Anderson Localization in 1-D Quantum Random Walk*

A.N. Bondarenko

Sobolev Institute of Mathematics, Novosibirsk State Technical University
630090, Novosibirsk, Akad. Koptyug pr., 4, Russia

V.A. Dedok

Novosibirsk State University
630090, Novosibirsk, Pirogova str., 2, Russia

***Abstract*-In this paper we intend to present some new results concerning two quantum models: quantum scattering model and discrete quantum random walk. We present the analytical solution of the 1-D quantum random walk and give an explicit formula of the quantum return probability. The exact solution provides weak Anderson localization in discrete quantum random walk theory. Connectivity between these theories is introduced.**

I. INTRODUCTION

Quantum scattering model provides a fundamental model for the emergence of global properties from local interactions. Periodic orbit scattering theory is considered in the connection with a genuine quantum phenomenon such as Anderson localization [1], which appears as a result of quantum interferences at the long time limit. Quantum transport in random media has been studied both experimentally and theoretically.

Both discrete and continuous models represent absence of diffusion firstly studied by Anderson [2]. Lattice models serve as a discretization of the continuous Schrödinger equation. Physical properties like electrical conductivity or localization of electrons have connected with spectrum (pure point, continuous…) of the random Schrödinger equation [3]. There are a lot of known results for models in large disorder or large dimensions. This is contrary to the regime of weak disorder.

In continuous models localization theory is connected with exponential decay of the wavefunction [4] provided by the theory of products of random matrices [5].

Quantum graphs are also studied in connection with laser tomography technology [12], propagation radiation in networks of optical fibers. Recent researches were inspired by possible applications to some models of nanoelectronic devices and quantum computing. For a list of references on quantum graphs, see [1, 9, 12, 13] and their references. Quantum mechanics provides a lot of enigmatic models that are unimaginably in a classical Newtonian word. In recent years the interest in quantum information theory is generated by the applications in quantum computing. Quantum walk algorithms [6] serve as the basis of solution of a number of problems. Quantum algorithms based on quantum random walks represent an attempt to increase speed of classical walks [7].

Scattering theory may serve a powerful tool to study properties of quantum random walks [8]. For investigation Anderson localization we are considering quantum return probability which characterize probability of the wave packet initially localized at a site occupies the same site after a given time.

We deal discrete time 1-dimensional quantum walk model which is a particular case of scattering on the line and derive a property corresponding to weak absence of diffusion in continuous model [11]. Finally we propose a hypothesis concerning the same property on fractal graphs.

II. QANTUM GRAPHS

Let us introduce a graph as a collection of bonds B (lines) joined in vertices V (nodes). The valence v_j of a vertex j is the number of bonds with common endpoint j. When vertices i and j are connected, we denote the connecting bond by $b=[i,j]$. If one fixes a direction of the bond $b=(i,j)$ we call this bond as oriented or directed from i to j. The same bond but oriented from j to i is $\tilde{b}=(j,i)$. A graph may contain multiply bonds or loops, but we shall consider graphs with simple geometry without multiply bonds or loops, unless explicitly specified.

We assign to each bond $b=(i,j)$ a coordinate $x_{(i,j)}$ which measures a distance along the bond. $x_{(i,j)}$ takes the value 0 at the vertex i and the value $l_{(i,j)}=l_{(j,i)}$ at

* This research was supported in part by RFFI foundation (grants 05-01-00171, 05-01-00559) and grants SS-1172.2003.1, UR-04.01.200.

the vertex j. Note, that $x_{(i,j)} = l_{(i,j)} - x_{(j,i)}$. The wavefunction $y(x) = [y_1(x),..., y_B(x)]^T$ is a B component vector where each $y_b(x)$ lives on its ownbond and satisfies the one-dimensional Schrödinger equation

$$-\frac{d^2}{dx^2} y_b(x) + u_b(x) y_b(x) = k^2 y_b(x) \qquad (1)$$

and boundary conditions at the vertices.

