

Spectral Properties of Schrödinger Operators on Decorated Graphs

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In the last few years, the spectral theory of the Laplace–Beltrami operator on periodic manifolds has attracted special attention (see, e.g., [1] and the references therein). Not the last of the reasons is the interest in the transport properties of carbon nanostructures composed of fullerenes and nanotubes [2], whose geometry is adequately modeled by the so-called hybrid manifolds, i.e., by topological spaces composed of manifolds of different dimensions. In this paper, we present several results concerning the spectrum of the Schrödinger operator on periodic decorated graphs, which are a special case of periodic hybrid manifolds and, in turn, include metric graphs (quantum networks) [3] as a special case.

In what follows, Γ denotes a certain oriented graph with the set V of vertices and the set E of edges. For each $v \in V$, we choose a compact Riemannian manifold M_v whose dimension does not exceed 3, and for each $e \in E$, we choose a segment

$$M_e = [a_1(e), a_2(e)] \subset \mathbb{R}, \quad \text{where } a_1(e) \leq a_2(e).$$

A topological space obtained from the disjoint union Y of manifolds M_v and segments M_e by gluing each point $a_1(e)$ (respectively, $a_2(e)$) to the manifold M_v , where v is the starting point (respectively, the endpoint) of the edge e , will be called a *decorated graph* X . We note that if all the manifolds M_v , $v \in V$, are zero-dimensional and all the segments M_e , $e \in E$, are nondegenerate, then the decorated graph is exactly a *metric graph*.

By Ξ we denote the disjoint union of the sets V and E . Then, under the natural definition of the space $L^2(X)$, we have the identification

$$L^2(X) \simeq \bigoplus_{\xi \in \Xi} L^2(M_\xi).$$

For each $\xi \in \Xi$, we choose a Schrödinger operator H_ξ in $L^2(M_\xi)$ determined by a second-order differential expression on M_ξ with sufficiently smooth coefficients and (for $\xi \in E$) by self-adjoint boundary conditions at the endpoints of the segment M_ξ . Then the Schrödinger operator on X can be defined as follows. Suppose that S_ξ is the restriction of H_ξ to the set of all functions defined on the domain $\mathcal{D}(H_\xi)$ and vanishing at the points of gluing, S is the direct sum of all S_ξ , and $\xi \in \Xi$. Any self-adjoint extension of the operator S will be called a *Schrödinger operator* on X . It is convenient to describe all the Schrödinger operators generated by S by using the Krein formula for resolvents. To do this, we denote the direct sum of all H_ξ by H^0 and, for each $\xi \in \Xi$, introduce an auxiliary Hilbert space \mathcal{G}_ξ whose dimension coincides with the deficiency number of

the operator S_ξ . Suppose that γ_ξ and Q_ξ are, respectively, the Γ -field and the Q -function of the pair (H_ξ, S_ξ) [4]; in particular, $\gamma_\xi(z)$ (respectively, $Q_\xi(z)$) is a bounded linear operator from \mathcal{G}_ξ to $L^2(M_\xi)$ (respectively, from \mathcal{G}_ξ to \mathcal{G}_ξ) for each regular value z of the operator H^0 . Now, we set

$$\mathcal{G} = \bigoplus_{\xi \in \Xi} \mathcal{G}_\xi, \quad \gamma = \bigoplus_{\xi \in \Xi} \gamma_\xi, \quad Q = \bigoplus_{\xi \in \Xi} Q_\xi.$$

Then the following formula determines a bijection between the resolvents of all self-adjoint extensions H of the operator S and the self-adjoint (generally, multivalued) operators Λ in \mathcal{G} :

$$(H - z)^{-1} = (H^0 - z)^{-1} - \gamma(z)[Q(z) - \Lambda]^{-1}\gamma^*(\bar{z}).$$

The extension of H corresponding to Λ will be denoted by H_Λ . An operator Λ is single-valued if and only if H_Λ and H^0 are disjoint, i.e.,

$$\mathcal{D}(H_\Lambda) \cap \mathcal{D}(H^0) = \mathcal{D}(S).$$

To simplify the subsequent statements, we assume that H_Λ and H^0 are disjoint. We note that, in fact, this assumption does not lead to a loss of generality: the graphs of all Λ are exactly Lagrangian subspaces in $\mathcal{G} \times \mathcal{G}$ with respect to the standard skew-Hermitian product [5]; obviously, the graphs of single-valued operators form Lagrangian planes in general position.

We shall consider periodic decorated graphs and gauge-periodic operators H_Λ on them. To do this, we assume that a discrete group G acts freely on a graph Γ ; in particular, the action of the group G on Ξ is given. Assuming that $M_{g\xi} = M_\xi$, $g \in G$, $\xi \in \Xi$, and the points of gluing are invariant under the action of G on Y , we obtain the natural action of G on X . Now, let σ be a 2-cocycle on G ranging in $\mathbf{U}(1)$. Closed linear operators A in $L^2(X)$ with $(G, \bar{\sigma})$ -invariant resolvents are said to be *gauge-periodic*. If we have $\sigma = 1$ in this case, then A is said to be *periodic*. In what follows, we assume that $H_{g\xi} = H_\xi$ for any $g \in G$. Then we can easily prove that the *Schrödinger operator H_Λ is gauge-periodic if and only if Λ is $(G, \bar{\sigma})$ -invariant*. Everywhere below, the *last condition is assumed to be satisfied*.

