dedicated to V.I.Arnold’s 60-th birthday

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Schrodinger Operators on Graphs and
Symplectic Geometry

Introduction. Hamiltonian Formalism of Analytical Mechanics has been systematically used after Poincare especially by people who created Quantum Mechanics in the 20’s. In pure mathematics, formalism of differential forms appeared as a by-product of Hamiltonian Theory formalized finally by E.Cartan. However, geometrical understanding of many important parts of Hamiltonian Formalism has not been elaborated on for a long period. For example, general definitions of such fundamental geometrical objects as Lagrangian Submanifolds in Symplectic (Hamiltonian) linear spaces (and in more general nonlinear symplectic manifolds as well) were finally formulated only in the 60’s. In particular, V.Arnold participated in this (see [1, 2]).

In the late 60’s, the present author observed that some algebraic version of Hamiltonian Formalism for rings with involutions plays a fundamental role in many constructions of Differential Topology (see [3]). As a reaction to this work, I.M.Gelfand observed (and pointed out to me in about 1971) that von Neumann’s construction of selfadjoint extensions for symmetric operators is based in fact on some Lagrangian planes in Hilbert spaces with symplectic scalar product.

The present work is in a sense a natural continuation of these old observations. An essential part of its results already was announced by the present author in a short note [4]. Let me point out here that we started at first to discuss graphs with A.Veselov as a continuation of a series of papers...
Discrete Schrödinger Operators on Graphs
Wronskians and Topology

We shall consider Graph $\Gamma$—i.e., one dimensional simplicial complex such that:

1. Only a finite number of edges $R_i$ (equal to $m_P$) can meet each other in any vertex $P$;
2. Graph $\Gamma$ has no ends, i.e. $m_P > 1$ for every vertex $P$. Two spaces of scalar complex-valued functions will be used:

The space of complex-valued functions $\psi_P$ depending on vertices $P$ and the space of functions $\psi_R$ depending on edges $R$. We do not formulate any global restrictions on these functions now.

We shall consider real self-adjoint (i.e. symmetric, in fact) operators $L$ acting on these spaces of functions:

\[
(L\psi)_P = \sum_{P,P'} b_{P,P'} \psi_{P'}, b_{P,P'} = b_{P',P} \quad (1)
\]
\[
(L\psi)_R = \sum_{R,R'} d_{R;R'} \psi_{R'}, d_{R,R'} = d_{R';R} \quad (2)
\]

Reality means that all coefficients are real.

**Definition 1** Operator $L$ will be called Finite Type iff for any point $P$ or edge $R$ there exists only a finite number of points $P'$ or edges $R'$ such that the coefficients above are nonzero. The Operator will be called an operator of Finite Order iff this number does not depend on $P$ or $R$. Order of operator is a maximal number of vertices (edges) in the minimal paths joining such pairs of vertices (edges) for which coefficients are nonzero. For the Second Order Operators on the vertices nonzero coefficients can be only $b_{P,P} = V_P$ and $b_{P,P'}$ iff $P \cup P' = \partial R$. In the case of edges nonzero coefficients can be only $d_{R,R} = V_R$ and $d_{R,R'}$ iff $R \cap R' \neq \emptyset$. We call coefficients $V_P$ and $V_R$ Potentials.
For any simplicial complex \( K \) and number \( k \) we have a boundary operator \( \partial \) from \( k \)-chains into \( k-1 \)-chains. We also have a scalar product where \( \delta \)-functions (i.e. functions taking value 1 on one of \( k \)-simplices only) give an orthonormal basis in subspace of finite chains (i.e. finite functions from \( k \)-simplices). Therefore we have an adjoint coboundary operator \( \partial^* \).

Combinatorial **Laplace-Beltrami Operators** \( \Delta_k \) on the spaces of \( k \)-chains are defined by the general formula

\[
\Delta_k = (\partial + \partial^*)^2 = \partial \partial^* + \partial^* \partial
\]

For the cases \( k = 0 \) and \( k = 1 \), Laplace-Beltrami operators on Graph \( \Gamma \) are the second order operators (Schrodinger Operators on the vertices and edges) such that

\[
\Delta_0 : b_{P,P'} = 1, P \bigcup P' = \partial R, V_P = -m_P
\]

\[
\Delta_1 : d_{R,R'} = 1, R \bigcap R' \neq \emptyset, V_R = -2
\]

**Example 1** Let Graph \( \Gamma \) is a line \( R^1 \), i.e., 1-simplices \( R \) and vertices \( P \) can be numerated naturally by the integers \( n \) such that boundary of the edge with number \( n \) is equal to the union of vertices with numbers \( n \) and \( n - 1 \). We always have \( m_P = 2 \) here. There is a natural one–to–one correspondance here between edges and vertices with the same numbers such that \( \Delta_0 = \Delta_1 \). Both operators can be considered as the same operator \( L_0 \) acting on the functions on the Lattice \( \mathbb{Z} \).

\[
(L_0 \psi)_n = \psi_{n-1} + \psi_{n+1}, n \in \mathbb{Z}
\]

\[-L_0 = \Delta_0 + 2 = \Delta_1 + 2\]

Two standard bases of solutions for the equation \( L_0 \psi = \lambda \psi \) can be given by the obvious formulas

\[
\psi_n^\pm = a_n^\pm, a_\pm = 1/2(\lambda \pm \sqrt{\lambda^2 - 4})
\]

\[
C_n = \frac{\psi_n^- a_+ - \psi_n^+ a_-}{a_+ - a_-}, S_n = \frac{\psi_n^+ - \psi_n^-}{a_+ - a_-}
\]

\[C_0 = 1, C_1 = 0, S_0 = 0, S_1 = 1\]

\[\psi^\pm = C + a_\pm S\]
More general operators $L$ on the Lattice $\mathbb{Z}$ appeared in the discretized Theory of Solitons (theory of Toda Lattice) beginning in 1974 (see in the survey and encyclopedia articles [7, 8]). They have form of the second order selfadjoint Schrodinger Operators on the graph $\Gamma = \mathbb{R}^1$ above

$$(L\psi)_n = c_{n-1}\psi_{n-1} + V_n\psi_n + c_n\psi_{n+1}$$

$$c_n = b_{n:n+1} = d_{n:n+1},$$

Solving the most fundamental problems of Spectral Theory for these operators for rapidly decreasing coefficients $c_n - 1, V_n$ and for periodic (quasiperiodic) coefficients, the so-called Wronskian for any pair of solutions has been used.

