Statistical properties of semiclassical solutions of the non-stationary Schrödinger equation on metric graphs.

V.L. Chernyshev[1,2] joint work with A.I. Shafarevich[1]

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Analysis on Graphs and its Applications Follow-up Meeting 2010

Outline

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The problem that we studied

We study properties of a time-dependent Schrödinger equation, in which the spatial variable varies within a metric graph Γ.

$$ih\frac{\partial\psi(x,t)}{\partial t} = -h^2\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x,t)\psi(x,t) \qquad (1)$$

We study properties of asymptotic, as $h \to 0$ (semiclassical), solutions.

The main effect of the related "branching" of the space is in the multiple reflection at the vertices of the graph, which leads to the occurrence of nontrivial statistical phenomena.

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These properties become especially clear when describing Gaussian packets (which were originally localized near a single point).

As initial data we have

$$\psi(x,0) = K \exp\left(\frac{i(a(x-x_0)^2 + b(x-x_0)+c)}{h}\right). \quad (2)$$

Here K, b and c are real numbers, $Im(a) > 0$.

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Terms and definitions

A *graph* Γ consists of a finite set $\mathcal{E}$ of intervals γ_j, $j = 1, \ldots, E$ called *edges*, and a partition of the set $\mathcal{V} = \{x_j\}$ of endpoints of the edges. The equivalence classes V_n, $n = 1, \ldots, V$ will be called *vertices* and the number of elements of V_n will be called the *valence* of V_n.

Every edge is identified with an interval of the real line. We introduce the space $L^2(\Gamma)$ of square integrable functions on the graph

$$L^2(\Gamma) = \oplus \sum_{j=1}^{E} L^2(\gamma_j)$$

with a standard scalar product

$$(f, g) = \int_{\Gamma} f(x)\overline{g(x)}dx. \tag{3}$$

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Definition. Let q be an arbitrary real valued continuous function on Γ, smooth on the edges. Then the *Schrödinger operator*

$$\widehat{H}\psi = -h^2 \frac{\partial^2 \psi(x)}{\partial x^2} + q(x)\psi(x) \tag{4}$$

is defined on the domain of functions from the Sobolev space $\psi \in H^2(\Gamma \setminus V) = \oplus \sum_{j=1}^{E} H^2(\gamma_j)$ satisfying the following boundary conditions at the vertices

1. ψ is continuous on Γ,
2. $$\sum_{x_j \in V_m} \alpha_j \frac{\partial \psi_j}{\partial x}(x_j) = 0, \quad \alpha_j \in \mathbb{R}, \quad m = 1, 2, \dots, V - K, \tag{5}$$
   at all inner vertices, *i.e.* vertices of the valence greater than one,
3. $\psi(a) = 0$ at all boundary vertices, *i.e.* having valence 1.

Definition. The *Neumann* transmission conditions can be written explicitly using normal derivatives $\partial_n \psi$ as

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Packet on a line

Let us first recall the scheme of constructing semiclassical Gaussian packets on a line.

V. P. Maslov, The Complex WKB Method for Nonlinear Equations. I. Linear Theory (Birkhäuser, Basel, 1994).

Proposition. The function

$$\psi(x,t) = \frac{K}{\exp\left(\int\limits_0^t \frac{p_l(t)}{q_l(t)}dt\right)} \exp\left(\frac{i(S_0(t) + S_1(t)(x - X(t)) + S_2(t)(x - X(t))^2)}{h}\right) \quad (6)$$

is a solution of Schrödinger equation up to $O(h^{3/2})$. Here

$$S_0(t) = c + \int\limits_0^t ((P(t))^2 - V_0(t))dt, \quad (7)$$

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$X(t)$ and $P(t)$ are solutions of the Hamiltonian system

$$\begin{aligned} \dot{X}(t) &= H'_p(X(t), P(t)) \\ \dot{P}(t) &= -H'_x(X(t), P(t)), \end{aligned} \tag{10}$$

with the initial data $X(0) = x_0$, $P(0) = b$,
The pair $q_l(t)$, $p_l(t)$ is a solution of the linearized system

$$\begin{aligned} \dot{q}_l &= 2p_l \\ \dot{p}_l &= -\frac{\partial^2 V}{\partial x^2} q_l. \end{aligned} \tag{11}$$

One can take the initial data for this system in the form $q_l(0) = 1$, $p_l(0) = 2a$.

On each edge the solution is constructed using two Hamiltonian systems, one of which determines the velocity of the packet, while the second, determines the shape of the packet.

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Propagation of Gaussian packets on an arbitrary graph.

