The Shrödinger operator on graphs and topology

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We shall define a Schrödinger operator for a one-dimensional simplicial complex (a graph) $\Gamma$ without ends (that is, at least two and only finitely many edges meet at any vertex), which acts on functions of vertices $T$ or edges $R$:

$$(L\psi)_T = \sum_{T'} b_{T:T'} \psi_{T'}$$

for $L_0 = \partial\partial^*$, $b_{T:T'} = 1$, $b_{T:T'} = -m_T$,

$$(L\psi)_R = \sum_{R'} d_{R:R'} \psi_{R'}$$

for $L_0 = \partial^*\partial$, $d_{R:R'} = 1$, $d_{R:R} = -2$.

Here the coefficients are real, symmetric, and non-zero only for nearest neighbours

$$T' \cup T = \partial R, \quad R \cap R' = T.$$

The coefficients $b_{T:T} = W_T$ and $d_{R:R} = W_R$ are called the potential, $m_T$ is the number of edges at a vertex, and $\partial$ is the boundary operator.

**Definition 1.** The Wronskian of a pair of solutions of $L\psi_i = \lambda\psi_i$, $i = 1, 2$, is the skew-symmetric bilinear expression

$$W_R = b_{T:T'} (\psi_{1T'} \psi_{2T'} - \psi_{2T} \psi_{1T'}), \quad T' \neq T,$$

$$W_R = \sum_{R' \cap R = T} d_{R:R'} (\psi_{1R'} \psi_{2R'} - \psi_{2R} \psi_{1R'}), \quad R' \neq R.$$  

Here $R = (TT')$ is an oriented edge, $W_{TT'} = -W_{T'T}$.  

\footnote{We began the discussion of this problem together with A. P. Veselov}
Theorem 1. The Wronskian of a pair of solutions is well defined as a 1-chain on $\Gamma$, whose boundary is equal to zero: $\partial W = 0$.

The proof follows in both cases by considering the quantity $(L\psi_1)\psi_2 - (L\psi_2)\psi_1$.

We consider a graph $\Gamma$ having $k$ ‘tails’ $(z_1, \ldots, z_k)$, $k \geq 1$: the tails $z_j$ are half-lines with edges $R_{jn}$, $n \geq 1$, and vertices $T_{j,n-1}$, $\partial R_{jn} = T_{jn} - T_{j,n-1}$. Suppose that the Schrödinger operator is ‘finite’, that is, for $n > n_0$ and all $j$ we have $L = L_0 + 2$ in both cases.

The equation $L\psi = \lambda\psi$ has solutions in $z_j$ as $n \to \infty$ of the form $\psi_{jn}^\pm = a_n^\pm$, $a_\pm = \frac{1}{2}(\lambda \pm \sqrt{\lambda^2 - 4})$. A basis of real solutions for $\lambda \in \mathbb{R}$ is:

$$C_{jn} = (a_-\psi_{jn}^+ + a_+\psi_{jn}^-)(a_+ + a_-)^{-1}, \quad S_{jn} = (\psi_{jn}^+ - \psi_{jn}^-)(a_+ - a_-)^{-1}. $$

These solutions are defined only on the tails. We introduce a ‘phase space’ $\mathbb{R}^{2k}$ with basis $(C_1, S_1, \ldots, C_k, S_k)$ and a skew-scalar product

$$\langle C_i, C_j \rangle = \langle S_i, S_j \rangle = 0, \quad \langle C_i, S_j \rangle = \delta_{ij}. $$

The operator $L$ determines the subspace $\Lambda_\infty^\lambda \subset \mathbb{R}^{2k}$ of vectors $\psi_\infty \in \Lambda_\infty^\lambda$, which can be extended to the whole graph $\Gamma$ as the solution

$$L\psi = \lambda\psi, \quad \psi = \psi_0 = (\psi_1^\infty, \ldots, \psi_k^\infty), \quad \psi_{j}^\infty = \alpha_j C_j + \beta_j S_j$$

in the tail $z_j$ for $n > n_0$.

Theorem 2. The subspace $\Lambda_\infty^\lambda$ is Lagrangian, that is, the scalar product on it is equal to zero.

