

## QUANTUM GRAPH OF SIERPINSKI GASKET TYPE IN ELECTRIC FIELD

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**ABSTRACT.** Quantum graph of Sierpinski gasket type with attached leads in an electric field is considered. We study the dependence of the transmission coefficient via the wave number of the quantum particle. It has strongly resonance character. The influence of the amplitude and the orientation of the electric field on the coefficient is investigated.

### 1. Introduction

Before the beginning of the twentieth century continuous mathematical objects were the main tool for scientific investigations. Classical analysis established a numerous new directions such as topology, differential geometry, functional and harmonic analysis and many others. That directions are actively developed in our days and seemingly will be dominating directions in the field of mathematical sciences in future.

At the same time, it has become clear that objects of nature has much more irregular structure than the objects of the classical analysis. A special interest is attracted by self-similar sets, or, as they are called, fractals (self-similarity, generally speaking, does not necessarily mean a linear similarity, and its synonym in this case is the word “like”). Of course, self-similar sets were studied in analysis earlier (e.g., the well-known Cantor set). But the intensive investigation started after the publication in 1977 of Mandelbrot book “The Fractal Geometry of Nature” [12] where the term “fractal” was introduced.

One can observe self-similarity in nature for different objects, e.g., leaves, trees, or patterns on animal skins. However, no existing object is completely self-similar, so fractals are only an approximation of real objects. Note that even a small change in the set of fractal parameters changes it dramatically, for example, leaf of fern and Sierpinski gasket presented in Figure 1, are fractals of the same type, differing by only a few parameters.

To describe physical phenomena related with the fractal-like objects, one needs the “analysis on fractals”. For example, the thermal diffusion is described

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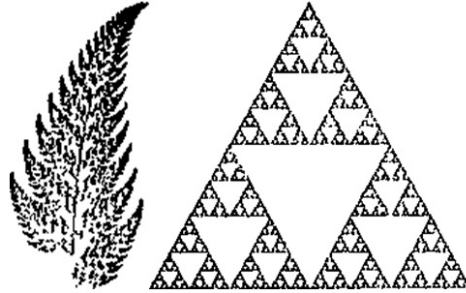


FIGURE 1. Simple fractals(fern's leaf and Sierpinski gasket)

by the heat equation

$$\frac{\partial u}{\partial t} = \Delta u,$$

where  $u = u(t, x)$ ,  $t$  is time,  $x$  is a coordinate vector and  $\Delta$  is the Laplace operator:  $\sum_{i=1}^n \frac{\partial^2}{\partial x_i^2}$ . Correspondingly, we need the Laplacian on a fractal set. However, fractals, like the Sierpinski gasket or the Koch curve, do not have a smooth structure and the conventional way of the derivative definition fails. There is a number of works dealing with the Laplace operator definition and properties.

One of the approaches to the definition of the Laplacian was considered in [6, 7, 8] by Kigami (it is so-called analytical approach). It can be used to describe the structure of harmonic functions, the Green's function and the solution of the Poisson equation. Here we consider a sequence of discrete Laplacians on graphs: let  $l(V_m) = \{f : V_m \rightarrow R\}$ . Then we define the linear operator  $L_m : l(V_m) \rightarrow l(V_m)$ , where

$$(L_m u)(p) = \sum_{q \in V_{m,p}} (u(q) - u(p))$$

for any  $u \in l(V_m)$  and any  $p \in V_m$ . This operator  $L_m$  is the discrete Laplacian on the graph  $G_m$ . This definition is given for a discrete graph. In the present paper we deal with a metric graph, more precisely, a quantum graph. The corresponding definition is given in the next section.

Another way to define the Laplacian is the so-called probabilistic method. Particularly, it was considered by Kusuoka in [9], where the "Brownian motion" on the Sierpinski gasket is constructed. Namely, Kusuoka considered a sequence of random steps on the graphs that are close to the Sierpinski gasket, and showed that the choice of a certain scale random steps are close to a diffusion process on the Sierpinski gasket. The work of Kusuoka was pioneering among papers in which the Laplacian on such a set was introduced.