Our goal is to invent and to use a natural analog of this quantity for any finite order Schrodinger Operator on the arbitrary Graph $\Gamma$ satisfying to the conditions above.

Consider any pair of solutions $L\psi = \lambda\psi, L\phi = \lambda\phi$ on the Graph $\Gamma$.

**Definition 2** The following quantity will be called Wronskian for any pair of solutions.

**For vertices:**

$$W = \sum_R W_R$$

$$W_R(\phi, \psi) = b_{P:P'}(\phi_P\psi_{P'} - \psi_{P'}\phi_P)$$

$$P \cup P' = \partial R$$

**For Edges:**

$$W = \sum_R W_R$$

$$W_R(\phi, \psi) = \sum_{R'} d_{R:R'}(\phi_{R'}\psi_{R'} - \psi_{R'}\phi_{R'})$$

$$R \cap R' = P$$

We can see that our formula for the Wronskian is very much the same as for the line in the case of vertices, but for the edges it is less obvious. For example, it contains summation along the edges $R'$ meeting our edge $R$ in one point $P$ only. Second boundary point $P'$ where $\partial R = P \cup P'$ does not appear in the sum. Therefore, in this case the correctness of our definition should be proved.
Theorem 1. For any pair of solutions $\phi, \psi$ of the second order difference equation $L\phi = \lambda \phi, L\psi = \lambda \psi$, Wronskian is a well-defined 1-chain $W$ on the Graph $\Gamma$ (i.e. a complex-valued function of the oriented edges $R = PP'$) whose boundary is equal to zero

$$\partial W = 0 \quad (11)$$

Therefore our Wronskian belongs to the first homology group $H = H^\text{open}_1(\Gamma, \mathbb{Z})$ modulo infinity (if Graph is noncompact). It defines an $H$-valued skew symmetric scalar product on the spaces of solutions.

Proof. In the case of vertices, Wronskian is obviously well-defined as 1-chain. From the equality $(L\phi)_P\psi_P - (L\psi)_P\phi_P = 0$ we extract immediately that

$$\sum_{P' \cup P = \partial R'} W_{R'} = 0$$

Here the edges are taken with such orientation that they end in $P$. However, this equality means precisely that $\partial W = 0$ by definition of the boundary operator.

Consider now the case of edges. Our formula above defines correctly this quantity as $W_{R,P}$ depending on the edge $R$ and its vertex $P$. Starting from the same equality $(L\phi)_R\psi_R - (L\psi)_R\phi_R = 0$ for the pair of solutions, we can see that the left-hand part is obviously equal to the sum of two expressions. One of them is precisely equal to $W_{R,P}$ as it was defined above for the case of edges. The second one is equal to the analogous sum $W_{R,P'}$ with point $P$ replaced by $P'$. So we have

$$W_{R,P} + W_{R,P'} = 0 \quad (12)$$

Therefore we have $W_{R,P} = -W_{R,P'}$. Wronskian is well-defined as a 1-chain. Consider now the boundary of it.

$$(\partial W)_P = \sum_{P \in R} W_R =$$

$$= \sum_{R' \neq R} \sum_{R} d_{R,R'}(\phi'\psi' - \psi'\phi')$$

$$R' \cap R = P, \phi' = \phi_{R'}, \phi = \phi_R$$
However, in the last sum any fixed pair $R, R'$ appears twice with opposite signs. Therefore the total sum is equal to zero. Our theorem is proved. 

**Higher Order Operators:** For the case of higher order Schrodinger operators acting on vertices, we define Wronskian in the same way as for the second order operators. For any pair of interacting vertices $P, P'$, we fix one simple path

$$I_{PP'} = R_1, R_2, \ldots, R_k, \partial I = P \cup P'$$

(14)

Elementary 1-chain associated with interacting pair $PP'$ is defined as before. Full Wronskian is a sum of these expressions along all interacting pairs of vertices:

$$W = \sum_{I} W_I, W_I = b_{P,P'}(\phi_{P'}\psi_P - \psi_{P'}\phi_P)$$

(15)

$$\partial W = 0$$

As before, it is easy to prove that

$$W \in H_1^{open}(\Gamma, Z)$$

For the complex solutions $\psi_P$, one may consider Wronskian $W(\psi, \bar{\psi})$ as a **Quantum Current**; its Topological property to be 1-cycle is a **Kirchhoff Law**.

**Multidimensional Simplicial Complexes:** For the natural classes of Schrodinger operators acting on the spaces of $k$-chains in Simplicial Complexes $K$ with $k > 1$, we can define analogous quantity (Wronskian) as a function on the set of all pairs $W_{S_k, S_{k-1}}$ (here we have a $k$-simplex and its $k-1$-face). It is exactly the class of operators for which $k$-simplices can interact if they have common ($k-1$)-face. This is an exact definition of this class of operators and of the Wronskian:

$$W_{S_k, S_{k-1}}(\phi, \psi) = \sum_{S_k' \cap S_{k-1} = S_{k-1}} b_{S_k' : S_{k-1}}(\phi' \psi - \psi' \phi)$$

(17)

$$\psi' = \psi_{S_k'}, \psi = \psi_{S_k}$$

\textsuperscript{3}It is strange, but the present author was not able to find this elementary fact in the literature (I asked several experts in the theory of graphs and operators on them). It does not surprise me for the edges, but I cannot believe that this fact is new for the case of vertices.
The following theorem is true.

**Theorem 2** 1. The full sum of "Wronskians" along all $k-1$-faces of every $k$-simplex is equal to zero;

2. The full sum of "Wronskians" along all $k$-simplices with common $k-1$-face is also equal to zero.

Proof of this theorem is exactly the same as for $k = 1$.

**Remark 1** For nontrivial applications of the theorems above we need to consider such classes of operators that for some $\lambda$ the space of solutions is at least 2-dimensional, otherwise our Wronskian will be identically equal to zero. There are two natural sources for that for the graphs:

1. Graph $\Gamma$ and operator $L$ admit nontrivial symmetry group.

2. Graph $\Gamma$ has several number of "Tails" at infinity and operator $L$ has asymptotically constant coefficients. It is exactly a case for which Scattering Theory can be developed. We shall do this in the next paragraph. In particular, we shall demonstrate that "Unitarity" of Scattering follows from the Topological Property of Wronskians established above.