Potentials u_b are real-valued functions defined on each edge such that

$$u_b \in L_1(b), \quad b = (i, j)$$

Boundary conditions are provided with continuity of a wavefunction in vertices and current conservation. The continuity condition requires that at each vertex i the value of the wavefunction is independent of the bond from where this vertex is approached. Current conservation is a condition on the derivatives of the wavefunctions at the vertices. In other words boundary conditions are specified as follows:

- continuity,

$$y_b(x)\big|_{x=0} = y_i, \quad y_b(x)\big|_{x=l_b} = y_j, \quad b = (i, j), \qquad (2)$$

- current conservation,

$$-\sum_{j<i} \frac{d}{dx} y_{j,i}(x)\big|_{x=l_{i,j}} + \sum_{j>i} \frac{d}{dx} y_{i,j}(x)\big|_{x=0} = a_i y_i. \qquad (3)$$

The last sum means a sum of the first derivatives over all outgoing bonds. The parameters a_i are free parameters which determine boundary conditions. In the case when $v_i = 2$ we may think about a_i as a δ-function potential. In general we will refer to them as vertex scattering potentials. Point out two special cases of potentials: Neumann and Dirichlet. Neumann boundary conditions are introduced by zero a_i's. Dirichlet boundary conditions are determined by $a_i = \infty$. The above model can serve as the Kronig-Penney model generalization to a multiply connected, yet one-dimensional manifold.

More generally boundary conditions can be determined by unitary transformations of wavefunction at each vertex – the scattering matrix related to a single vertex [9].

To define scattering matrix we turn a compact graph which consists of finite sets of vertices and bonds into scattering system by coupling to some its vertices set of leads to infinity. We may think about such external lead as a half-line while internal bond is thought as a closed interval.

We extend wavefunction to external leads. Each component should satisfy the Schrödinger equation on a half-line with a potential u_b such that

$$\int_0^\infty (1+|x|)|u_b(x)|\,dx < \infty.$$

In the case where all potentials are zero this operator is called by Laplace operator on the graph and we will denote it by L.

Let n be the count of external leads. The $n \times n$ scattering matrix S(k) is defined by looking at the solutions of Schrödinger equation having the following asymptotics on the long legs:

$$y_j^i(x,k) = \begin{cases} s_{ji}(k)\exp(ikx), & i \neq j \\ \exp(-ikx) + s_{ii}sxp(ikx), & i = j \end{cases} \qquad (4)$$

The Schrödinger equation (1) always have asymptotics (4) [10], so the scattering matrix

$$S(k) = \begin{pmatrix} s_{11}(k) & s_{12}(k) & \dots & s_{1n}(k) \\ s_{21}(k) & s_{22}(k) & \dots & s_{2n}(k) \\ \dots & \dots & \dots & \dots \\ s_{n1}(k) & s_{n2}(k) & \dots & s_{nn}(k) \end{pmatrix}$$

is well defined. Boundary conditions (2), (3) provide S-matrix to be unitary. Diagonal elements of the scattering matrix S(k) are called reflection coefficients, we will denote them by $R_{ii}(k)$. Other elements are called transmission coefficients and are denoted by $T_{ij}(k)$.

III. DISCRETE QUANTUM RANDOM WALKS

Before presenting quantum random walk recall classical one. Consider a person with a coin in their hand. They start, say, at the origin of a line and at every time step flip the coin. Each of two possible outcomes of the flipping directs the distinct direction, "left" and "right". Then they move one step in the tossing direction.

Consider now the quantum walk in one dimension. A quantum particle that moves freely on integer points on the line has an additional degree of freedom called chirality, which takes values "left" and "right". The quantum walk of such particle may be described by two operators: a rotation (or "flip" as in the classical case) operator and a shift operator, and is divided into two steps. On the first step the chirality undergoes a rotation (in general a unitary transformation). The next step is moving the particle according to its final chirality state.

As an example consider "Hadamar walk" where the chirality undergoes a Hadamar transformation. Figure 1 depicts two stage of the quantum random walk.

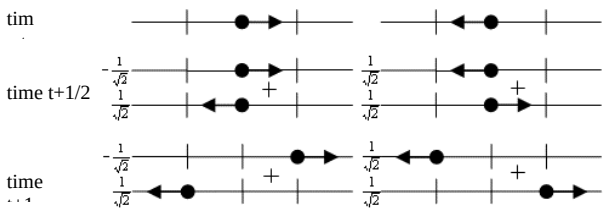

Fig. 1. The dynamics of the quantum Hadamar walk

Let R and L denote "right" and "left" chirality states. The Hadamar walks in these terms is described as follows

$$\begin{array}{l} |L\rangle \to \frac{1}{\sqrt{2}}\left(|L\rangle + |R\rangle\right) \\ |R\rangle \to \frac{1}{\sqrt{2}}\left(|L\rangle - |R\rangle\right) \end{array}. \qquad (5)$$

We start from studying properties of the Hadamar quantum walk. More general cases we shall study may be described by an unitary transformation C ("coin-tossing operator") of the chirality state at each vertex of the graph and a shift operator S which moves the quantum particle according to its chirality state. One step of the quantum walk is given by $U = S \cdot (C \otimes I)$. The action of S is following $S|a,v\rangle = |a,u\rangle$ where u is a-th neighbour of the vertex v.