Proposition

Let Γ be a star graph, with the single vertex a of valence n. Let the initial data have the form (2), where the point x_0 is on one of the egdes. Then solution of

$$\widehat{H}\psi(x,t) = ih\frac{\partial\psi(x,t)}{\partial t} + O(h^{3/2})$$

is, in any finite time, a finite sum of Gaussian packets, i.e. functions of the form $\exp\left(\frac{iS^j(x,t)}{h}\right)\varphi^j(t)$,
$S^j = S_0^j(t) + (x - x_j(t))S_1^j + S_2^j(x - x_j(t))^2, \;\; Im\, S_2^j > 0.$

The packet that came to the vertex a is divided into n packets traveling on the edges. At each of the edges the solution is determined by two Hamiltonian systems.
The initial values for the amplitudes are determined by the following formulas.
For the "reflecting" Gaussian packet:

$$\varphi_0^{(1,2)}(\beta) = \frac{\alpha_1 - \alpha_2 - \cdots - \alpha_n}{\alpha_1 + \alpha_2 + \cdots + \alpha_n} \varphi_0^{(1,1)}(\beta). \qquad (12)$$

For the "transmitted" Gaussian packets:

$$\varphi_0^{(k,1)}(\beta) = \frac{2\alpha_1}{\alpha_1 + \alpha_2 + \cdots + \alpha_n} \varphi_0^{(1,1)}(\beta), \qquad (13)$$

where $k = 2, \ldots, n$.
Here β is the time when the initial packet came to vertex a.

Propagation of Gaussian packets on an arbitrary graph.

If the operator $\widehat{H}$ is self-adjoint, then this solution differs from the exact solution of the non-stationary Schrödinger equation by not more than $O(h^{1/2})$.

Consider the Neumann transmission condition (the self-adjoint case). At vertex amplitude is divided in accordance with the following ratio: $2/n$ for each transmitted packet and $2/n - 1$ for reflected packet.

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These formulas enable us to describe the propagation in the case of an arbitrary graph. We obtain a solution of (1) on a subgraph of the original graph, and this subgraph contains the point at which the initial data are given.

$$\Psi(x,t)=\sum_{j=1}^{N(t)}\exp\left(\frac{iS^j(x,t)}{h}\right)\varphi^j(t).$$

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is a semiclassical solution of the Cauchy problem for the non-stationary Schrödinger equation with initial conditions of a special form.

We consider the asymptotical behavior of function $\Psi(x,\, t)$ as $t\to\infty$. Namely, we will see how the number of Gaussian packets $N(t)$ changes in time.

Note that this problem differs from the task of describing the asymptotic solution of the Schrödinger equation at $t\to\infty$, as the error estimation is valid only for finite times. From a physical point view, this means that we are considering big t, but much smaller than $1/h$.

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Preliminary remarks

- In this section, we consider only finite graphs with compact edges. We choose the transmission conditions at the vertices in such a way that the Schrödinger operator is self-adjoint.
- From formulas of the previous section it follows that, if a Gaussian packet passes through a vertex of degree v, then this leads to the occurrence of exactly v new Gaussian packets.
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Asymptotics for $N(t)$

The number of paths on a graph is growing exponentially with time. Question is: what will happen to the number of packets?

Asymptotics for $N(t)$

Theorem (1)

Let graph Γ be compact and clean. Suppose, moreover, that the numbers $t_1, \ldots t_E$ are linearly independent over the $\mathbb{Q}$. Then the function $N(t)$ with increasing t can be represented as

$$N(t) = Ct^{E-1} + o(t^{E-1}), \tag{14}$$

where C is a positive constant, and E is the number of edges in the graph.

Lemma about a star graph

Lemma. Consider a star graph.

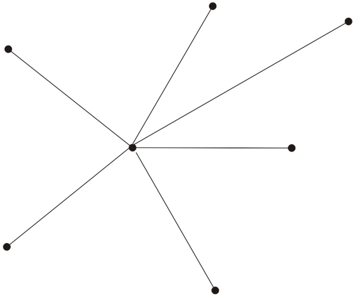


Figure: Star graph

Lemma about a star graph

The following formula holds for this graph:

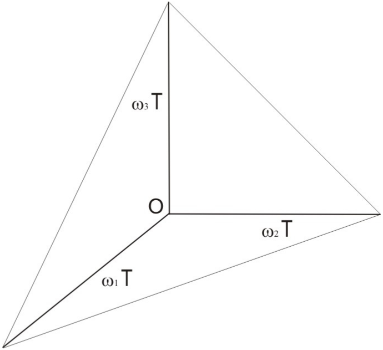
$$N(t) = \sum_{k=1}^{v-1} (v-k) \sum_{1 \le i_1 < i_2 < \cdots < i_k \le v} W\left(\triangle_k\left(\omega_1 t/2, \ldots, \omega_k t/2\right)\right), \tag{15}$$

here $W\left(\triangle_k\left(\omega_1 t/2, \ldots, \omega_k t/2\right)\right)$ is the number of integral points that are lying on the sides of a k-dimensional simplex $\triangle_k\left(\omega_1 t/2, \ldots, \omega_k t/2\right)$ with vertices $\omega_1 t/2, \ldots, \omega_k t/2$ on the coordinate axes. Only sides incidental to the origin of coordinates are taken into account, except for sides of lower dimension.