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**Scattering Theory for Graphs with Tails and Symplectic Geometry**

We consider graphs with $k$ tails here. It means precisely that outside of the finite domain this Graph is isomorphic to the union of $k$ positive half lines ("Tails") $z_1, z_2, \ldots, z_k$. Let us choose some initial vertices $P_j, j = 1, 2, \ldots, k$ in these tails and attribute to them the number of the tail and zero. Other vertices in the same tail behind $P_j$ will be naturally numerated by the number of the tail and positive integers $n \in \mathbb{Z}^+$. We attribute to the edge $R = (n, n - 1)$ number $n$, as in paragraph 1 for the line, $n = 0, 1, 2, \ldots$.

Any Graph $\Gamma$ with $k$ tails can be naturally represented in unique way as a union of the finite subgraph without ends $\Gamma' \subset \Gamma$ with some number of Trees attached to it in the vertices $Q_l, l = 1, \ldots, s$. Obviously we have $s \leq k$ because every tree contains at least one tail (maybe more).
**Definition 3** We call Graph $\Gamma'$ the **Basis** of our Graph $\Gamma$. Points $Q_l$ from which Trees grow up in the Graph $\Gamma$ will be called **Nests**. Several trees can grow up from one nest. Connected Graph $\Gamma$ is Topologically trivial iff its basis $\Gamma'$ is equal to one point. We call graphs $\Gamma$ with $k$ tails **Diagrams** for which Scattering Processes naturally can be defined.

Consider now a class of second order Schrödinger Operators $L$ on Graph $\Gamma$ with $k$ tails acting on the vertices or on the edges such that outside of the finite domain we have in the tails for $n \geq n_0$ and all $j = 1, \ldots, k$:

$$-L = -L_0 = \Delta_i + 2, i = 0, 1 \quad (18)$$

Outside of this finite ”domain of interaction” our equation $L\psi = \lambda\psi$ has solutions in the tails $\psi_{jn}^\pm$ and $C_{jn}, S_{jn}$ for $j = 1, \ldots, k$ and $n > n_0$, described above (see formulas (6,7) in paragraph 1).

**Definition 4** **Symplectic space** $H^{2k}$ with basis $C_1, S_1, \ldots, C_k, S_k$ and real-valued skew scalar product such that

$$<C_j, C_p> = <S_j, S_p> = 0$$
$$<C_j, S_p> = \delta_{jp}, j, p = 1, \ldots, k \quad (19)$$

will be called an **Asymptotic Symplectic Space**.

Solutions $\psi_{jn}^\pm$ in the tails can be expressed as complex linear combinations in the same basis with natural linear extension of the same scalar product.

**Definition 5** **Vector** $\psi_{ass} \in H^{2k}$ such that there is a continuation of it as a solution $\psi$ on the whole Graph $\Gamma$ will be called an **Asymptotic Vector** for the operator $L$; $\lambda$-dependent linear space $T_\lambda$ of all asymptotic vectors $\psi_{ass} \in T_\lambda$ for the operator $L$ will be called **Space of Symplectic Scattering Data** for $L$.

**Theorem 3** For any selfadjoint real second order Schrödinger Operator $L$, the corresponding linear space of Symplectic Scattering Data is **Lagrangian** subspace in the Asymptotic Symplectic Space for every complex value of $\lambda$. 
Proof. We shall demonstrate that this fact is, in fact, topological. It follows from Theorem 1 which claims that Wronskians are homological cycles in our Graph for every pair of solutions \( \phi, \psi \).

At the same time, we know the following elementary topological properties of tails in the connected graphs:

1. Any piece of tail \( z_j \) may appear as a nonzero part of 1-cycle only if all edges of this tail belong to this cycle with the same coefficient;

2. Individual tail \( z_j \) never has a continuation to Graph \( \Gamma \) as a cycle containing other tails with coefficients equal to zero. The difference between any pair of tails \( z_j - z_p \) can be continued to Graph \( \Gamma \) as a cycle such that other tails do not participate in it.

For the Wronskian of two solutions on \( \Gamma \) we have

\[
W(\phi, \psi) = \sum_{j=1}^{j=k} \alpha_j z_j + (\text{finite}) = \sum_{p=2}^{p=k} \beta_p (z_1 - z_p) + (\text{finite})
\]

From this equality we conclude that

\[
\sum_{j=1}^{j=k} \alpha_j = 0
\]

At the same time we know that this sum is exactly a skew symmetric scalar product of asymptotic vectors:

\[
\sum_{j=1}^{j=k} \alpha_j = < \phi^{ass}, \psi^{ass} >
\]

Therefore our theorem is proved.

Our Schrodinger Operators will be considered now as a selfadjoint operators in the Hilbert Spaces of square integrable functions \( L^2_0(\Gamma) \) for two cases: vertices \( i = 0 \) and edges \( i = 1 \) as before. The subset of \( \delta \)- functions \( \delta_P \in L^0_2 \) or \( \delta_R \in L^1_2 \) contains functions equal to 1 on some vertex (edge), and zero otherwise.

For trivial reasons we always have a continuous spectrum with multiplicity equal to \( k \) for \( |\lambda| \leq 2 \). Therefore the results of paragraph 1 are very useful here.
Sometimes we may have exceptional discrete eigenvalues for $|\lambda| \leq 2$ drown in the continuous spectrum (see below). A "Normal" discrete spectrum appears for $|\lambda| > 2$

**Definition 6** We call the Scattering Zone of Spectrum the area where $|\lambda| \leq 2, \lambda \in \mathbb{R}$. The interval of real $|\lambda| > 2$ we call the Zone of Normal Discrete Spectrum, for which every eigenfunction has exponential decay in all tails and is nonzero at least in one tail. **Exceptional Discrete Spectrum** may appear for any real $\lambda$. It is such that corresponding eigenfunctions are identically equal to zero in all tails.

