + \sum_{j>i} \frac{kC_{i,j}}{\sin(kL_{i,j})}(-\varphi_i \cos(kL_{i,j}) + \varphi_j) = \lambda_i \varphi_i, \qquad \forall i.$$

T. Kottos, U. Smilansky, Ann. Phys. **76 ,** 274 (1999)

The Schrödinger equation on graphs: Eigenvalues

Spectral equation

$$\det\left(h_{i,j}(k)\right) = 0$$

where

$$h_{i,j} = \begin{cases} -\sum_{m \neq i} C_{i,m} \cot\left(kL_{i,m}\right) - \dfrac{\lambda_i}{k}, & i = j \\ C_{i,j}\left(\sin\left(kL_{i,j}\right)\right)^{-1}, & i \neq j. \end{cases}$$

T. Kottos, U. Smilansky, Ann. Phys. **76 ,** 274 (1999)

Transparent boundary conditions

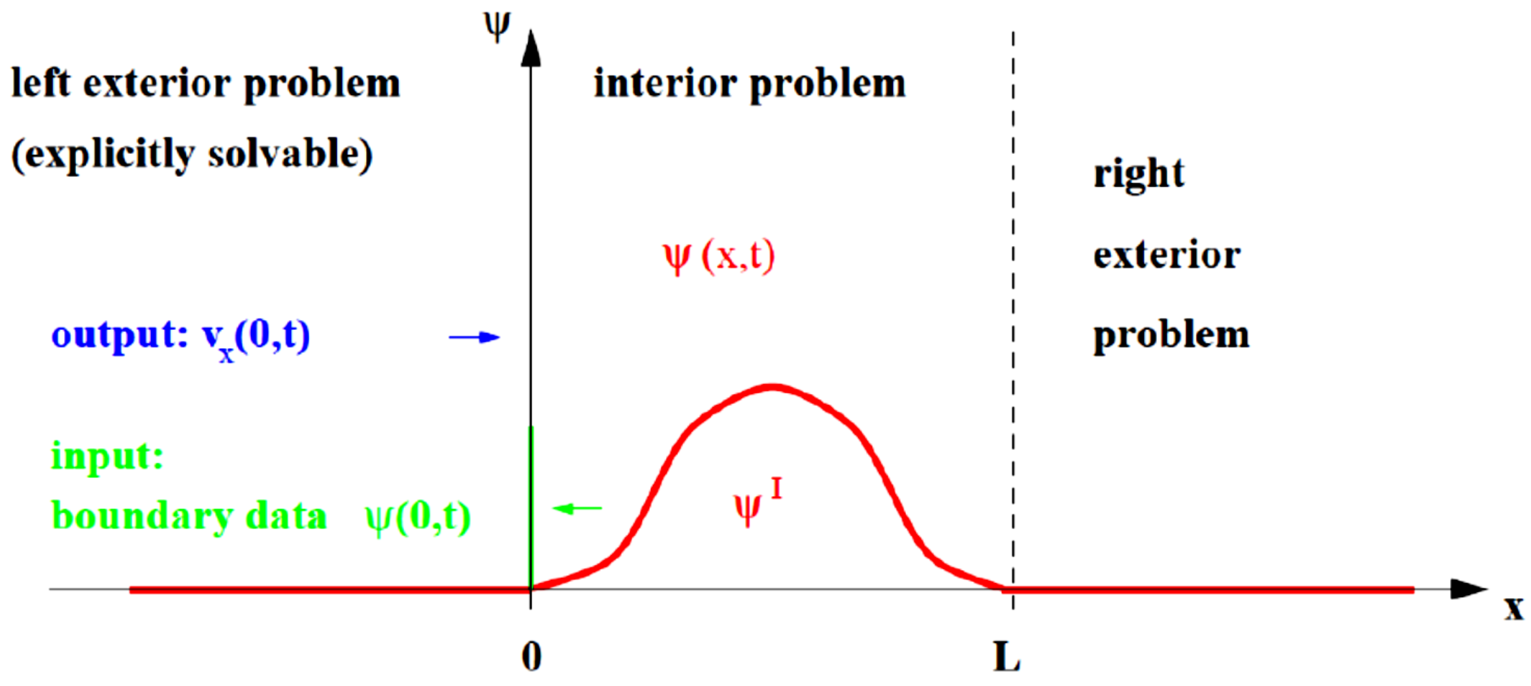
- For a given finite domain, Ω, the TBC sare imposed in such a way that the solution of a PDE in Ω corresponds to that in the whole space, i.e., the wave/particle moving inside/outside the domain does not 'see' the boundary of the domain.