Lemma about a star graph

Writing out the leading asymptotic term, we obtain the formula

$$N(t) = \frac{1}{2^{v-1}(v-1)!}\frac{(t_1+\ldots+t_v)}{t_1\cdot\ldots\cdot t_v}t^{v-1}+o(t^{v-1}). \qquad (16)$$



Formula for the leading coefficient

Theorem (2)

Let Γ be a compact finite clean graph and consists of one connected component. Then for almost all linearly independent over $\mathbb{Q}$ numbers $t_1, \ldots t_E$, the leading coefficient, with increasing t, for the number of Gaussian packets can be determined by the following formula:

$$C = \frac{1}{2^{V-2}(E-1)!} \frac{\sum_{j=1}^{E} t_j}{\prod_{j=1}^{E} t_j}. \tag{17}$$

Here V is the number of vertices, and E is the number of edges in the graph.

Number-theoretical references

We take into account some number-theoretical assertions related to the evaluation of the number of points with integral coordinates occurring in an extending polyhedron. The results in this area strongly depend on the rationality or irrationality of the coordinates of the vertices of the polyhedron.

- The results in the rational case are related to the Ehrhart polynomials (and quasipolynomials) see
  E. Ehrhart, "Sur les polyèdres rationnels homothétiques à n dimensions", C. R. Math. Acad. Sci. Paris 254, 616-618 (1962).
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  For the references related to the current state of investigations in this area see:
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- The results related to the case of irrational coordinates originate from the Hardy and Littlewood paper "The Lattice Points of a Right-Angled Triangle", Proc. London Math. Soc. 20 (2), 15-36 (1921), where the case of a right-angled triangle on the plane was treated.

  For the references related to the current state of investigations in this area see:
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  M. M. Skriganov, "Ergodic Theory on SL(n), Diophantine Approximations and Anomalies in the Lattice Point Problem", Invent. Math. 132 (1), 1-72 (1998).

Outline

The number of packets on an interval posed on an edge.

Theorem (3)

Let Γ be a compact clean graph, which consists of one connected component. Consider an interval cd on one of the edges, with the passage time being equal to τ. Then for almost all linearly independent over $\mathbb{Q}$ numbers $t_1, \dots t_E$, denoting the time of passage of the edges,

$$\frac{N_{cd}(t)}{N(t)} \to \frac{1}{t_1 + t_2 + \cdots + t_E}\tau. \tag{18}$$

The number of packets on an interval posed on an edge.

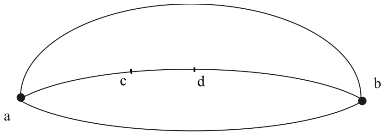

Figure: An example of graph with selected interval

The number of packets on an interval

Remark. Note that the Gaussian packets for almost all incommensurable t_j are uniformly distributed (for a given potential and given initial conditions) with respect to the time of passage of the edge. Obviously, this does not mean that the packets are uniformly distributed with respect to the spatial coordinate.

An open problem

An open problem: description of distribution of packets and calculation of asympotics for the number of packets when $t_j, j = 1 \ldots E$ are not linearly independent over $\mathbb{Q}$.

Propagation of energy on infinite regular rooted trees

Let us define an *energy on an edge* γ_j as

$$E_{\gamma_j} = \int\limits_{\gamma_j} |\psi^{(k,j)}(x,t)|^2 dx$$

Let us consider an infinite regular rooted tree.
The starting vertex has degree one. Other vertices all have the same degree v. All edges have the same length l.

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Energy on infinite regular trees

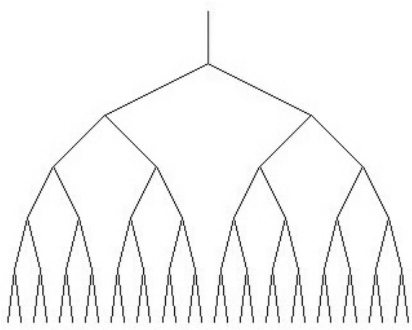

Figure: Binary tree.

Will $E_{\gamma_j} \to 0$ for all edges, as $t \to \infty$?

In the case of $v = 3$ (binary tree) a quarter of the energy will stay on the first edge. The half of the energy will stay on the first edges.

In the case of arbitrary valence v, $\frac{v-2}{v-1} E(0)$ will stay.

Figure: Energy vs levels of the tree, v=3.

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Energy E vs levels of the tree after 10000 steps. Cases of $b = 2$, $b = 3$ and $b = 4$.

l	$E, b = 2$	$E, b = 3$	$E, b = 4$
1	0,250000	0,444444	0,562499
2	0,125000	0,148148	0,140625
3	0,062500	0,049383	0,035156
4	0,031250	0,016461	0,008789
5	0,015625	0,005487	0,002197
6	0,007813	0,001829	0,000549
7	0,003906	0,000610	0,000137
8	0,001953	0,000203	0,000034
9	0,000976	0,000068	0,000009
10	0,000488	0,000023	0,000002
11	0,000244	0,000008	0,000001

Energy on infinite regular trees

Figure: Energy vs levels of the tree, v=11.

Thank you for your attention.

The work was partially supported by the grants MK-943.2010.1 and NSh-3224.2010.1.