In the Scattering Zone we have

$$\psi_{jn}^\pm = \exp\{\pm i\theta_j(\lambda)\} = a_n^\pm, n > n_0$$  \hspace{1cm} \theta(\lambda) \in \mathbb{R}, |\lambda| \leq 2$$

In the Zone of Normal Discrete Spectrum we have

$$\theta(\lambda) \in i\mathbb{R}, i^2 = -1$$

So in the last zone both solutions $\psi^\pm$ are real. One of them has exponential decay for large $n$:

$$\psi_j^+ \to \infty, n \to \infty, j = 1, \ldots, k$$

$$\psi_j^- \to 0, n \to \infty$$

Let us denote the open halflines on the real $\lambda$ line by

$$I_+ = (2 < \lambda < \infty), I_- = (-2 > \lambda > -\infty)$$

Using the result of the previous Theorem we have a pair of mappings

$$T^+: I_+ \to \Lambda_k, T^-: I_- \to \Lambda_k$$

defined by the Lagrangian Planes $T_\lambda$ for both cases $\lambda \in I_{\pm}$. Here $\Lambda_k$ is a **Lagrangian Grassmanian** whose points are Lagrangian $k$-planes in $H^{2k}$. There is a canonical codimension 1 cycle (see [8])

$$Z \subset \Lambda_k$$

containing all Lagrangian planes with a nonempty intersection with a set of directions $\sum_j \kappa_j \psi_j^-$. You may say that this cycle contains all singularities of the projection, when you project Lagrangian planes into the linear span of all vectors $\psi_j^+$ forgetting halfbasis $\psi_j^-$. 

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Corollary 1  Normal discrete eigenvalue appears exactly where the Lagrangian Plane $T_\lambda$ crosses the cycle $Z$. Therefore two ”Morse Indices” are defined; they characterize topological properties of normal spectra for $\lambda > 2$ and $\lambda < 2$: they are the intersection indices of the curves $T^\pm$ with the cycle $Z$ defined above.

We can see that decay of any eigenfunction belonging to the Hilbert space should be exponential here (or it should be equal to zero in all tails—see later).

Remark 2  I did not clarified yet whether these intersection indices are exactly equal to the numbers of eigenvalues (i.e. all crossing points for the generic case have sign +) or not.

Let us define now Scattering Matrix for Operator $L$. Consider the Scattering Zone $|\lambda| \leq 2$ where our basic complex solutions

$$\psi_{jn}^\pm = \exp\{\pm in\theta_j(\lambda)\}$$

are complex adjoint to each other. Take them as a basis for the complexified Symplectic Space $H^k_c$ where Lagrangian subspace $T_\lambda$ is given by the theorem above. Generically this subspace can be interpreted as a graph for the linear map from halfbasis $\psi^+ = (\psi_j^+)$ to the halfbasis $\psi^- = (\psi_j^-)$

$$\psi_p^+ \to \sum_j s_{jp}\psi_j^-$$

$$\psi^+ \to S(\lambda)(\psi^-)$$

This corresponds to the choice of basis in the form

$$e_t = \psi_t^+ + \sum_j s_{jt}\psi_j^- \in T_\lambda$$

Corollary 2  In the Scattering Zone the Scattering Matrix $S_\lambda$ is always unitary $S \in U_k$ and symmetric $S^t = S$

Proof. For $k = 2$, the relationship between Lagrangian planes and real unimodular matrices was mentioned as an example in the elementary textbook
of Arnold (see [4]): From the Lagrangian plane in $H^4$, we come to the standard Monodromy Matrix $M \in SL_2(R)$ which maps basis $C_1, S_1$ into the basis $C_2, S_2$. This matrix was always in use in Classical Math Literature for the second order Sturm–Liouville operator on the line. Coming to the complex bases $\psi_j^\pm$ and $\psi_j^\pm, j=1,2$, we get a monodromy matrix in the group $SU_{1,1}$ which is isomorphic to $SL_2(R)$. Monodromy matrix is unimodular because of wronskian property. Algebraic transform from this to the Scattering Matrix has the standard name of Caley Transformation in this case. It was used by quantum physicists in the Scattering Theory for the Schrödinger Operators. Let us point out that standard Quantum Scattering Matrix $S'$ on the line differs from our $S$ by the multiplication on permutation matrix $P$ from one side: $S' = SP$. For example, diagonal elements of $S$ are equal to the Reflexion Coefficient, not to Transmission Coefficient as in standard matrix $S'$. The famous Reflectionless Operators have Antidiagonal Scattering Matrix $S$ in our sense for $k = 2$. For any $k$ we immediately deduce from lagrangian property that

$$<\psi_j^+ + \sum_l s_{jl} \psi_l^-, \psi_p^+ + \sum_q s_{pq} \psi_q^-> = (s_{jp} - s_{pj}) <\psi^+, \psi^-> = 0$$

$$<\psi^+, \psi^-> = \sqrt{\lambda^2 - 4} \neq 0$$

Therefore our Scattering Matrix is symmetric.

To prove unitarity we need to use reality of the Lagrangian plane. Consider now a real basis in the plane $\Lambda$:

$$\left(\sum_l t_{lj} e_l\right) = T(\psi^+) + TS(\psi^-) \quad (29)$$

Its adjoint has a form

$$\bar{T}\bar{S}(\psi^+) + \bar{T}(\psi^-) \in \Lambda_k$$

$$\bar{\psi}^+ = \psi^-$$

From that we conclude

$$\bar{S}^{-1}\bar{T}^{-1}\bar{T} = S = S^t$$

because we are coming to the same basis $e \in \Lambda$. This line proves unitarity of $S$. Our Corollary is proved.
Remark 3 We can start with real basis in $T_\lambda$ of the form

$$\bar{A}(\Psi^+) + A(\Psi^-)$$

From the same arguments as above we deduce that $A$ is a unitary matrix, and

$$S = AA^t \in U_k$$

This is an imbedding of the space $\Lambda_k$ in $U_k$ as a set of all symmetric unitary matrices.

Let us describe now an Exceptional Discrete Spectrum. The following simple theorem is true.

**Theorem 4** Exceptional Discrete Eigenfunctions are completely defined by the eigenfunctions $\phi$ on the basis $\Gamma'$ equal to zero in all nests (case of vertices).

$$L'\phi = \lambda\phi (L' = DLD)$$

$$\phi(P_l) = 0, l = 1, \ldots, s$$

Here $D^2 = D$ is the projection operator from functions on $\Gamma$ to the functions on $\Gamma'$, putting all values outside subgraph equal to zero.