- Then such boundary conditions provide absence of the back scattering at the given point (or domain boundary) makes it transparent.

Transparent boundary conditions

- **<u>The general procedure for constructing transparent boundary conditions on a real line:</u>**
- 1. Split the original PDE evolution problem into coupled equations: the interior and exterior problems.
- 2. Apply a Laplace transformation to exterior problems on Ωext.
- 3. Solve (explicitly, numerically) the ordinary differential equations in the spatial unknownx.
- 4. Allow only “outgoing” waves by selecting the decaying solution asx→±∞.
- 5. Match Dirichlet and Neumann values at the artificial boundary.
- 6. Apply (explicitly, numerically) the inverse Laplace transformation

Transparent boundary conditions



Schrödinger edition: Construction idea for transparent boundary conditions

M. Ehrhardt and A. Arnold, Discrete Transparent Boundary Conditions for the Schrodinger Equation, *Rivista di Mathematica della Universita di Parma*, Volume 6, Number 4 (2001), 57-108.

Transparent boundary conditions

Interior problem:

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

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

$$\partial_x \Psi(0,t) = (T_0 \Psi)(0,t)$$

$$\partial_x \Psi(L,t) = (T_L \Psi)(L,t)$$

$T_{0,L}$ denote the Dirichlet-to-Neumann maps at the boundaries.

Transparent boundary conditions

$T_{0,L}$ are obtained by solving the two exterior problems:

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

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

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

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

$$(T_L\Phi)(t) = \partial_x \, v(L,t)$$

and analogously for T_0.

Transparent boundary conditions

The right TBC at $x = L$:

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

The left TBC at $x = 0$ is obtained as

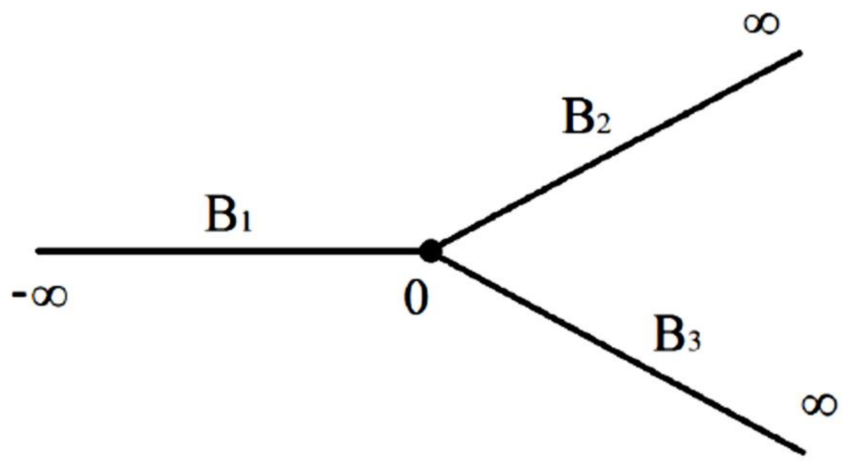
$$\partial_x \Psi(x = 0, t) = -\sqrt{\frac{2}{\pi}} e^{-i\frac{\pi}{4}} \frac{d}{dt} \int_0^t \frac{\Psi(L, \tau)}{\sqrt{t - \tau}} d\tau$$

Transparent quantum graphs

Time-dependent Schrödinger equation for star graph with 3 bonds (in units $\hbar = m = 1$)

$$i\partial_t \Psi_b = -\frac{1}{2}\partial_x^2 \Psi_b, \qquad\qquad b = 1,2,3$$

The coordinates assigned to bond B_1 is $x \in (-\infty;\ 0)$ and $B_{1,2}$ are $x \in (0;\infty)$.