An analytical result concerning to the Laplacian construction was obtained by Kigami in [6] using the Dirichlet Forms. See also book [8].

Later, the spectral properties of the Laplacian on the Sierpinski gasket was studied by Teplyaev in [15]. In particular, he gave the rigorous proof of the formulas describing the spectrum and the projection operators to the eigenspaces for the quantum graph, like the Sierpinski gasket. He also describes the eigenvectors and eigenvalues for such graphs.

The scattering problem for the Schrödinger equation arises in many physical situations. The Schrödinger operator is the quantum analogue of the classical evolution operator. The quantum graph is a popular model for studying the quantum dynamics in mesoscopic system (see, e.g., [4], [11], [14] and references therein).

This shows the importance of the problem of constructing the scattering matrix for fractal lattices. The solution of this problem in the lack of an electric field was considered by Blinova, Popov and Sandler in [2], as well as Bondarenko and Dedok in [3]. As a result, recurrence formulas have been obtained for the scattering matrices.

At the same time, the scattering problem for such graphs in the presence of an electric field has not been studied yet. The solution of this problem is the aim of this work. We construct a solution of the single-particle Schrödinger equation in the homogeneous electric field on the edges, take into account the Kirchhoff conditions at the vertices of the quantum graph and construct the solution of the scattering problem. We construct the scattering matrix and investigate the dependence of the transmission and the reflection coefficients on the wave number  $k$ . We consider the resonance effects, i.e., a strong change in the coefficients under small change in the parameters. Such dependence is described for different values of the amplitude and the direction of the field.

## 2. Model of Sierpinski gasket quantum graph

In this work we will study a quantum graph in electrical field. The quantum graph is a metric graph with a Hamiltonian determined on it. To describe the model, let us introduce some definitions related to graphs.

Graph  $G(V, B)$  consists of a nonempty set  $V$  (the set of vertices) and set  $B$  of unordered pairs of different elements of the set  $V$ .  $B$  is the set of edges (bonds). If the set  $B$  consists of ordered pairs, then the graph is called oriented. We are interested in a model of non-oriented graph.

For given vertices  $i$  and  $j$  we denote as  $[i, j]$  an undirected edge connecting vertices  $i$  and  $j$ ; in this case,  $b = [i, j] = [j, i]$ . Vertex  $i$  and edge  $[i, j]$  are called the incident;  $j$  and  $[i, j]$  are incident too. Now, we need to consider non-compact graphs, meaning graphs consisting of a compact part (a finite number of edges of finite lengths) and infinite edges, connected with some vertices. For infinite edges we use the notation  $(i, \infty)$ .

The number of edges  $[m, i]$  having a common vertex  $i$ , is called the degree (valence) of vertex  $i$ .

We associate the interval  $[a_i, a_j] = [0, l_{(i,j)}]$  of the corresponding length with each edge  $(i, j)$  of finite length. We associate a semi-axis  $[0, \infty) = [a_k, \infty)$  with each infinite edge. We denote the coordinate on the edge  $[a_i, a_j]$  by  $x_{(i,j)} \in [a_i, a_j]$  (similarly, for  $x_{(i,\infty)} \in [a_i, \infty)$ ), assuming, by definition, that  $x_{(j,i)} = l_{(i,j)} - x_{(i,j)}$ . We construct our model using these definitions.