Remark 4 In the case of edge operators we call 'edge-nest' any edge $R$ outside of $\Gamma'$ touching some vertex-nest $P_l$. After that replacement all theorems containing the word 'nest' remain true for edge operators.

Proof of this theorem is very simple. Every such eigenfunction on the basis $\Gamma'$ can be continued to $\Gamma$, taking zero value in all tails. This gives us an exact one-to-one correspondence between exceptional eigenvalues in $\Gamma$ and such special eigenvalues in $\Gamma'$, equal to zero in all nests.

**Corollary 3** The property of Operator $L$ to have at least one exceptional eigenvalue has codimension not less than the number of nests or edge-nests (in the space of all real selfadjoint Schrodinger Operators with finite domain where operator is different from the standard constant operator $L_0$). In particular, it is always not less than one, and Generic Operators have no exceptional spectra. After generic small perturbation of $L$ all discrete eigenvalues with $|\lambda| \leq 2$ disappear.
Proof of this corollary immediately follows from the fact that finite Graph \( \Gamma' \) has only a finite number of eigenvalues. Without the symmetry group, corresponding eigenfunctions are generically nonzero in the nests (edge-nests).

**Remark 5** For the Graphs and operators with nontrivial symmetry group this simple counting of parameters does not work. Exceptional eigenvectors may necessarily appear in some symmetric cases—see examples 2 and 3 below.

**Remark 6** As Misha Gromov often explains in his lectures, Hyperbolic Geometry is visible from the infinity as one-dimensional one. Therefore we may conclude, that for the discrete groups in 2D Lobachevski Plane with Noncompact Fundamental Domain of finite volume, Spectral Theory of the Laplace-Beltrami Operator should look in a sense ‘similar’ to the one on the graphs with \( k \) tails. We discussed this analogy with D.Kazdan, who pointed out to me that for arithmetic subgroups there are many discrete eigenvalues drown in the continuous spectrum. They disappear after nonarithmetic perturbation, as Peter Sarnak pointed out. In the case of graphs with \( k \) tails, we have simplified version of this picture for operators with symmetry: exceptional eigenvalues disappear after generic nonsymmetric perturbation.

**Example 2** Let \( k = 1 \). Our Graph \( \Gamma \) is equal to finite subgraph \( \Gamma' \), plus tail attached to it at one point (nest \( P_1 \)). For generic graphs \( \Gamma \), we have only Lagrangian plane \( T_{\lambda} \), which is one dimensional, and no exceptional eigenvalues. In the area where the operator is free (i.e. in the tail \( n > n_0 \)), we have one real solution \( \phi = a\psi^+ + b\psi^- \) for every real \( \lambda \). In the Scattering Zone \( |\lambda| \leq 2 \), we have

\[
\begin{align*}
\tilde{\phi} &= \phi, \tilde{\psi}^+ = \psi^-, b = a \\
|b/a| &= 1, \lambda \in [-2, 2]
\end{align*}
\]

By definition of the Scattering Matrix, we have here

\[
s(\lambda) = b/a \in U_1
\]

For the Zone of Normal Discrete Spectrum \( |\lambda| > 2 \), we have an analytic continuation of scattering coefficient \( s(\lambda) \) which has no sense of scattering anymore. Its poles \( a = 0 \) give us points of normal discrete spectrum \( \lambda_m \).
If exceptional spectrum drown in the continuous one exists for this operator, we have an eigenfunction \( \phi' \) equal to zero in the tail. So we have a two-dimensional eigenspace and can consider Wronskian as a skew scalar product.

Wronskian \( W(\phi, \phi') \) for this exceptional value of \( \lambda \) is equal to some finite cycle \( z \in H_1(\Gamma') \). For the graphs and operators with \( Z_2 \)-symmetry this possibility is generic, i.e., in general it cannot be destroyed by perturbation.

To illustrate the last statement, consider Graph \( \Gamma \) with one tail and triangle \( \Gamma' = 0AB \) attached to the vertex 0. Its vertices are numerated by nonnegative integers and letters A, B, P = ..., n, ..., 0, A, B with edges \( R_n = [n, n-1], R_A = [0A], R_B = [0B], R_{AB} = AB \). Take coefficients of the vertex Schrodinger Operator \( L \) in the form

\[
v_n = 0, n > 0, v_0 = u, v_A = v, v_B = w, b_{n,n-1} = 1, n > 0, b_{0,A} = a, b_{0,B} = b, b_{A,B} = c
\]

We have following set of equations:

\[
\begin{pmatrix}
  u - \lambda & a & b \\
  a & v - \lambda & c \\
  c & b & w - \lambda
\end{pmatrix}
\begin{pmatrix}
  \psi_0 \\
  \psi_A \\
  \psi_B
\end{pmatrix}
= \begin{pmatrix}
  -\psi_1 \\
  0 \\
  0
\end{pmatrix}
\]

For the exceptional eigenvector we need such solution that \( \psi_1 = \psi_0 = 0 \). It leads to the condition:

\[
\lambda_{ex} = w - bca^{-1} = v - acb^{-1}
\]

If \( |\lambda_{ex}| < 2 \), we have an exceptional eigenvalue drown in the continuous spectrum.

\( Z_2 \)-symmetry leads to the following coefficients:

\[
v = w, a = b
\]

Here we have \( \lambda_{ex} = c \).

**Example 3** Let us consider vertex operators for \( k = 2 \). We have two tails here and one or two nests in the Graph \( \Gamma' \). For almost all \( \lambda \) we have here well-defined Monodromy Matrix as on the line. However, on the line monodromy was well-defined for all \( \lambda \).
Here we may have isolated "singular" values of $\lambda$ for which Lagrangian plane $T_\lambda$ is special: a monodromy map from the free basis of one tail into free basis of the another tail does not exist. It happens if our Lagrangian plane has a basis $\phi_1, \phi_2$ such that $\phi_1 = 0$ in the second tail and $\phi_2 = 0$ in the first tail.

**Wronskian** $W(\phi_1, \phi_2)$ is equal to some finite cycle in $\Gamma'$ for such 'singular' $\lambda = \lambda^*$.

It might happen even in the Scattering Zone as a generic possibility. Such singular values $\lambda = \lambda^*$ may be real, or they may appear by the complex adjoint pairs.