Transparent quantum graphs

Kirchhoff-type boundary conditions

Continuity condition:

$$\alpha_1 \Psi_1(0,t) = \alpha_2 \Psi_2(0,t) = \alpha_3 \Psi_3(0,t)$$

Current conservation condition:

$$\frac{1}{\alpha_1}\partial_x \Psi_1(x=0,t) = \frac{1}{\alpha_2}\partial_x \Psi_2(x=0,t) + \frac{1}{\alpha_3}\partial_x \Psi_3(x=0,t)$$

Transparent quantum graphs

Interior problem for B_1:

$$i\partial_t \Psi_1 = -\frac{1}{2}\partial_x^2 \Psi_1, \qquad x < 0, \qquad t > 0$$

$$\Psi_1(x, 0) = \Psi^I(x)$$

$$\partial_x \Psi_1(0, t) = (T_+ \Psi_1)(0, t)$$

Transparent quantum graphs

Exterior problems for $B_{2,3}$:

$$i\partial_t \Psi_{2,3} = -\frac{1}{2}\partial_x^2 \Psi_{2,3}, \qquad x > 0, \qquad t > 0$$

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

$$\Psi_{2,3}(0,t) = \Phi_{2,3}(t), \qquad t > 0, \qquad \Phi_{2,3}(0) = 0$$

$$\left(T_+ \Psi_{2,3}\right)(t) = \partial_x \Psi_{2,3}(0,t)$$

Transparent vertex boundary conditions

At the vertex ($x = 0$) for bonds $B_{2,3}$ using continuity VBC we get

$$\partial_x \hat{\Psi}_{2,3}(x=0,s) = -\sqrt[+]{-2is}\,\frac{\alpha_1}{\alpha_{2,3}}\hat{\Psi}_1(x=0,s)$$

Laplace transformed Kirchhoff rule (at $x = 0$):

$$\partial_x \hat{\Psi}_1 = \frac{\alpha_1}{\alpha_2}\partial_x \hat{\Psi}_2 + \hat{\Psi}_1 = \frac{\alpha_1}{\alpha_3}\partial_x \hat{\Psi}_3 = -\sqrt[+]{-2is}\,\alpha_1^2\left(\frac{1}{\alpha_2^2} + \frac{1}{\alpha_2^2}\right)\hat{\Psi}_1$$

J. R. Yusupov, K. K. Sabirov, M. Ehrhardt, and D. U. Matrasulov, Phys. Lett. A **383**, 2382 (2019).

Transparent vertex boundary conditions

An inverse Laplace transformation yields the TBC at the vertex:

$$\partial_x \Psi_1(x=0,t) = -\sqrt{\frac{2}{\pi}} e^{-i\frac{\pi}{4}} \alpha_1^2 \left(\frac{1}{\alpha_2^2} + \frac{1}{\alpha_3^2}\right) \frac{d}{dt} \int_0^t \frac{\Psi_1(0,\tau)}{\sqrt{t-\tau}} d\tau$$

This condition coincides with transparent boundary condition (at $x = 0$), when the factor $\alpha_1^2 \left(\frac{1}{\alpha_2^2} + \frac{1}{\alpha_3^2}\right)$ is equal to one.

MJ. R. Yusupov, K. K. Sabirov, M. Ehrhardt, and D. U. Matrasulov, Phys. Lett. A **383**, 2382 (2019).