We name a graph that correlates to Sierpinski gasket  $n$ -th rank as the  $n$ -th iteration graph. Also we call vertices, connected with four edges, the internal vertices. There are  $2 * 3^n$  such vertices. There are three vertices, connected with 2 edges only. These vertices are named the external vertices. We assume also that there are half-lines (infinite edges) connected with these vertices. Ultimately, such graph consists of  $3^n$  finite edges and 3 infinite edges. Generally speaking, such a graph should contain  $\frac{3^n+3}{2}$  vertices. However, it is easy to calculate that all internal vertices are merging all four edges incident to this vertex, external vertices are joining of ends of two finite edges and one half-infinite edge. We will correlate two variables with each vertex – one will represent the value of the function at our vertex, another – the value of its derivative. We will identify the first type of our variables by expressions “ $f_1$ ”, “ $f_2$ ” and so forth; the second type – by “ $g_1$ ”, “ $g_2$ ” and so on. We assume all edges equal.

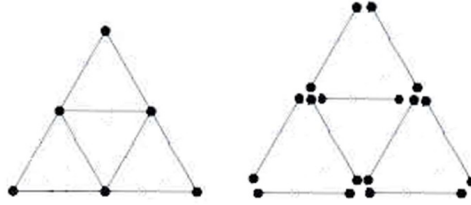


FIGURE 2. Model of the graph of second rank in the cases when we consider one common vertex for incident edges (simple graph) and when we consider all edges ends

We can consider the scattering problem on our graph as follows. Suppose that each semi-infinite edge is input - output for quantum particles. We consider the one-particle scattering problem and choose one of these edges, calling it the “input”. We will call “outputs” another self-infinite edges. Also, we assume that the particle can get from the outside only through this “input” (it does not violate the generality, since our graph is symmetric by the symmetry of an equilateral triangle). Then, we obtain the problem of scattering by a triangle with three outputs (see Fig. 3).

We assume that the uniform electric field is only within finite edges of the graph. Then, at each edge of the graph, we can represent the 1D potential as a potential for the projection of the vector electric field  $\vec{E}$  to the relevant edge:

$$E_x = (\vec{E}, \vec{x}).$$

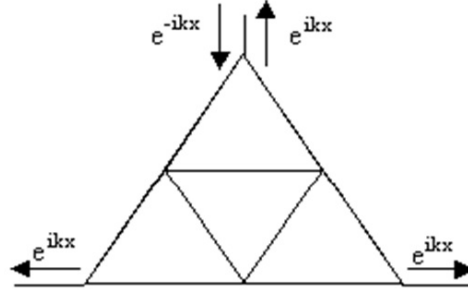


FIGURE 3. Transmitting and reflected waves on the graph

Here  $x$  is the coordinate along this edge,  $|\vec{x}| = 1$ . The change of the direction of the vector field is equivalent to a rotation of our graph in the space (if our graph is embedded in 2D). The direction will specify by an angle from 0 to  $\pi$ , where zero corresponds to the field directed vertically downward (in accordance with Fig. 3),  $\pi/2$  - the field is directed from left to right,  $\pi$  - the field is directed vertically upwards.

The Hamiltonian  $H$  acts in

$$\mathcal{H} = \left(\oplus \sum_{j=1}^k L_2(a_{2j-1}, a_{2j})\right) \oplus \left(\oplus \sum_{i=1}^3 L_2[a_i, \infty)\right).$$

It is the orthogonal sum of the operators defined on each edges:

$$H\psi = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi - E_x x \psi,$$

where  $\hbar$  is the Planck's constant,  $m$  is the particle mass. The domain of the operator is as follows

$$(1) \quad \text{dom } \mathcal{H} = \left\{ \psi \mid \psi \in C(\Gamma) \cap H^2(\Gamma - V), \sum_{e \in B_v} \frac{d\psi}{dx_e}(v) = 0 \right\}.$$

Here  $H^2$  is the Sobolev space ( $W_2^2$ ).