To illustrate the last statement, we consider two cases:

1. $\Gamma'$ is a triangle $[0AB]$ where the vertex 0 is a nest for both tails.
2. $\Gamma'$ is a triangle $[0_10_2A]$ where the vertices $0_1, 0_2$ are the nests.

In the Case 1 we have vertices

$$P = ..., n_1, ..., 0_1 = 0, ..., n_2, ..., 0_2 = 0, A, B$$

and coefficients

$$b_{n_i; n_{i-1}} = 1, n_i > 0, i = 1, 2, b_{0; A} = a, b_{0; B} = b, b_{A; B} = c, v_0 = w, v_A = u, v_B = v$$

As elementary calculation shows, we have solution $\psi_i$ equal to zero in the tail $i = 1$ or $i = 2$ iff

$$(u - \lambda^*)(v - \lambda^*) = c^2$$

Here we have real $\lambda^*$ only, and $W(\psi_1, \psi_2) = 0$

In the Case 2 we have vertices

$$P = ..., n_1, ..., 0_1, ..., n_2, ..., 0_2, A, n_i \geq 0$$

and coefficients

$$b_{n_1; n_{1-1}} = b_{n_2; n_{2-1}} = 1, n_i > 0, b_{0_1; 0_2} = a, b_{0_1; A} = b, b_{0_2; A} = c, u = v_0_1, v = v_0_2, w = v_A$$

After elementary calculations we have

$$\lambda^* = bca^{-1}, W(\phi_1, \phi_2) = bca^{-1}[0_10_2A] \in H_2(\Gamma, R)$$

Here $\phi_i = 0$ in the tail with number $i, i = 1, 2$, and $\phi_i(A) = 1$. Exceptional eigenvalues with eigenfunctions equal to zero in both tails do not exist for this simple graph.
For the cases $k \geq 3$ the situation is much more complicated.

Let us point out here that a very simple argument leads to the existence of discrete spectrum $\lambda_q > 4$ for Laplace-Beltrami operators. Apply operator $L$ to the set of $\delta$-functions. Consider the square of norm

$$(L\psi, L\psi) = ||L\psi||^2$$

and the maximum of it for all $\delta$-functions. We denote this maximum by $M_L$. For the Laplace-Beltrami operators, we shall use $L = \Delta + 2$ as before. This choice of constant is optimal for this estimate. If this quantity is bigger than 4, we conclude that discrete spectrum exists for $L$. Moreover, this estimate is certainly nonexact. So, discrete eigenvalue $\lambda_q > 2$ exists also if our estimate is exactly equal to 4 on the set of $\delta$-functions. We are coming finally to the following estimates sufficient for the existence of discrete spectrum in most cases:

1. Vertices

$$M_L = \max_P (\sum_{P'} b^2_{P,P'} + V_P^2) \geq 4$$

For the vertex Laplace-Beltrami, we have $M_L = \max_P \{ m_P + (m_P - 2)^2 \}$

2. Edges

$$M_L = \max_R (\sum_{R'} d^2_{R,R'} + V_R^2) \geq 4$$

For the edge Laplace-Beltrami, we have $M_L = \max_R \{ m_P - 1 + m_{P'} - 1 \}$ where $P \cup P' = R$. It is easy to improve last inequalities, replacing the Operator $L$ by $L^2$. Sasha Veselov obtained better estimates for the case of vertices, for example, as he privately informed me.

Factorization of Schrodinger Operators on Graphs

**Definition 7** We call Schrodinger Operator $L$ acting on vertices or edges factorizable if it can be represented in the form

$$L + C = Q Q^+, C = \text{const}$$

Table 7

\[ L + C = Q^+ Q + U_R \]

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Factorization is **special** if function $U_R$ is equal to constant. For the case of vertices we consider only special factorization. Here operators $Q, Q^+$ are real adjoint to each other. An Operator $Q^+$ maps functions of vertices into functions of edges by the following formula

$$ (Q^+ \psi)_R = \sum_P c_{R:P} \psi_P $$

$$ (Q \psi)_P = \sum_R c_{R:P} \phi_R $$

We call factorization **formal** if coefficients of operators $Q, Q^+$ are not real (and they are not adjoint actually to each other).

Elementary substitution of this into our equations leads to the following result:

**Theorem 5** Representation of Operator $L$ in the factorized form is equivalent to the set of equations:

1. For vertices

$$ b_{P,P'} = c_{R:P} c_{R':P'}, \: P \neq P' $$

$$ V_P + C = \sum_{P \in R} c_{R:P}^2 $$

2. For edges

$$ d_{R,R'} = c_{R:P} c_{R':P}, \: R \cap R' = P $$

$$ V_R + C = c_{R:P}^2 + c_{R':P}^2 + U_R $$

**Corollary 4** For Operators $L$ acting on edges: part of our factorization equations for the quantities $c_{R:P}$ through $d_{R:P}$ provides a complete set of algebraic equations for any given vertex $P$. **This set of equations is overdetermined** for such $P$ that $m_P > 3$. Compatibility conditions (in the form of algebraic constraint for the coefficients of operators) should be satisfied for factorization in this case. If all coefficients $d_{R:P}$ are positive for all closed neighbors $R \neq R'$, the solution $c_{R:P}^2$ is also positive. There is a formal factorization $L = QQ^t + U_P$ such that the squares of coefficients $c_{R:P}^2$ are uniquely defined by the equation of factorization above.
**Corollary 5** For operators acting on vertices: let all coefficients \( b_{P,P'} \) are strictly positive for all closest neighbors \( P \neq P' \). Take any finite contractible ("tree-like") subgraph \( \Gamma'' \) in the Graph \( \Gamma \) and its initial vertex (nest) \( P_0 \in \Gamma'' \). Take any value of the constant \( C \) and any function \( c_{R,P} \) given along the boundary of \( \Gamma'' \) except the point \( P_0 \), where edges \( R \) look inside of our selected subgraph from the boundary vertices \( P \). There is a special formal factorization of \( L \) with functions \( c_{R,P}^2 \) uniquely defined by this data in the subgraph \( \Gamma'' \). There is a value of the constant \( C \) depending on the subgraph \( \Gamma'' \) such that all quantities \( c_{R,P}^2 \) are positive.

Proof of this easy follows from the form of the factorization equations: we solve the equations above for the quantities \( c_{R,P}^2 \) in both cases. Let me point out that factorization is purely local in the case of edges. So we proved our corollary for the case of edges.