In one-dimensional case the dynamics is described by the next wavefunction. Let $Y(n,t) = \begin{pmatrix} y_L(n,t) \\ y_R(n,t) \end{pmatrix}$ be the two component vector of the chirality amplitudes of the particle at point n at time t. The upper component denotes chirality left state and the lower component denotes chirality right state. The Hadamar quantum walk is given by the following transformation

$$Y(n,t+1) = \begin{pmatrix} 0 & 0 \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} Y(n-1,t) + \qquad (6)$$

$$\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & 0 \end{pmatrix} Y(n+1,t) = M_+ Y(n-1,t) + M_- Y(n+1,t),$$ for matrices M_+, M_- defined appropriately. If the particle starts from the origin with chirality state "right" we have the initial conditions $Y(0,0) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$, $Y(n,t) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ if $n \neq 0$.

To solve the problem it is convenient to cast it in the Fourier domain. The spatial Fourier transform of the wavefunction Y(n,t) is given by

$$\tilde{Y}(k,t) = \sum_n Y(n,t) e^{ikn}. \qquad (7)$$

In particular for $Y(0,0) = \begin{pmatrix} a \\ b \end{pmatrix}$, $Y(n,0) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ we have $\tilde{Y}(k,0) = \begin{pmatrix} a \\ b \end{pmatrix}$.

In the Fourier domain (6) has more simple representation, indeed

$$\tilde{Y}(k,t+1) = \sum_n \left(M_+ Y(n-1,t) + M_- Y(n+1,t)\right) e^{ikn} =$$

$$e^{ik} M_+ \sum_n Y(n-1,t) e^{ik(n-1)} + e^{-ik} M_- \sum_n Y(n+1,t) e^{ik(n+1)} =$$

$$\left(e^{ik} M_+ + e^{-ik} M_-\right) \tilde{Y}(k,t).$$

Thus

$$\tilde{Y}(k,t+1) = M_k \tilde{Y}(k,t)$$

with M_k defined above.

Thus we have the simple form of the recurrence in Fourier space which gives $\tilde{Y}(k,t) = M_k^t \tilde{Y}(k,0)$.

The corresponding inverse Fourier transform given by

$$Y(n,t) = \frac{1}{2\pi} \int_{-\pi}^{\pi} Y(k,t) e^{-ikn} dk \qquad (8)$$

returns the basis in real space.

For the "left" chirality initial state we have

$$\tilde{y}_L(k,t) = \frac{1}{2}\left(1 + \frac{\cos k}{\sqrt{1+\cos^2 k}}\right) e^{-ig_k t}$$

$$+ \frac{(-1)^t}{2}\left(1 - \frac{\cos k}{\sqrt{1+\cos^2 k}}\right) e^{ig_k t}, \qquad (9)$$

$$\tilde{y}_R(k,t) = \frac{e^{ik}}{2\sqrt{1+\cos^2 k}}\left(e^{-ig_k t} - (-1)^t e^{ig_k t}\right),$$

where $g_k = \arcsin\frac{\sin k}{\sqrt{2}}$.

The inverse Fourier transformation (8) of (9) can be written in the form

$$y_L(n,t) = \frac{1+(-1)^{n+t}}{2} \int_{-\pi}^{\pi} \frac{dk}{2\pi}\left(1 + \frac{\cos k}{\sqrt{1+\cos^2 k}}\right) e^{-i(g_k t + kn)},$$

$$y_R(n,t) = \frac{1+(-1)^{n+t}}{2} \int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{e^{ik}}{\sqrt{1+\cos^2 k}} e^{-i(g_k t + kn)}. \qquad (10)$$