To find the solution of the scattering problem, we should solve the Schrödinger equation at each edge:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi - E_x x \psi = k^2 \psi.$$

By simple replacement of variable (see, e.g., [10], [13]),

$$\xi = \left(\frac{2mE_x}{\hbar^2}\right)^{\frac{2}{3}} \left(x + \frac{k^2}{E_x}\right),$$

we transform our equation to the Airy equation  $\psi'' + \xi\psi = 0$ . The general solution is a linear combination of the Airy functions:

$$\psi(x) = AAi(-\xi) + BBi(-\xi).$$

Consider the basic cell for our graph, i.e., the triangle with three connected leads (Fig. 4).

We assume that the electric field acts at the triangle only and does not act at the attached leads. Correspondingly, the solution at the leads 1, 2, 3 has the form

$$\psi_j = C_j \exp ikx + D_j \exp -ikx, j = 1, 2, 3.$$

At the edges 12, 23, 13 (of lengths  $L$ ) one has the Schrödinger operator with the electric field. Let the angle between  $\mathbf{E}$  and edge 13 is  $\alpha$ . Then, the corresponding projections are:  $E_{12} = E \cos(\alpha - \pi/3)$ ,  $E_{23} = E \cos(\alpha + \pi/3)$ ,  $E_{13} = E \cos \alpha$ . At each edge, we replace the variable:

$$\xi_{jn} = (x + \frac{k^2}{E_{jn}})(\frac{2mE_{jn}}{\hbar^2})^{2/3} = qE_{jn}^{2/3}(x + \frac{k^2}{E_{jn}}), \quad q = (\frac{2m}{\hbar^2})^{2/3}$$

which leads to the Airy equation. The solution is

$$\psi_{jn}(x) = A_{jn}Ai(-\xi_{jn}) + B_{jn}Bi(-\xi_{jn}),$$

where Ai, Bi are the Airy functions.

To find the reflection and transmission coefficients for the basic cell, we consider the conditions at vertices. It leads to the following system:

$$\begin{aligned} C_1 + D_1 &= A_{12}Ai(-qk^2E_{12}^{-1/3}) + B_{12}Bi(-qk^2E_{12}^{-1/3}), \\ C_1 + D_1 &= A_{13}Ai(-qk^2E_{13}^{-1/3}) + B_{13}Bi(-qk^2E_{13}^{-1/3}), \\ ikC_1 - ikD_1 - A_{12}E_{12}^{2/3}qAi'(-qk^2E_{12}^{-1/3}) \\ &\quad - B_{12}E_{12}^{2/3}qBi'(-qk^2E_{12}^{-1/3}) - A_{13}E_{13}^{2/3}qAi'(-qk^2E_{13}^{-1/3}) \\ &\quad - B_{13}E_{13}^{2/3}qBi'(-qk^2E_{13}^{-1/3}) = 0, \\ C_2 + D_2 &= A_{12}Ai(-qE_{12}^{2/3}(L + k^2E_{12}^{-1})) + B_{12}Bi(-qE_{12}^{2/3}(L + k^2E_{12}^{-1})), \end{aligned}$$