Transparent quantum networks

Continuity condition:

$$\alpha_1 \Psi_1(0,t) = \alpha_2 \Psi_2(0,t) = \alpha_3 \Psi_3(0,t)$$

Current conservation condition:

$$\frac{1}{\alpha_1} \partial_x \Psi_1(x=0,t) = \frac{1}{\alpha_2} \partial_x \Psi_2(x=0,t) + \frac{1}{\alpha_3} \partial_x \Psi_3(x=0,t)$$

Condition for transparency the continuity and current conservation:

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

J. R. Yusupov, K. K. Sabirov, M. Ehrhardt, and D. U. Matrasulov, Phys. Lett. A **383**, 2382 (2019).

Transparent vertex boundary conditions

Similarly, the results for *B*2 (*B*3) can be obtained considering exterior problems for $B_{1,3}$ $(B_{1,2})$:

$$\partial_x \Psi_2(x=0,t) = \sqrt{\frac{2}{\pi}} e^{-i\frac{\pi}{4}} \alpha_2^2 \left(\frac{1}{\alpha_1^2} + \frac{1}{\alpha_3^2} \right) \frac{d}{dt} \int_0^t \frac{\Psi_2(0,\tau)}{\sqrt{t-\tau}} d\tau$$

and

$$\partial_x \Psi_3(x=0,t) = \sqrt{\frac{2}{\pi}} e^{-i\frac{\pi}{4}} \alpha_3^2 \left(\frac{1}{\alpha_1^2} + \frac{1}{\alpha_2^2} \right) \frac{d}{dt} \int_0^t \frac{\Psi_3(0,\tau)}{\sqrt{t-\tau}} d\tau$$

Transparent quantum graphs

Thus, in order to have transparent vertex boundary condition for B_1 the following constraint must be fulfilled:

$$\frac{1}{\alpha_1^2} = \frac{1}{\alpha_2^2} + \frac{1}{\alpha_3^2}$$

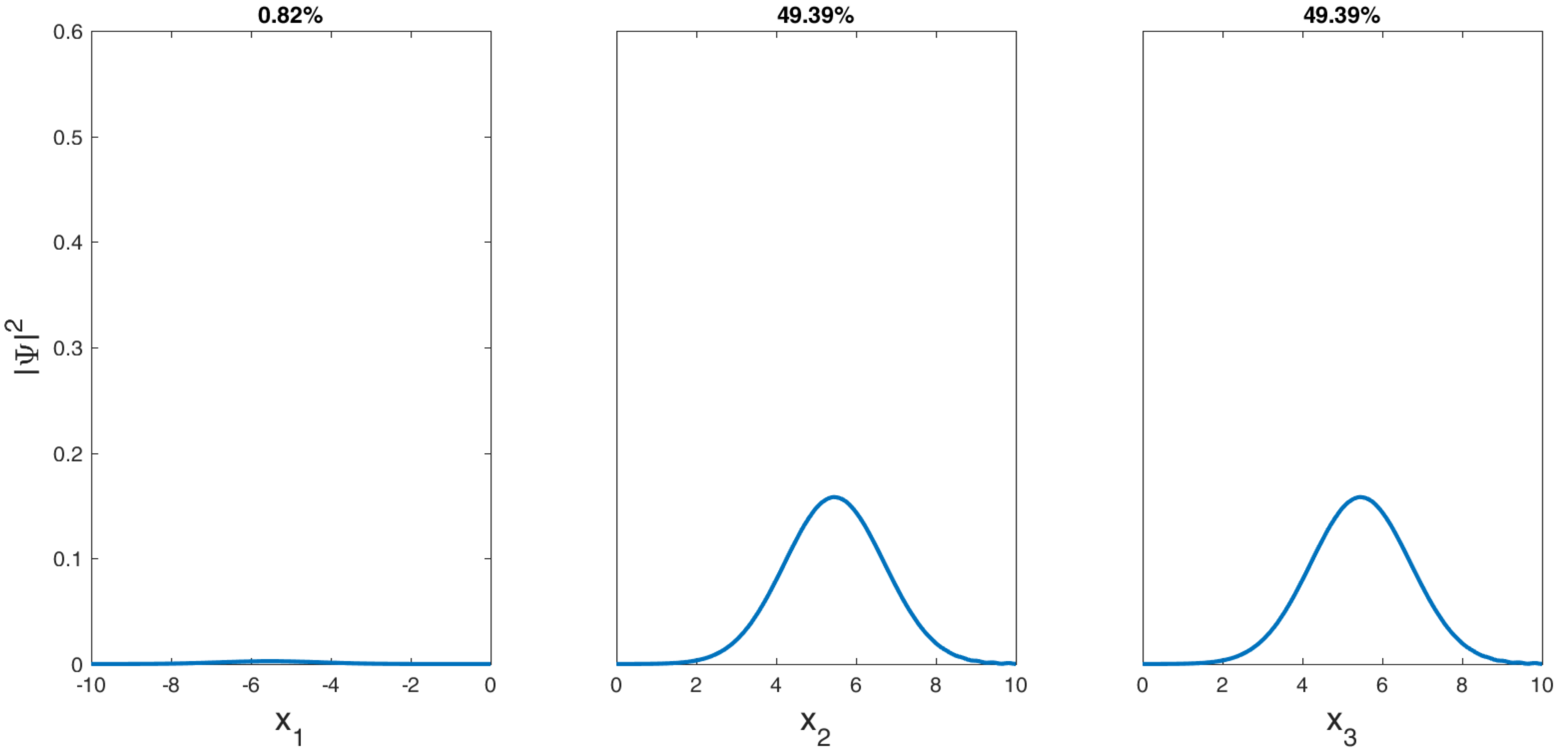
Similarly, the results for B_2 (B_3):