For the "right" initial chirality state we have similar expressions

$$\tilde{y}_L(k,t) = \frac{e^{-ik}}{2\sqrt{1+\cos^2 k}}\left(e^{-ig_k t} - (-1)^t e^{ig_k t}\right),$$

$$\tilde{y}_R(k,t) = \frac{\sqrt{2}e^{ig_k} - e^{ik}}{2\sqrt{1+\cos^2 k}} e^{-ig_k t} + \qquad (11)$$

$$\frac{(-1)^t}{2} \frac{\sqrt{2}e^{-ig_k} + e^{ik}}{\sqrt{1+\cos^2 k}} e^{ig_k t}.$$

In the real space (11) can be expressed as

$$y_L(n,t) = \frac{1+(-1)^{n+t}}{2} \int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{e^{-ik}}{\sqrt{1+\cos^2 k}} e^{-i(g_k t + kn)}, \qquad (12)$$

$$y_R(n,t) = \frac{1+(-1)^{n+t}}{2} \int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{\sqrt{2}e^{-ig_k} - e^{-ik}}{\sqrt{1+\cos^2 k}} e^{-i(g_k t + kn)} .$$

The amplitudes vanish for even t and odd n (respectively, odd t and even n) as one can expect from the definition of the walk.

IV. QUANTUM RANDOM WALK RETURN PROBABILITY

Now we can calculate the probability of observing of the quantum particle at any given point n at any given time t from the wavefunction derived above. It given by

$$P(n,t) = |y_L(n,t)|^2 + |y_R(n,t)|^2 . \qquad (13)$$

We shall derive asymptotic expression for return probability P(0,t) for the large time limit. Let's start from the computer simulation of return probability. Consider now three cases of the initial chirality state: "left", "right" and "symmetric".

From fig. 2, 3 and 4 we can suppose that return probability of the quantum random walk doesn't depend on initial state.

Numerical simulation gives $\approx \frac{2}{\pi t}$ decreasing of return probability. Straight line in fig. 2, 3, 4 represents the plot of the $2/(\pi t)$ in log-log scale. We shall derive this result analytically below using stationary phase method.

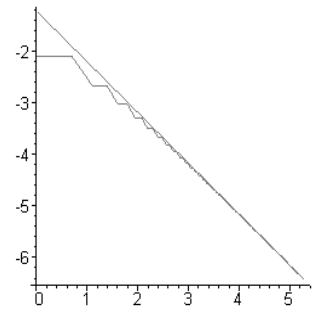

Fig. 2. Return probability in log-log scale for "left" initial state $(1,0)^T$.

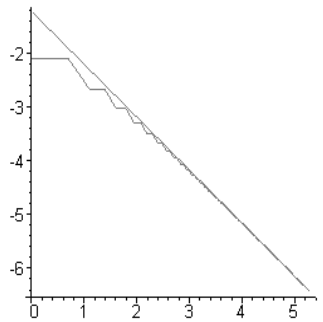

Fig. 3. Return probability in log-log scale for "right" initial state $(0,1)^T$.

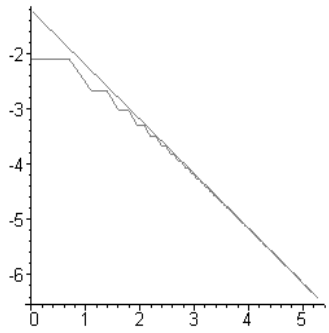

Fig. 4. Return probability in log-log scale for "symmetric" initial state $(1/\sqrt{2}, 1/\sqrt{2})^T$.

Let $n = 0$, the phase function $h(k) = g(k) = \arcsin(\sin k/\sqrt{2})$ has two stationary points

$$k_1 = -\frac{\pi}{2}, k_2 = \frac{\pi}{2} .$$

The leading terms for the "left" initial state are (we assume that t is even)

$$y_L(t) = \sqrt{\frac{2\pi}{t}}\left(\frac{1}{2\pi} + O(t^{-1})\right) e^{it\frac{\pi}{4} - i\frac{\pi}{2}} + \qquad (14)$$

$$\sqrt{\frac{2\pi}{t}}\left(\frac{1}{2\pi} + O(t^{-1})\right) e^{-it\frac{\pi}{4} + i\frac{\pi}{2}}, \quad t \to \infty ,$$

$$y_R(t) = \sqrt{\frac{2\pi}{t}}\left(-\frac{i}{2\pi} + O(t^{-1})\right) e^{it\frac{\pi}{4} - i\frac{\pi}{2}} + \qquad (15)$$

$$\sqrt{\frac{2\pi}{t}}\left(\frac{i}{2\pi} + O(t^{-1})\right) e^{-it\frac{\pi}{4} + i\frac{\pi}{2}}, \quad t \to \infty .$$