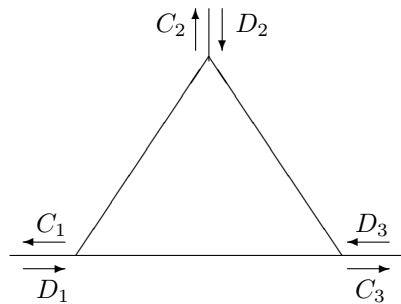


FIGURE 4. SG of 0 order

$$\begin{aligned}
 C_2 + D_2 &= A_{23}\text{Ai}(-qk^2E_{23}^{-1/3}) + B_{23}\text{Bi}(-qk^2E_{23}^{-1/3}), \\
 ikC_2 - ikD_2 + A_{12}E_{12}^{2/3}q\text{Ai}'(-qE_{12}^{2/3}(L + k^2E_{12}^{-1})) \\
 &+ B_{12}E_{12}^{2/3}q\text{Bi}'(-qE_{12}^{2/3}(L + k^2E_{12}^{-1})) \\
 &- A_{23}E_{23}^{2/3}q\text{Ai}'(-qk^2E_{23}^{-1/3}) \\
 &- B_{23}E_{23}^{2/3}q\text{Bi}'(-qk^2E_{23}^{-1/3}) = 0, \\
 C_3 + D_3 &= A_{13}\text{Ai}(-qE_{13}^{2/3}(L + k^2E_{13}^{-1})) + B_{13}\text{Bi}(-qE_{13}^{2/3}(L + k^2E_{13}^{-1})), \\
 C_3 + D_3 &= A_{23}\text{Ai}(-qE_{23}^{2/3}(L + k^2E_{23}^{-1})) + B_{23}\text{Bi}(-qE_{23}^{2/3}(L + k^2E_{23}^{-1})), \\
 ikC_3 - ikD_3 + A_{13}E_{13}^{2/3}q\text{Ai}'(-qE_{13}^{2/3}(L + k^2E_{13}^{-1})) \\
 &+ B_{12}E_{13}^{2/3}q\text{Bi}'(-qE_{13}^{2/3}(L + k^2E_{13}^{-1})) \\
 &+ A_{23}E_{23}^{2/3}q\text{Ai}'(-qE_{23}^{2/3}(L + k^2E_{23}^{-1})) \\
 &+ B_{23}E_{23}^{2/3}q\text{Bi}'(-qE_{23}^{2/3}(L + k^2E_{23}^{-1})) = 0.
 \end{aligned}$$

Of course, this system can be solved explicitly, but for computation, it is more suitable to solve it numerically when it is needed in the procedure (it is very fast process). The solution of the system can be represented in the following form (it is a conventional form for any linear system with three inlets (which are outlets simultaneously)):

$$\begin{aligned}
 (2) \quad C_1 &= a_{11}D_1 + a_{12}D_2 + a_{13}D_3, \\
 C_2 &= a_{21}D_1 + a_{22}D_2 + a_{23}D_3, \\
 C_3 &= a_{31}D_1 + a_{32}D_2 + a_{33}D_3,
 \end{aligned}$$

where  $D_i, C_i, i = 1, 2, 3$  - are amplitudes of input and output waves on each input respectively (see above) and coefficients  $a_{jm}$  are simply computed by solving the previous system. This representation is appropriate not only for the triangle graph (SG on zero order) but for the SG graph of any order. One can see that if there is no electric field, the problem has a symmetry property and the system (2) can be essentially simplified:

$$\begin{aligned}
 C_1 &= \beta(D_2 + D_3) + \alpha D_1, \\
 C_2 &= \beta(D_1 + D_3) + \alpha D_2, \\
 C_3 &= \beta(D_1 + D_2) + \alpha D_3,
 \end{aligned}$$

where  $\alpha(k)$  and  $\beta(k)$  are complex coefficients of reflection and transmission, correspondingly.

Having a solution of the system for the triangle graph in the form (2) with  $a_{jm} = a_{jm}^0$  ("0" means the order of the SG), one can consequently obtain the solution for the SG of  $n$ -th order, i.e., to get the recurrent relation for the coefficients  $a_{jm}^n$ . To do this, it is necessary to consider a graph composed from the triangles (i.e., from the SG of  $n - 1$ -th order), see Fig. 5.

For the case of absence of the electric field, the recurrent formulas have simple forms (see [2]), namely, for the reflection ratio:

$$\alpha_n = \alpha_{n-1} + \frac{2\beta_{n-1}(\alpha_{n-1} + \frac{\beta_{n-1}^2}{1-\alpha_{n-1}})}{1 - (\alpha_{n-1} + \beta_{n-1})(\alpha_{n-1} + \frac{\beta_{n-1}^2}{1-\alpha_{n-1}})},$$

and for the transmission ratio:

$$\beta_n = \frac{(1 + \frac{\beta_{n-1}}{1-\alpha_{n-1}})\beta_{n-1}^2}{1 - (\alpha_{n-1} + \beta_{n-1})(\alpha_{n-1} + \frac{\beta_{n-1}^2}{1-\alpha_{n-1}})}$$

for SG of  $n$ th order, by terms of SG of  $(n - 1)$ -th order.