$$\frac{1}{\alpha_2^2} = \frac{1}{\alpha_1^2} + \frac{1}{\alpha_3^2}$$

and

$$\frac{1}{\alpha_3^2} = \frac{1}{\alpha_1^2} + \frac{1}{\alpha_2^2}$$

Transparent quantum graphs



J. R. Yusupov, K. K. Sabirov, M. Ehrhardt, and D. U. Matrasulov, Phys. Lett. A **383**, 2382 (2019).

Dirac Particles in Transparent Quantum Graphs

The Dirac equation (in unitis $\hbar = c = 1$):

$$i\partial_t\phi_j = -i\,\partial_x\chi_j + m\phi_j,$$
$$i\partial_t\chi_j = -i\,\partial_x\phi_j - m\chi_j.$$

Vertex boundary conditions are imposed in the form of weighted wave functions continuity

$$\alpha_1\phi_1(0,t) = \alpha_2\phi_2(0,t) = \alpha_3\phi_3(0,t),$$

and generalized Kirchhoff rule

$$\frac{1}{\alpha_1}\chi_1(0,t) = \frac{1}{\alpha_2}\chi_2(0,t) + \frac{1}{\alpha_3}\chi_3(0,t).$$

J. R. Yusupov, K. K. Sabirov, Q.U. Asadov, M. Ehrhardt, and D. U. Matrasulov, ArXiv:2004.07838 (To appear in PRE)

Dirac Particles in Transparent Quantum Graphs

Transparent boundary condition:

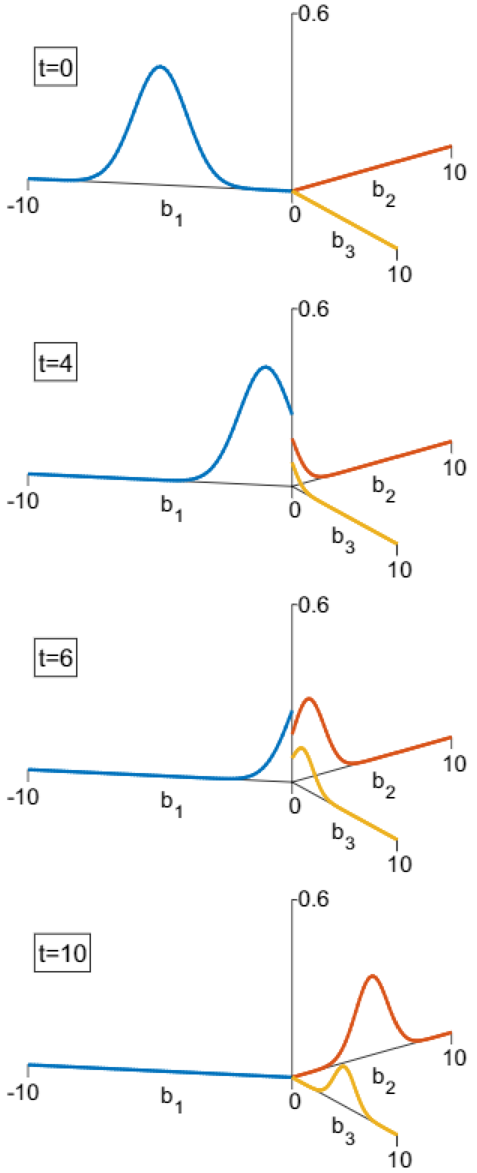
$$\chi_1(0,t) = A\,[\frac{d}{dt}\int_0^t I_0\big(m(t-\tau)\big)\phi_1(0,\tau)d\tau + im\int_0^t I_0\big(m(t-\tau)\big)\phi_1(0,\tau)d\tau],$$