The proof follows from Theorem 1. In fact, for any pair of solutions $\psi_1, \psi_2$ on $\Gamma$ we have $W = \sum_{j=1}^{k} \kappa_j z_j + \text{(finite)}$, where the $z_j$ are the tails. Only the differences $z_i - z_j$ can be extended to cycles on $\Gamma$ modulo $\infty$. Therefore we have $W = \sum_{l \geq 2} \mu_l(z_1 - z_l) + \text{(a finite cycle)} = \sum_{j=1}^{k} \kappa_j z_j + \text{(a finite chain)}$. Hence the theorem follows:

$$\sum_{j=1}^{k} \kappa_j = 0 = \langle \psi_1^\infty, \psi_2^\infty \rangle.$$

\[2\text{In 1971 I. M. Gelfand told the author about an interesting idea on the relation between self-adjoint extensions of symmetric operators and Lagrangian planes. This was Gel’fand’s reaction to the author’s paper [2], built round the relation between Hamiltonian formalism and differential topology.} \]
We represent the graph $\Gamma$ in the form $\Gamma = \Gamma' \cup K_1 \cup \cdots \cup K_s$, where the $K_i$ are trees growing from the vertices (‘nests’) $T_i \in \Gamma'$, with $\Gamma'$ a finite graph without ends (‘the base’), $s \leq k$.

**Theorem 3.** The dimension of the spaces of solutions of $L\psi = \lambda\psi$ on $\Gamma$ is always at least $k$. It is strictly greater than $k$ if and only if the Schrödinger operator $L'$, restricted to the base $\Gamma'$ has a ‘singular’ eigenvalue $\lambda'_p$, where $\psi'_p(t_l) = 0$ at all nests $l = 1, \ldots, s$. In this case and only in this case the operator that associates the vector $\psi_{\infty} \in \Lambda^\infty_\lambda$ with the solution of $L\psi = \lambda\psi$ has a non-trivial kernel.

The spectrum of the operator $L$ in the Hilbert space $L^2_\varepsilon(\Gamma) = H_\varepsilon, \varepsilon = 0, 1$ (vertices and edges) can be divided into a continuous part $|\lambda| \leq 2$ (scattering zone) and a discrete spectrum in the zones $\lambda < -2, \lambda > 2$. Points of the discrete spectrum inside the zone $|\lambda| \leq 2$ are possible only if localized on $\Gamma'$, where $\lambda = \lambda'$ is a singular eigenvalue. The algebraic properties of the scattering zone (unitarity) are entirely determined by Theorem 2. For $|\lambda| > 2$ we have $a_+a_- = 1, a_+ \in \mathbb{R}$. We consider a Lagrangian plane $\Lambda^-_\lambda \subset \mathbb{R}^{2k}$ with basis $\Psi_j^-, j = 1, \ldots, k$, decreasing at infinity.

**Proposition 1.** A point $\lambda \in \mathbb{R}$, is a point of the discrete spectrum for $L$ in $H_\varepsilon$ ($\varepsilon = 0, 1$) if $\Lambda^\infty_\lambda \cap \Lambda^-_\lambda$ is non-empty or $\lambda = \lambda'_p$ is a singular eigenvalue on the base $\Gamma'$. The Morse indices of eigenvalues for $\lambda \in [2, \infty]$ and $\lambda \in [-\infty, -2]$ are well-defined and equal to the algebraic numbers of the normal discrete eigenvalues. There is necessarily a discrete spectrum if: $\max_T (\sum b^2_{T,T'} + W^2_T) > 4, \max_R (\sum d^2_{R,R'} + W^2_R) > 4, \text{ or } \max_q |\lambda'_q| > 4$ for the spectrum of base $\Gamma'$.

**References**

[1] S. P. Novikov and I. A. Dynnikov, *Russian Math. Surveys* 52:5 (1997), 175–234.

[2] S. P. Novikov, *Izv. Akad. Nauk SSSR Ser. Mat.* 34 (1970), 253–288, 475–500; English transl. in *Math. Ussr-Izv.* 4 (1970).