### 3. Discussion

Let us perform a numerical investigation of the reflection ratio depending on the wave number  $k$ , for SG of  $n$ -th order. More or less obvious method for the transmission ratio calculation is explicit solving of the linear system arising from the boundary conditions. Still this approach has essential drawback, the number of calculations grows exponentially when increasing the SG order. We will use another method. It is based on ideas described in the previous section. Let us consider SG of the zero order. Its behaviour is described by 9 equations with twelve unknowns (there are three equations for each node). Such a redundancy of unknowns could be explained by the fact that any entering waves may be arbitrary, and after that state of all leaving and interior waves could be determined unambiguously. By eliminating unknowns describing waves on the interior edges one could get 3 equations with 6 unknowns.

Now we could analyze SG of  $n$ -th order, it is constructed from three SG of  $(n - 1)$ -th order and for each of them one already knows describing equations, moreover some unknowns from one SG are unknowns from another. Connecting

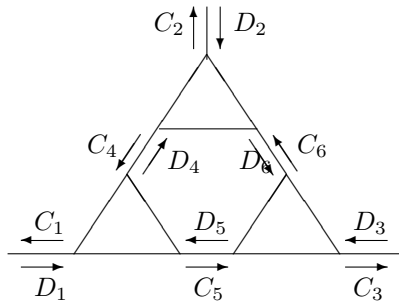


FIGURE 5. SG of  $n$ -th order composed of three SG's of  $(n - 1)$ -th order, nonzero distance between SG's is added only for better clearance, this distance gives zero phase shift



all them together, as we do it in the previous section, we would receive 9 equations with 12 unknowns. After that, we may eliminate unknowns describing interior edges, and thus we would get 3 equations with 6 unknowns describing system of  $n$ -th order already. By continuing this iteration procedure, we can find the linear system describing SG of any order. In the electric-field case the recursion formulas were obtained, but they are too complex to be printed in the text. In addition to symmetric SG (as in the case of the electric field absence), such approach allows one to introduce local heterogeneities (such as changing lengths of some edges, or adding a point-like potential into nodes).

Let us describe some numerical results. Recall that the graph edge is taken 1. The dependence of the transmission coefficient on the wave number  $k$  has strongly resonance character. To describe the behavior, it is more convenient to use a logarithm of the coefficient instead of the coefficient (see Fig. 6, 7).

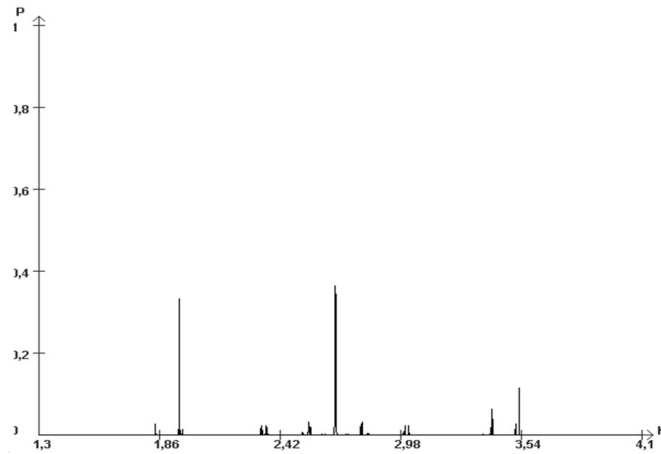


FIGURE 6. The transmission coefficient via  $k$  for the SG of the sixth order.

The increasing of the SG order leads, naturally, to the decreasing of the transmission. One can observe the effect of the resonance (i.e., the value of  $k$  for which the transmission is close to one) conservation. At the same time new resonances appear. See Fig. 8.

