Real Self-Adjoint Operators on Graphs

Symplectic and Topological Phenomena

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Discrete Operators on Graphs.

These investigations were started by the present author in the late XX Century. By definition, graph is an one-dimensional simplicial complex Γ (see Fig 1) . We assume that only finite number m_P of edges meet each other in the vertex $P \in \Gamma$, and this number is bounded $n_P < m$ for all P (see Fig 2).

Fig 1

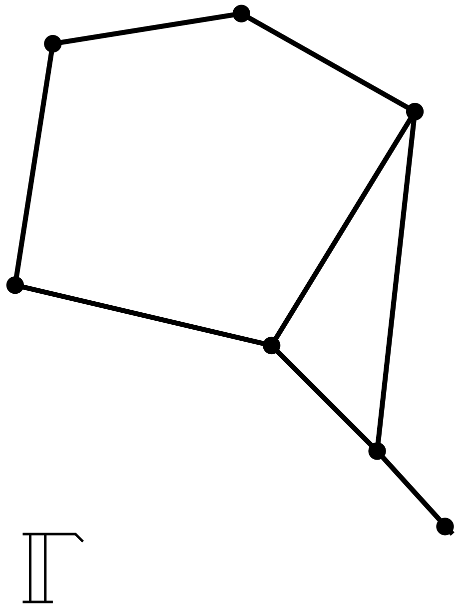
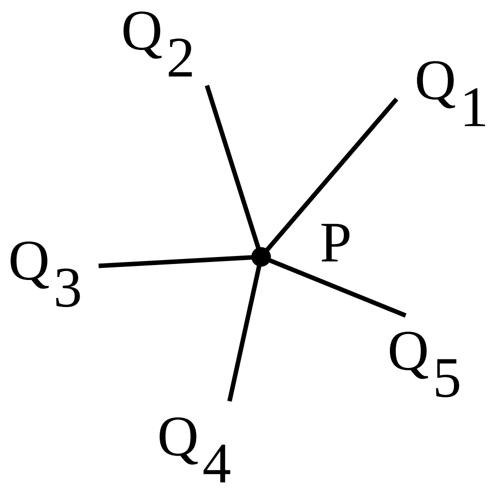


Fig 2



$m_P = 5$

Discrete self- adjoint real operator L acts on the space of functions of vertices

$$L\psi(P) = \sum_Q b_{PQ}\psi(Q)$$

such that b_{PQ} are real and $b_{PQ} = b_{QP}$.

The order of L is equal to $2d$

where $d = max_{b_{PQ} \neq 0} d(PQ)$. Operators acting on the functions of simplices of higher dimension in the simplicial complex K can be reduced to the operators acting on vertices of baricentrical subsivision K'.

The Symplectic Form. Topological Properties

For the pair of solutions $L\psi = \lambda\psi, L\phi = \lambda\phi$ we define the "Symplectic Inner Product" as a chain: $W(\psi, \phi) =$

$$\sum_{[PQ]} (\psi(P)\phi(Q) - \phi(P)\psi(Q)) b_{PQ}[PQ]$$

where $[PQ]$ is the selected shortest path (chain) with property $\partial[PQ] = Q - P$.

Theorem. For every pair of solutions we have $\partial W = 0$, so

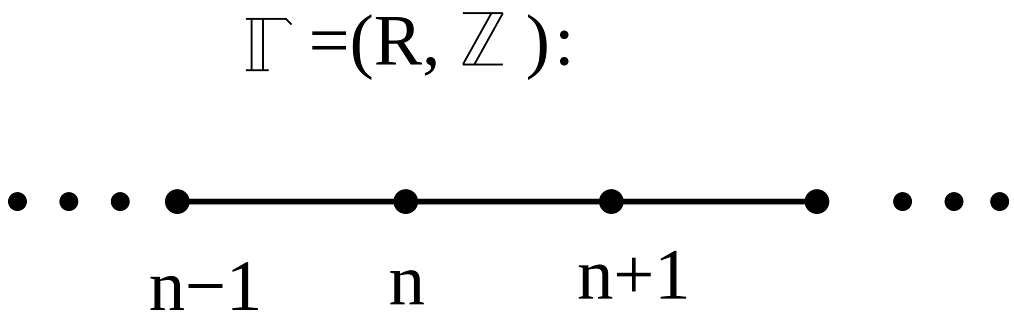
$$W(\phi,\psi) = -W(\psi,\phi) \in H_1^{open}(\Gamma, R)$$

For the second order operators we have

$$W = \sum(\psi(P)\phi(Q) - \phi(P)\psi(Q))b_{PQ}[PQ]$$

for the edges $[PQ]$. This quantity appeared in the theory of Toda Lattice for $\Gamma = (R, Z)$ (see Fig 3) but nobody used it before for the spectral theory of more general graphs.