For the "right" initial state we have similar expressions

$$y_L(t) = \sqrt{\frac{2\pi}{t}}\left(\frac{i}{2\pi} + O(t^{-1})\right) e^{it\frac{\pi}{4} - i\frac{\pi}{2}} + \qquad (16)$$

$$\sqrt{\frac{2\pi}{t}}\left(-\frac{i}{2\pi} + O(t^{-1})\right) e^{-it\frac{\pi}{4} + i\frac{\pi}{2}}, \quad t \to \infty ,$$

$$y_R(t) = \sqrt{\frac{2\pi}{t}}\left(\frac{1}{2\pi} + O(t^{-1})\right) e^{it\frac{\pi}{4} - i\frac{\pi}{2}} + \qquad (17)$$

$$\sqrt{\frac{2\pi}{t}}\left(\frac{1}{2\pi} + O(t^{-1})\right) e^{-it\frac{\pi}{4} + i\frac{\pi}{2}}, \quad t \to \infty .$$

Using (14)-(17) we derive the quantum return probability (13). It doesn't depend on initial state and for even t

$$P(0,t) = \frac{2}{\pi t} + O(t^{-2}), \; t \to \infty .$$

The classical return probability for the symmetric walk for even t is

$$P_{cl}(0,t) = C_t^{t/2} / 2^N \approx 1/\sqrt{\pi t}\ ,\ t \to \infty\ ,$$

thus, quantum random walk spreads faster that classical one.

Random walk is called recurrent if $\sum_t P(0,t) = \infty$. Evidently, quantum walk is recurrent as well as classic is.

In continuous walk model this means weak absence of diffusion [11] or weak localization.

So we prove

Theorem 1. Hadamar quantum random walk is recurrent and weak localized for the "left" and "right" initial chirality states.

V. QUANTUM RANDOM WALKS AND QUANTUM SCATTERING THEORY

Consider now a simple 1-D scattering model consisting of N scattered points and 2 infinite leads (fig. 5). Let scattering matrices are equal Hadamar matrix at each vertex for the sake of simplicity and the length of all finite bonds is 1.

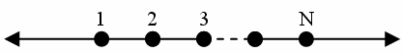

Fig. 5. Simple scattering system.

We proved [12] the ways decomposition formulae for scattering data

$$s_{ll'}(k) = \sum_C a(C) e^{ikl(C)}\ . \qquad (18)$$

For the model being discussed (18) may be rewritten as

$$s_{ll'}(k) = \sum_n \sum_{C_n} a(C_n) e^{ikn} \qquad (19)$$

where C_n denotes n-periodic orbit.

Let expand our model by adding the other integer points (fig. 6)

Ошибка!

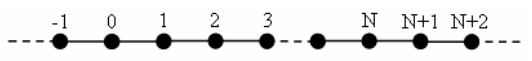

Fig. 6. Extended model

with identity scattering matrices. Put a quantum particle with the "right" chirality state at the point $n = 0$, $t = -2$. Scattering matrices will play a role of the "coin-tossing" operators. Applying quantum step procedure (8) we can obtain probability amplitudes of being the quantum particle at the point $n = 0$ at any given time. Evidently, wavefunction of the particle at the point $n = 0$ has vanishing "right" amplitude except time $t = -2$. Notice, that chirality rotation corresponds to scattering amplitudes multiplication. Easy to obtain $y_L(0,0) = 1/\sqrt{2}$, $y_L(0,2) = -1/(2\sqrt{2})$ and so on. If N is sufficiently large the reflection coefficient $R_{11}(k)$ has the following decomposition

$$R_{11}(k) = \frac{1}{\sqrt{2}} - \frac{1}{2\sqrt{2}} e^{2ik} - \ldots,$$

so, the coefficient (19) is the Fourier transform of the probability amplitude of being at point 0.

Theorem 2. Reflection coefficient $R_{11}(k)$ is the Fourier transform (7) of the "left" probability amplitude of the quantum particle walk defined by extended scattering system (fig. 6).

Remark. Other scattering coefficients have the same property for the quantum random walk appropriately defined.