In the case of electric field we have no symmetry in the transmission coefficients. We will call the transmission coefficient that corresponds to the transmission from the bottom left input to the top output by “the left transmission coefficient” (the right transmission coefficient, correspondingly, is that from the bottom right input to the top output). Fig. 9 shows the variation (and shift to the left) of the left transmission coefficient under the increasing of the amplitude of the electric field  $E$ ,  $\theta = 0$ ,  $\theta$  is the angle between the field vector and the normal to the bottom of the triangle. Here and below we show

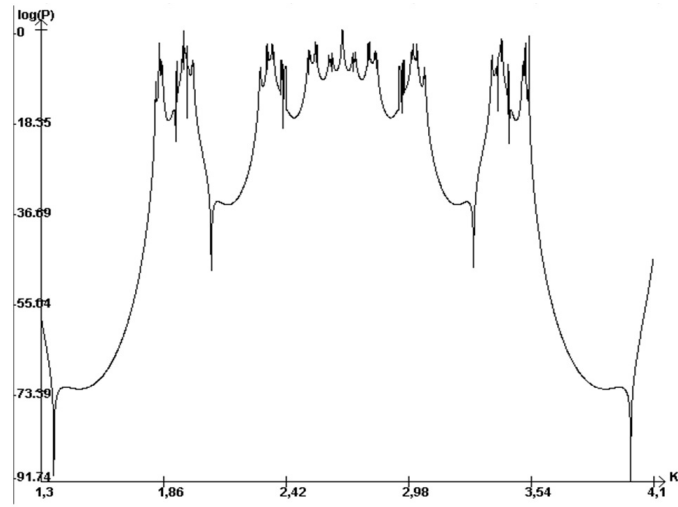


FIGURE 7. The logarithm of the transmission coefficient via  $k$  for the SG of the sixth order.

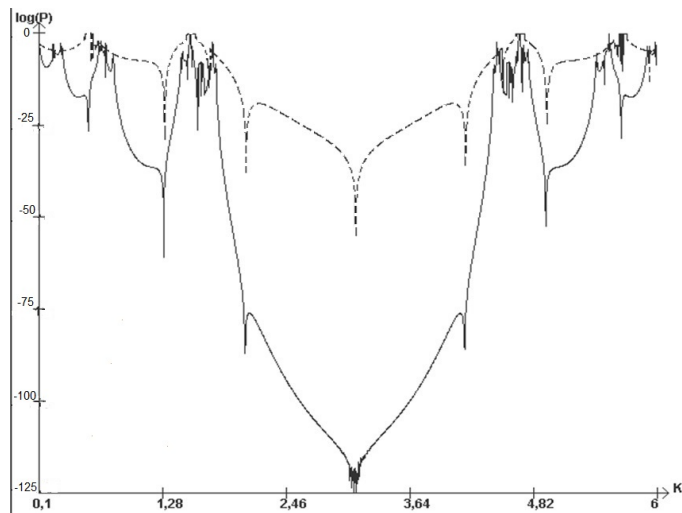


FIGURE 8. Conservation of resonances with increasing of the SG order from the third (dashed line) to the fifth (solid line)

pictures for the SG of the sixth order. The shift of resonances in this situation is shown better in the logarithmic scale (Fig. 10).

If one varies the angle  $\theta$ , then the shift of the peaks is also observed (Fig. 11)