Fig 3



For the complex solution $\Psi = \psi + i\phi$ we can define a "Current" in the Quantum State Ψ as

$$2iJ = W(\Psi, \bar{\Psi}) = W(\psi, \phi)$$

It satisfies to the classical "Kirchhof Law" $\partial J = 0$(see Fig 4).

This quantity was extended by the present author and A.Schwarz to nonlinear lagrangian systems on graphs as a homology-valued closed two-form on the space of solutions of Euler-Lagrange equation.

Continuous Operators on Graphs:

Continuous second order operator $L = -\partial_{x_i}^2 + u_i(x_i)$ acts on the functions $\psi : \Gamma \to R$ such that $\psi = \psi_i(x_i)$ in every edge $R_i = [P, Q]$ between two vertices parametrized by the coordinate x_i. Here we assume that graph Γ is a minimal cell complex such that more than two edges enter every vertex. For infinite graphs we may have tails $R_i = [Q, \infty]$ parametrized by $x_i \in [a, \infty] \subset R$. Our potentials assumed to be continuous including the endpoints. For the construction of self-adjoint operator we need to formulate some "junction conditions" in all vertices. Let any vertex P be given, and $R_i = [Q_i, P]$ be all m_P edges entering it with coordinates $x_i \in [a_i, b_i] = R_i$ where b_i corresponds to the vertex P. We have a linear space $H_P^{2m_P}$ with coordinates $\psi_i(P), \psi'_i(P)$ and symplectic form

$$\Omega_P = \sum_i d\psi_i(P) \wedge d\psi'_i(P)$$

For every vertex P and number $\lambda \in R$ a Lagrangian Subspace should be selected

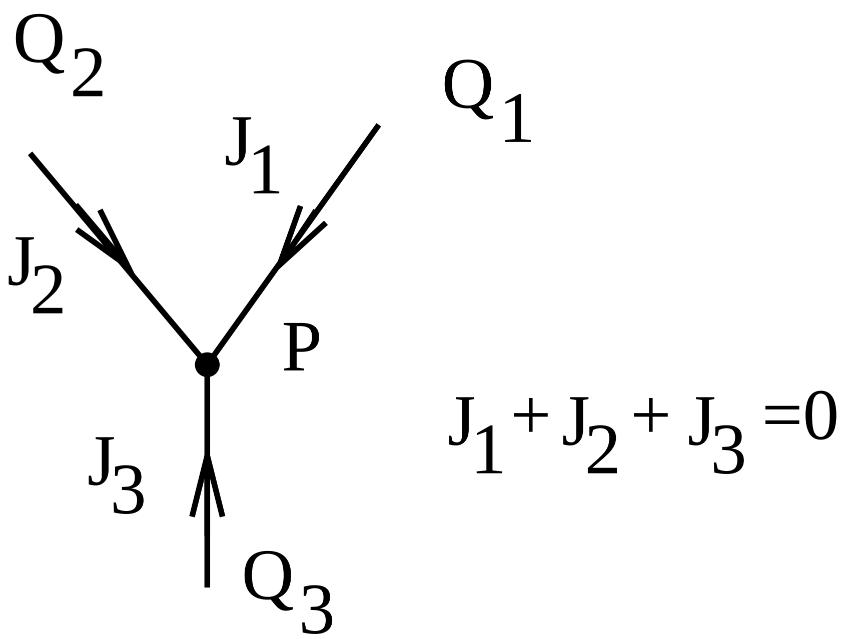
$$L(P, \lambda) \subset H^{2m_P}$$

We require that in every vertex all set of boundary values $\psi_i(P), \psi'_i(P)$ belongs to the subspace $L(P, \lambda)$ for the solutions $L\psi = \lambda\psi$. Then the expression $W(\psi, \phi) =$

$$\sum_i (\psi'_i \phi_i - \phi'_i \psi_i)[Q_i, P_i]$$

is well-defined as an open one-chain in Γ such that $\partial W = 0$. A Current $J(\Psi)$ is defined for the complex quantum state $\Psi = \psi + i\phi$ as $2iJ = W(\Psi, \bar{\Psi})$ such that "The Classical Kirchhof Law" $\sum_i J([Q_i, P]) = \partial J|_P = 0$ is valid (see Fig 4). No problem to extend this construction to the higher order operators.