Consider the case of vertices more carefully. From the data on the boundary of subgraph \( \Gamma'' \) we can find unique real solution for the squares \( c_{R,P}^2 \) for any real constant \( C \). However these quantities might take negative value. This leads to complex solutions in terms of \( c_{R,P} \). After that we find signs of \( c_{R,P} \) from the very simple part of our equation which does not contain squares, using initial data.

To prove the last part of the Corollary, we need to take constant \( C \) large enough and special initial data on the boundary of subgraph \( \Gamma'' \). We take large enough values of \( c_{R,P}^2 \) on the boundary after choosing a large constant \( C \). Here the edges \( R \) are attached to the boundary points \( P \) from inside of \( \Gamma'' \). Solving the factorization equation in the direction to the endpoint \( P_0 \) we shall go through the number of steps (layers) in \( \Gamma'' \), such that \( c_{R,P}^2 \) will be small, of the order \( C^{-1} \) for the edges looking from outside to the layer vertices. After that we shall find that the values of \( c_{R,P}^2 \) will be large and closed to \( C \) for the edges looking inside of layers. This ansatz is selfconsistent. Therefore we are coming to the desired positive solution. Corollary is proved.

**Conjecture:** Let coefficients \( d_{R,R'} \) and their inverse \( d_{R,R'}^{-1} \) for \( P \neq P', R \neq R' \) are positive and bounded. Let Graph \( \Gamma \) is contractible and all numbers \( m_P \) are also bounded. There is some positive value of \( C \) that Operator \( L \) admits a real factorization.

Probably, this statement follows from the little improvement of the same arguments as last Corollary.
Until now we did not investigate factorization for the graphs with non-trivial topology.

Appendix: Two Remarks

1. Nonlinear equations. 2. Fermionic Quadratic Forms

We shall discuss here the continuous analog of our constructions for the case of vertices and nonlinear generalizations. After that we describe some properties of real fermionic quadratic forms.

1. Consider any smooth manifold $M$ with Riemannian metric and the linear selfadjoint Schrödinger Operator $L$ acting in the space of the scalar functions. This operator can be obtained from the variational principle

$$S\{\psi\} = \int_M \left( \sum a^k(x) \psi_k \psi_j + U(x) |\psi|^2 \right) \sqrt{g(x)} d^n x$$

$$\psi_k = \partial_k \psi$$

in the Hilbert space of square integrable functions, where $g(x)$ is determinant of the Riemann tensor in the local coordinate system $x^1, \ldots, x^n$. What Gelfand told me in 1971 is that the expression

$$\int_B ( (L\psi) \phi - (L\phi) \psi ) \sqrt{g(x)} d^n x$$

for the arbitrary pair of functions $\psi, \phi$ is nonzero for the domain $B$. Using the Stokes formula, it can be reduced to the boundary $\partial B = D$. It leads to the integral

$$\int_B ( (L\psi) \phi - (L\phi) \psi ) \sqrt{g(x)} d^n x = \int_D W(\phi, \psi) d\gamma$$

Here $d\gamma$ means corresponding area element on the boundary. As we can see, what we get along the boundary is in fact an analog of Wronskian in our terminology. For the selfadjoint extension of operator $L$ in the domain $B$ you need to take boundary conditions in the form of some Lagrangian Plane in the last space of pairs $(\psi, \phi) \in H$ of functions on the boundary.

In the main part of this work, we defined and used a discrete analog (for the Graph $\Gamma$) of the quantity $W$ which is now the density of vector field
$W^j(x)\sqrt{g(x)d^n x}$ on the manifold $M$ in the continuous case. Our scheme corresponds in this case to the following: we take any 1-form $\omega_i(x)dx^i$ with compact support on $M$; $W$ can be considered as a 1-chain on $M$ ("current")

$$<z,\omega> = \int_M \omega_i(x)W^i(x)\sqrt{g}d^n x$$

For the pair of solutions $(\psi,\phi)$ of the equation $L\psi = \lambda\psi$, we are coming to the 1-cycle associated with current $W$.

We did not clarify any continuous analogs of the cases $k > 0$.

After the very useful discussion of our first work [4] with A.Schwarz in Maryland in December 1997, we came to the conclusion that this construction has a natural generalization to the nonlinear case: we may construct a closed $H$-valued 2-form on the space of solutions for nonlinear variational problems in both cases—continuous and discrete, i.e., on $M$ and on the Graphs $\Gamma$. Here $H = H_{1}^{open}(\Gamma, Z)$ for graphs, and $H$ is a divergenceless current for manifolds. Construction of this 2-form immediately follows from this work, applying it to the operator of second variation along the solution $f$, to the pair of variations for $\lambda = 0$: $W_f(\delta\psi, \delta\phi) = \Omega$

This form is closed for $\lambda = 0$. I will publish details in the next work.

**Remark 7** In one-dimensional case there is a natural class of continuous operators—the Schrodinger Operators on Graphs such that in every edge $R_i$ a self-adjoint second order standard Schrodinger Operator $L_i$ is given, characterized by the set of real potentials $v_i(x), x \in R_i$ given in all edges $R$ as the functions continuous in the closed edge (i.e. including boundary). For any vertex $P$ we have $k = m_P$ edges $R_i$ ending in it. Consider Symplectic Space $R_{P}^{2k}$ given as a direct sum of 2-spaces $R^2_i$ associated with every edge $R_i$

$$R_{P}^{2k} = R^2 \oplus \ldots \oplus R^2$$

with canonical coordinates $p_i, q_i \in R^2_i$. For any solution $L_i\psi_i(x) = \lambda\psi_i(x)$ in the edge $R_i$, we have boundary values $\psi(P), \psi'(P) \in R^2_i$. Let for any vertex $P$ a Lagrangian Plane $\Lambda_P \subset R_{P}^{2k}$ is given. We call set of solutions $L_i\psi_i(x) = \lambda\psi_i(x), x \in R_i$ solution of the real selfadjoint operator $L$
on the graph iff in any vertex $P$ full set of the boundary values
belongs to the Lagrangian Planes $\Lambda_P$.