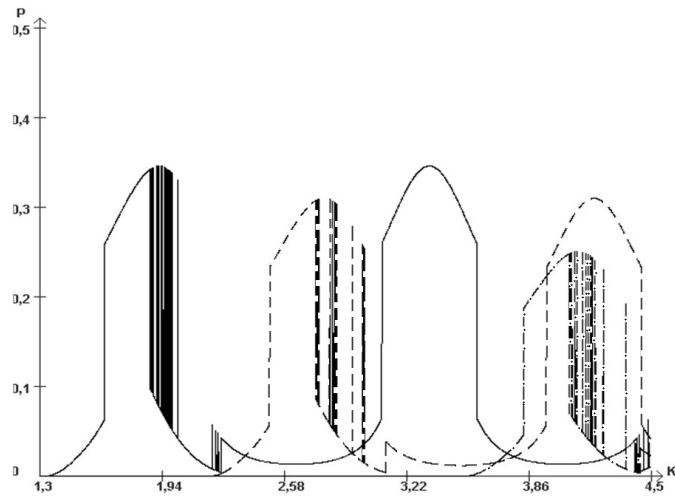


FIGURE 9. Variation of the left transmission coefficient with increasing field resulted in a shift of peaks passing to the left;  $E = 1$  - dash-dot line,  $E = 5$  - dashed line,  $E = 10$  - solid line.

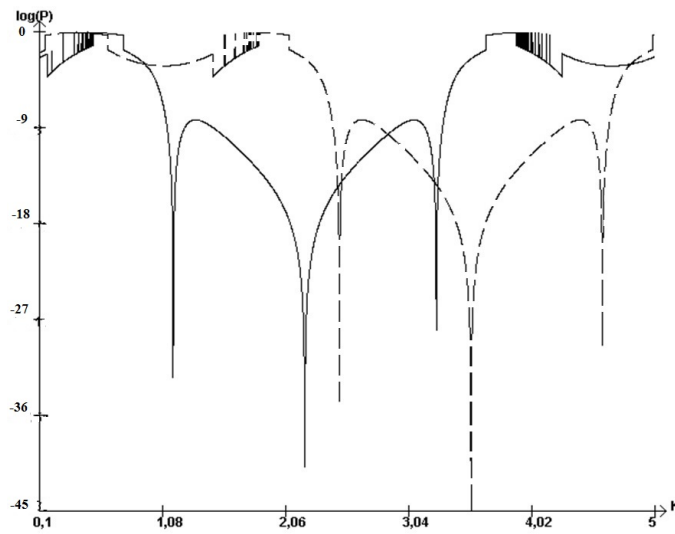


FIGURE 10. Variation of the left logarithmic transmission coefficient as the field increases with a shift of resonances to the left;  $E = 1$  - dashed line,  $E = 20$  - solid line.

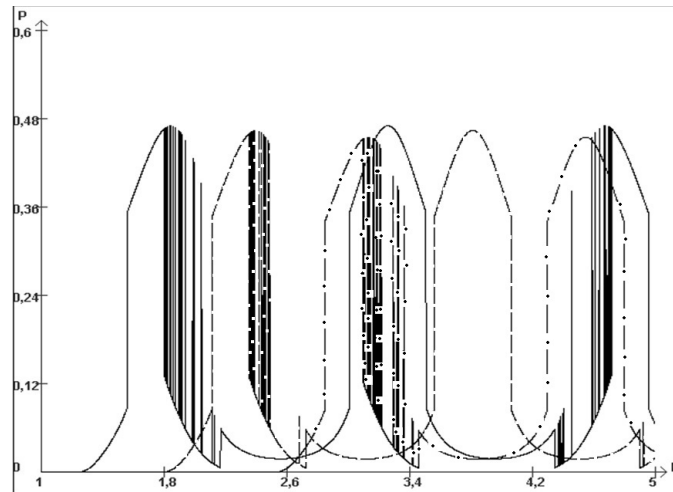


FIGURE 11. Change of the left transmission coefficient when the angle varies:  $\theta = 0$  - dash-dot line,  $\theta = \pi/18$  - dashed line,,  $\theta = \pi/9$  - solid line;  $E = 100$ )

One can observe the corresponding behavior for the right transmission coefficient. As has been mentioned, we showed the pictures for the sixth order SG. Our approach allows us to obtain the corresponding results for the graphs up to the fifteenth order (the effects are similar, but the number of resonances is, of course, greater).

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