Fig 4



Kirchhoff Law

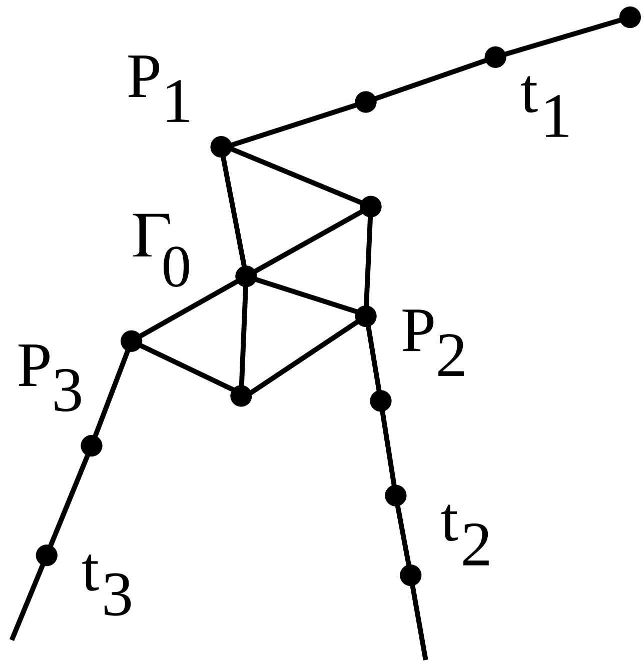
Remark:

Let me point out that the idea of connection of self-adjoint extensions of symmetric operators with symplectic geometry was communicated to me by I. Gelfand in early 1970s. However, I found applications of it only in the late 1990-s.

Graphs with Tails. The Lagrangian Property.

Consider now the Graph $\Gamma = \Gamma_0 \cup [P_i, \infty_i]$ consisting of the finite subgraph Γ_0 with finite number of tails $t_j = [P_j, \infty_j]$ attached to the vertices $P_j \in \Gamma_0, j = 1, 2, ..., r$ (see Fig 5).

Fig 5

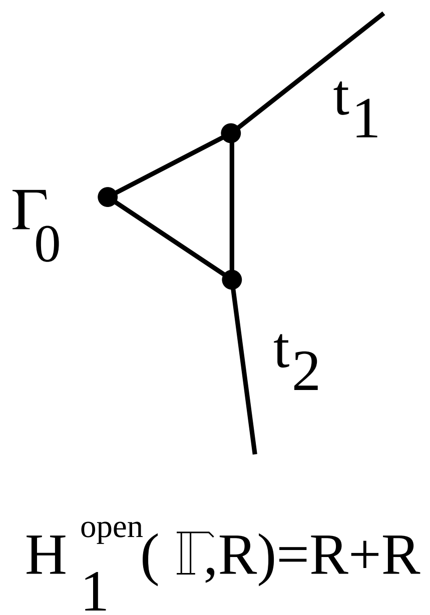


tails t_i

Let L be a real discrete or continuous second order operator on Γ which is "free at infinity". It exactly means that $L \to L_0$ (rapidly enough) in every tail where $L_0 = -\partial_x^2$ for the continuous case and $L_0\psi_n = \psi_{n+1} + \psi_{n-1} - 2\psi_n$ in the discrete case. We have (see Fig 6)

$$H_1^{open}(\Gamma) = H_1(\Gamma_0) \oplus R_{tails}^{r-1}$$

Fig 6



We define the "Asymptotic Space at Infinity" H^{2r}_{as} consisting of all functions ψ asymptotically well-defined nearby of all infinities and satisfying to the equation $L\psi = \lambda\psi$. This space has dimension $2r$ for the second order operator L. It has a natural symplectic form Ω because the form W is a standard scalar-valued form in every tail with canonical basis of solutions $C_i, S_i, W(C_i, S_i) = 1$. It corresponds to the basis C, S: $C(0) = 1, C(1) = 0, S(0) = 0, S(1) = 1$ for the operator L_0 acting on the functions of discrete variable $n \in Z$. We have $\psi^{\pm} = a_{\pm}^{n}, a_{\pm} = 1/2(\mu \pm \sqrt{\mu^2 - 4})$ where $\mu = \lambda + 2$ and $\psi^{\pm} = C + a_{\pm} S$. By definition, $\Omega(C_i, S_j) = \delta_{ij}, \Omega(C_i, C_j) = \Omega(S_i, S_j) = 0$. For the continuous case $C_i = \cos(kx), S = k^{-1}\sin(kx), \psi^{\pm} = \exp(\pm ikx)$.

Theorem. For every λ the subspace of solutions defined for all graph Γ is lagrangian $L_\lambda \subset H^{2r}_{as}$. Its dimension is equal to r.