We may replace operators $L_R$ by the Monodromy Matrices $M_R \in SL_2(R)$:
\[ M_R : R^2_P \to R^2_{P'}, \partial R = P \cup P' \]

All set of vertices can be considered as some kind of 'boundary' for the
Schrodinger Operator $L = \cup L_R$ (union along all edges). The whole set of
Lagrangian Planes $\Lambda = \cup \Lambda_P$ is some sort of 'selfadjoined extension' for the
Operator $L$. As P.Kuchment informed me in May 1998, these operators have
been considered by mathematical and theoretical physicists for some concrete
problems of Solid State Physics and Superconductivity in the late 80-s, who
formulated self-adjoint junction condition in vertices in the classical von
Neumann-Krein form. The most popular conditions are following:

1. $\psi_i(P) = \psi_j(P) = \psi(P), \sum_i \psi_i'(P) = \alpha \psi(P)$

2. $\psi_i'(P) = \psi_j'(P) = \psi'(P), \sum_i \psi_i(P) = \alpha \psi'(P)$

Here indices $i, j$ as before numerate all edges coming to the vertex $P$. (see [11])
B.Pavlov with N.Gerasimenko obtained also some results in the Scattering Theory for such operators (see [12]). We shall compare their results with
our ideas in the next work. In the works of P.Kuchment and A.Figotin a
pseudodifferential model on graphs was developed for photonic crystals (see
for example [13]). Certainly, no one of them discussed such problems in
terms of Symplectic Geometry.

Consider now any subgraph $\Gamma_1 \subset \Gamma$ such that $\partial R \subset \Gamma_1$ implies $R \subset \Gamma$. Therefore the subgraph $\Gamma_1$ attached to the other part of the Graph $\Gamma$ by
some edges $R_1, \ldots, R_p$ ending in the vertices $P_i \in \Gamma_1$ and in the vertices
$P_i' \in (\Gamma \text{minus} \Gamma')$. For any selfadjoint real Schrodinger Operator $L$ on $\Gamma$ we
can define naturally the $\lambda$-dependent Lagrangian Plane $\Lambda_{\Gamma_1}$ in the Symplectic
Space $R^{2p} = R^2_{P_1} \oplus \ldots \oplus R^2_{P_p}$ generated by the values of the solutions $L_i \psi_i = \lambda \psi_i$ along the edges $R_i$ and their first derivatives in the vertices $P_i$. All
interaction of this subgraph with other part depends on this Lagrangian Plane.
In a sense we may consider such subgraph equipped by the Lagrangian Plane
as some more complicated kind of Selfinteracting Vertex with $\lambda$-dependent boundary conditions.
2. **Fermionic Quadratic Forms.** Let us consider now a finite dimensional real linear space $R^n$ with basis $e_j$ and total space of external powers

$$\Lambda^*(R^n) = \sum_{k=0}^{n} \Lambda^k(R^n)$$

Let us associate with every basic vector $e_j$ a Fermionic Creation Operator $a_j$; we associate a vacuum vector $\eta$ with unity $1 \in R = \Lambda^0 \subset \Lambda^*(R^n)$:

$$e_j = a_j(\eta)$$

The total space of exterior powers has a natural basis

$$a_{j_1} \ldots a_{j_k}(\eta), j_1 < \ldots < j_k$$

for all $j, k$.

**Definition 8** A Real Fermionic Quadratic Form is a selfadjoint operator $L$ with real coefficients acting on the total space of exterior powers, written in the form:

$$L = A_{pq}a_p a_q + B_{pq}a^*_p a_q + C_{pq}a^*_p a^*_q + \text{const}$$

Here the Annihilation Operators $a^*_p$ are adjoint to the Creation Operators $a_p$. They satisfy to the ”canonical” relations

$$a_p a_q = -a_q a_p, a^*_p a_q + a_q a^*_p = \delta_{pq}$$

We have obviously

$$A_{pq} = -A_{qp}, B_{pq} = B_{qp}, C_{pq} = -A_{pq}$$

**Theorem 6** Take the new (noncanonical) basis $a^\pm_j = a^*_j \pm a_j$ An Operator $L$ has the form

$$L = D_{pq}a^+_p a^-_q + \text{const}, D = A + B$$
**Definition 9** A Bogolyubov Transformation or Canonical Transformation is an isomorphism of this Clifford Algebra given by the change of canonical basis:

\[ a_p = \sum P_{pq} b_q + \sum Q_{pq} b_q^* \]

\[ a_p^* = \sum Q_{pq} b_q + \sum P_{pq} b_q^* \]

Here new basis \( b_j^*, b_j \) satisfies to the same algebraic relations as the original one (both of them should be canonical).

**Theorem 7** For any Canonical Transformation both matrices \( O_\pm = P \pm Q \) are orthogonal \( O_\pm \in O_n(R) \). The Transformation Rule for the matrix \( D \) is following:

\[ D = O_+ D' O_- \]

where

\[ L = D_{pq} a_p^+ a_q^- = D'_{rs} b_r^+ b_s^- \]

This theorem can be easily proved by the direct elementary verification. As a corollary from this we have

**Corollary 6** An operator \( L \) can be reduced to the diagonal form using Bogolyubov Transformations above and Transformation Rule for matrix \( D = A + B \). Eigenvalues \( \mu_{j_1 j_2 ... j_k} \) of the Operator \( L \) in the space \( \Lambda^*(R^n) \) can be computed in the following way:

\[ \mu_{j_1} + ... + \mu_{j_k} = \mu_{j_1 ... j_k}, j_1 < ... < j_k \]

where \( \mu_j \) are the eigenvalues of the 'Absolute Value Operator'

\[ |L| = \sqrt{L^* L} \]

in the space \( R^n \)

This algebraic statement has been found as a lemma in the present author’s Appendix to our joint work with Misha Shubin (see [10]). In this Appendix I developed a nice analytic Witten-like approach trying to find right analog of the Morse Inequalities for the Vector Fields on real manifolds: necessity to diagonalize an arbitrary Real Fermionic Quadratic Form appears naturally here.
(Let us remind that in the Witten’s approach to the Morse inequalities for ordinary functions we have $A_{pq}=0$; therefore only one orthogonal matrix has been used for the diagonalization). Several experts in Quantum Field Theory pointed out to the present author that this elementary observation has never appeared in the literature, so I decided to repeat it here once more. (The last one was A.Schwarz who told me that in the December 1997.)

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