where $A_1 = \alpha_1^2(\alpha_2^{-2} + \alpha_3^{-2})$ и $I_0(z)$ – Bessel's function

Sum rule: $$\frac{1}{\alpha_1^2} = \frac{1}{\alpha_2^2} + \frac{1}{\alpha_3^2}$$

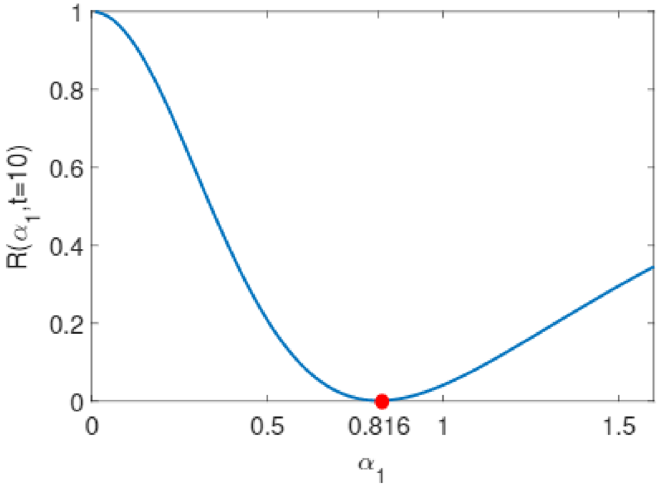
J. R. Yusupov, K. K. Sabirov, Q.U. Asadov, M. Ehrhardt, and D. U. Matrasulov, ArXiv:2004.07838 (To appear in PRE)

Dirac Particles in Transparent Quantum Graphs



The position probability density $\left|\varphi_j(x,t)\right|^2 + \left|\chi_j(x,t)\right|^2$ plotted at different time moments for the regime when the sum rule is fulfilled (no reflection occurred): $\alpha_1 = \sqrt{2/3}$, $\alpha_2 = 1$ and $\alpha_3 = \sqrt{2}$.

Dependence of the vertex reflection coefficient R on the parameter α_1 when the wave packet splitting time elapses ($t = 10$). For fixed $\alpha_2 = 1$ and $\alpha_3 = \sqrt{2}$, $R = 0$ when $\alpha_1 = \sqrt{2/3} \approx 0.816$ (red dot).



Summary

- The concept of Transparent boundary conditions is applied to quantum graphs;
- Physically acceptable constraint for the reflectionless transmission at the vertex is derived in the form of sum rule;
- Reflectionless transmission of solitons through the vertex of a star graph is shown by solving the problem numerically;
- The approach can be directly extended to arbitrary graph topologies.

Outlook

- Transparent optical fiber networks;
- Ballistic (reflectionless) particle transport in branched nanostrctures and nanoscale networks;
- Ballistic transport of charge carriers (e.g., excitons, polarons, solitons) in branched conducting polymers.
- Experimental realization in microwave networks

Further reading

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