Proof: Let $W(\psi, \phi) = \sum_{j=1}^{j=r} a_j t_j + (finite)$ where t_j are the tails, and $\sum_{j=1,\dots,r} a_j =$

$\Omega(\psi, \phi)$. But $\partial W = 0$, so we can express it through the basic open cycles $t_1 - t_2, ..., t_1 - t_r$. Finally we obtain: $W = \sum_{q=2,...,r} b_q(t_1 - t_q) = \sum_{j=1,...,r} a_j t_j$ modulo finite cycles. So we have $\Omega(\psi, \phi) = \sum a_j = 0$. We conclude that codimension of such subspace is at least r. At the same time it is defined by r linear equations. Therefore its dimension is exactly r. Theorem is proved.

The Spectral Properties. Scattering Matrix.

Our operators have continuous spectrum in presence of tails for $-4 \leq \lambda \leq 0$ in the discrete case and $\lambda \geq 0$ for the continuous case. We call them " The Scattering Zones". The Scattering Matrix $S_{lj}(\lambda)$ is defined by the solution $L\psi = \lambda\psi$ such that:

$$\psi = \psi_j^+ + \sum_l S_{lj}\psi_l^-$$

where $\psi_j^\pm$ are well defined in the tails $t_j$as above, and $\bar{\psi}_j^+ = \psi_j^-$

Theorem. Scattering Matrix S is Unitary and Symmetric $S_{lj} = Sjl$.

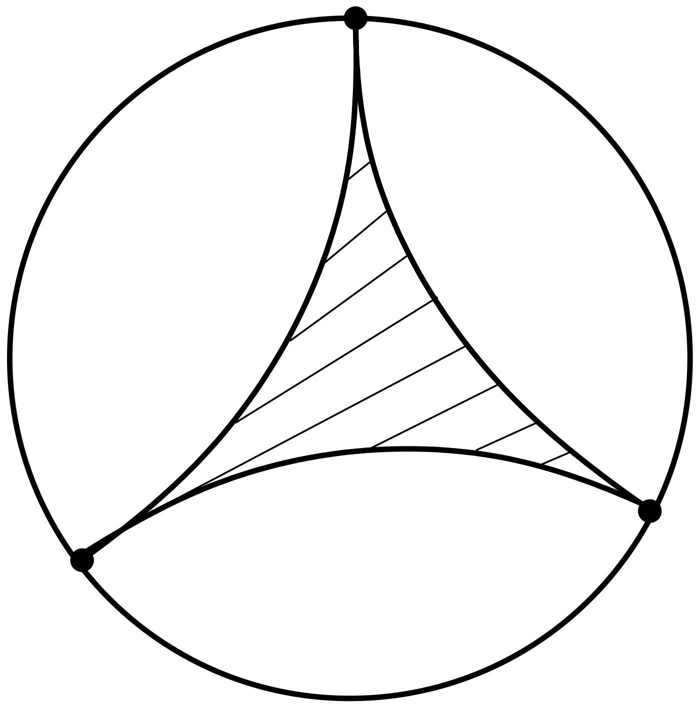
Unitarity of Scattering was known long ago. For the graphs with tails it was studied for the continuous operators in 1980s (Pavlov and Gerasimenko, Exner and Seba). However, the symmetry property remained unknown till our works (1997). Let me point out that it is easily visible from the viewpoint of symplectic geometry. What is a set of unitary symmetric matrices? If $S^t = S$, we can express S as $S = AA^t$ where $A \in U_r$. For every matrix $O \in O_n, B = AO$, one have the same S:

$$AA^t = AOO^tA^t = BB^t = S$$

Therefore $A \in U_r//O_r$. But this is exactly the "lagrangian grassmanian" or manifold of all lagrangian subspaces in the space H^{2r}.

Let me mention also that the "normal" discrete eigenvalues are such that corresponding eigenfunctions have exponential decay at infinity, and eigenvalue is not in the scattering zone. For graphs however, there exists the ”unnormal” eigenvalues such that eigenfunctions are equal to zero in all tails. Corresponding eigenvalues may belong to the scattering zone. Such operators are nongeneric: these eigenvalues can be destroyed by the generic perturbation. However, in presence of the discrete symmetry they might became stable relative to the symmetry-preserving perturbations. There exists an interesting analogy between this theory and spectral theory of the Laplace-Beltrami operators in the hyperbolic (Lobatchevski) space for the discrete groups with finite volume and r ”ends” at infinity (see Fig 7). This geometry looks like ”graph” from the far distance.

Fig 7



Hyperbolic space H^2

Fundamental domain with 3 "ends"