Next, we assume that G acts on Γ with finitely many orbits. We let F denote the fundamental set of the action of G on Ξ , i.e., a subset Ξ containing a single representative of each orbit. By $C_r^*(G, \sigma)$ we denote the reduced twisted group C^* -algebra of the group G with factor σ [6], and by \mathcal{H}_f (respectively, by \mathcal{G}_f) the space $\bigoplus_{\xi \in F} L^2(M_\xi)$ (respectively, $\bigoplus_{\xi \in F} \mathcal{G}_\xi$). The space of all compact linear operators in the Hilbert space \mathcal{H} will be denoted by $\mathcal{K}(\mathcal{H})$, and the standard trace in

$$C_r^*(G, \sigma) \otimes \mathcal{K}(\mathcal{H}_f)$$

will be denoted by Tr . Since \mathcal{G}_f is a finite-dimensional space, the following theorem significantly simplifies the study of the spectrum of the gauge-periodic operator H_Λ (in this theorem and in what follows, we identify the spaces $L^2(X)$ and \mathcal{G} with $l^2(G, \mathcal{H}_f)$ and $l^2(G, \mathcal{G}_f)$, respectively).

Theorem 1. *Let Λ belong to the C^* -algebra $C_r^*(G, \sigma) \otimes \mathcal{K}(\mathcal{G}_f)$. Then the resolvent of the operator H_Λ belongs to $C_r^*(G, \sigma) \otimes \mathcal{K}(\mathcal{H}_f)$.*

The assumption of Theorem 1 is satisfied for the very important case in which Λ is a bounded operator in \mathcal{G} and its standard matrix representation has only finitely many nonzero diagonals. Moreover, we assume that G is equipped with a left-invariant metric ρ . Then, using the methods proposed in [7], we can prove the following theorem.

Theorem 2. *Suppose that Λ is a bounded operator and there exist constants C and $\delta > 0$ such that, for all $\alpha, \beta \in G$, the matrix elements $\Lambda(\alpha, \beta)$ satisfy the condition*

$$\|\Lambda(\alpha, \beta)\| \leq C\eta(\rho(\alpha, \beta))^{-1-\delta},$$

where $\eta(R)$ is the number of elements in the ball of radius R . Then $\Lambda \in C_r^*(G, \sigma) \otimes \mathcal{K}(\mathcal{G}_f)$.

In what follows, we assume that H_Λ is semibounded below, which is the case under very general assumptions on H_ξ and Λ . We fix a real number $E' < \inf \text{spec}(H^\Lambda)$ and, for $E \notin \text{spec}(H^\Lambda)$, define

$$N(E) := \begin{cases} \text{Tr } P_{[E', E]}, & E \geq E'; \\ 0, & E < E', \end{cases}$$

where P is the spectral projection operator for H_Λ .

Corollary 1. *Under the assumptions of Theorem 1, the values of $N(E)$ lie in a countable set of real numbers $\text{Tr}(K_0 C_r^*(G, \sigma))$, where K_0 is the corresponding component of the K -functor on the category of C^* -algebras.*

It is said that the pair (G, σ) has the *Kadison property* if the traces of all nonzero self-adjoint projection operators from $C_r^*(G, \sigma) \otimes \mathcal{K}(l^2)$ are bounded away from zero. In particular, each pair $(\mathbb{Z}^m, 1)$, $m \geq 1$, has the Kadison property; more examples can be found in [8].

Corollary 2. *If, under the assumptions of Theorem 1, the pair (G, σ) has the Kadison property, then the spectrum of the operator H_Λ has a zone structure.*

It is said that the C^* -algebra A has the *RR I_0 property* if A has an exact state F such that each self-adjoint element from A can be approximated (with arbitrary accuracy) by an element with finite spectrum whose spectral projection operators are arbitrarily small on F [9]. The proof of the following corollary is based on an argument from [10].

Corollary 3. *Suppose that the assumptions of Theorem 1 are satisfied. Suppose additionally that the C^* -algebra $C_r^*(G, \sigma) \otimes \mathcal{K}(\mathcal{H}_f)$ has the RR I_0 property. Then the operator H_Λ can be approximated with arbitrary accuracy in the sense of uniform resolvent convergence by operators with a Cantor spectrum from $C_r^*(G, \sigma) \otimes \mathcal{K}(\mathcal{H}_f)$.*

Next, we assume that G is an Abelian group without torsion; then $G \simeq \mathbb{Z}^d$, and, in G , we fix the standard metric ρ of the group \mathbb{Z}^d .

Theorem 3. *Suppose that*

$$\Lambda(\alpha, \beta) \leq c_1 \exp(-c_2 \rho(\alpha, \beta))$$

with constants $c_1, c_2 > 0$. Then H_Λ has a zone spectrum without any singular continuous component.

Remark. Simple examples show that, under the assumptions of Theorem 3, the operator H_Λ can have eigenvalues.

In [11], one can find examples of the Schrödinger operator on a periodic decorated graph X , $\dim X \geq 2$, whose spectrum has infinitely many gaps, i.e., for which the Bethe–Sommerfeld hypothesis is not true [12]. We show that this hypothesis is not true for a rather wide class of periodic decorated graphs.

Theorem 4. *Suppose that G acts transitively on the set of vertices of the graph Γ . Suppose that the operator H_v (which is independent of v in this case) has infinitely many eigenvalues whose multiplicity is greater than the degree of the vertex v (which is also independent of v). Suppose also that all segments M_e are degenerate. Then, when the points of gluing are in general position, the spectrum of H_Λ has infinitely many lacunas both in the sense of the Lebesgue–Riemann measure and in the sense of the Baire category.*

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