Notice, that the Hadamar quantum walk is the extreme case of recurrent random walk which spreads faster then classical one. It is well known that the classical walk isn't recurrent in 3 and larger dimensions. We are trying to extend our results over large dimensions.

Consider now finite-ramified Sierpinski gasket which is defined by the following scheme (fig. 7)

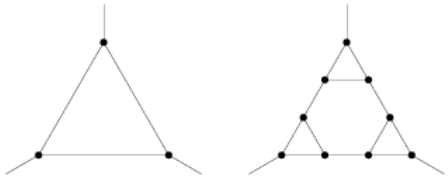

Fig.7. Finite-ramified Sierpinski gasket

Quantum surgery methods and the renormalization scheme [13, 14] provide us to calculate scattering data for any given stage of the Sierpinski gasket. Numerical experiments show that the absolute value of the reflection coefficient moves away from zero (fig. 8) with the next gasket stage

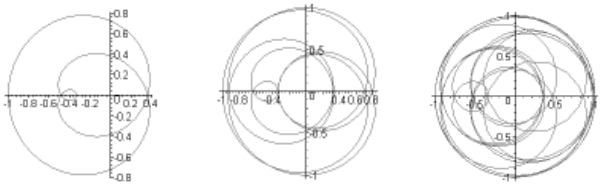

Fig. 8. Reflection data of the 1st, 2nd and 3rd stages of the Sierpinski gasket

and approach to 1. This observation means that the gasket reflection doesn't vanish over all frequencies range and gives us an ability to formulate a hypothesis

Hypothesis. Quantum random walk on the fractal Sierpinski gasket is recurrent and weak localized.

ACKNOWLEDGEMENTS

This research was supported in part by RFFI foundation (grants 05-01-00171, 05-01-00559) and grants SS-172.2003.1, UR-04.01.200.

REFERENCES

[1] H. Schanz, U. Smilanski, "Periodic-orbit theory of the Anderson localization on graphs," *Phys. Rev. Lett.*, vol. 84, pp. 1427-1430, 2000.

[2] P.W. Anderson, "Absence of diffusion in certain random lattices," *Phys. Rev.*, vol. 109, pp. 1492-1505, 1958.

[3] W.-M. Wang, "Localization and universality of Poisson statistics for the multidimensional Anderson model at weak disorder", *Invent. Math.*, vol. 146, pp. 365-398, 2001.

[4] M.V. Berry, S. Klein, "Transparent mirrors: rays, waves and localization," *Eur. J. Phys.*, vol. 18, pp. 222-228, 1997.

[5] H. Furstenberg, "Non commuting random products," *Trans. Amer. Math. Soc.*, vol. 108, pp. 377-428, 1963.

[6] A. Nayak, A. Vishwanath, "Quantum walk on the line," *preprint: quant-ph/0010117*, www.arxiv.org.

[7] J. Kempe, "Quantum random walks – an introductory overview," *preprint: quant-ph/0303081*, www.arxiv.org.

[8] E. Feldman, M. Hillery, "Quantum walks on graphs and quantum scattering theory," *preprint: quant-ph/0403066*, www.arxiv.org.

[9] T. Kottos, U. Smilansky, "Periodic orbit theory and the spectral statistics for quantum graphs," *Ann. Phys.*, vol. 274, pp. 76-124, 1999.

[10] P. Kurasov, F. Stenberg, "On the inverse scattering problem on branching graphs," *J. Phys. A: Math. Gen.*, vol. 35, pp. 101-121, 2002.

[11] K. Ishii, "Localization of Eigenstates and Transport Phenomena in the One-Dimensional Disordered System," *Prog. Theor. Phys. Suppl.*, no. 53, pp. 77-138, 1973.

[12] A.N. Bondarenko, V.A. Dedok, "Inverse scattering problem on quantum graphs in optical tomography technology," *The 7th Korea-Russian International Symposium on Science and Technology. University Ulsan, Republic Korea*, vol. 3, pp. 105-110, 2003.

[13] A.N. Bondarenko, V.A. Dedok, "Surgery of quantum graphs," *The 8th Korea-Russian International Symposium on Science and Technology. Tomsk. Russia.*, vol. 2, pp. 108-111, 2004.

[14] N. Bondarenko, V.A. Dedok, "Spectral surgery of quantum graphs", Sib. Journ. Ind. Math., vol. 7, no. 4(20), pp. 16-28, 2004.