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QUANTUM GRAPHS FEATURING UNUSUAL SELF-ADJOINT EXTENSIONS

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Abstract. We present an example of a simple quantum graph with “vertices at infinity”, which appear due a strongly attractive potential making the spectral problem quantum-mechanically incomplete. We construct the appropriate self-adjoint extensions of the formal graph Hamiltonian, and derive their spectral properties.

Keywords: Quantum graphs, self-adjoint extensions, discrete spectrum.

1. Introduction

This paper is devoted to the memory of *Miloslav Havlíček*, my teacher, colleague and dear friend for no less than six decades, who passed away last year. We worked together on various problems, for instance, the dynamics of open quantum systems or canonical realisations of Lie algebras. We also wrote and rewrote, coauthored by late Jiří Blank, a book on Hilbert space operators in quantum physics which became, for many, a standard reference source. I always admired in Miloslav his ability to go to the core of a question; he liked examples that were not overly technical but expressed the essence of the problem. For this paper, I choose an example showing an unusual behaviour of quantum graphs; I hope he would like it.

The term *quantum graphs* is a common shorthand for models describing quantum-mechanical dynamics on metric graphs, described mostly by an appropriate Schrödinger operator, however, Dirac, nonlinear Schrödinger, and other operators are also considered in this context. The idea can be traced back to a simple model in quantum chemistry [1], but the concept attracted attention only half a century later, motivated in part by development of microfabrication techniques in solid-state physics. Since then there was a lot of activity in this area; for the current state of art we refer to the monographs [2–4].

One of the most common classes of quantum graphs concerns Schrödinger dynamics on a graph consisting of a compact core in the form of a finite graph to which a finite number of semiinfinite “leads” is connected; one usually investigates spectral and scattering properties of such systems in dependence on the topology and geometry of the core and coupling of the wave functions at the graph vertices. The leads in these problems play mostly a “service role” only, bringing the particles in and out; they communicate mutually only through the core. The aim of this note is to show that this may not be the case if the potential of the corresponding Schrödinger operator makes the problem *quantum-mechanically incomplete* in the language of Reed and Simon [5, App. to Sec. X.1].

We consider the simplest situation of this type when the core is restricted to a single vertex in which N halfline edges meet; the vertex coupling is supposed to be free of any interaction being described by Kirchhoff conditions, cf. (2) below. The potential on the edges is attractive and decreases with the fourth power of the distance from the vertex. We consider only star graphs with a genuine branching, $N \geq 3$. The case $N = 2$, equivalent to the motion on line, is discussed in detail in [6], including topics we do not touch here, such as approximations of self-adjoint extensions or Feynman path-integral expression of the time evolution.

2. Star graph with limit-circle lead ends

Consider a star graph consisting of N halfline edges connected at a single vertex. The state Hilbert space of the system is $\mathcal{H} = \sum_j^{\oplus} L^2(\mathbb{R}_+)$, its elements being written as $\psi = \{\psi_j\}$. We are interested in the operator $H\colon\; H\psi = \{H\psi_j\}$ acting as

$$(H\psi_j)(x) = -\psi_j''(x) - x^4\psi_j(x); \tag{1}$$

the domain $D(H)$ of H is chosen to consist of functions from $\sum_j^{\oplus} C_0^\infty(\mathbb{R}_+)$ satisfying the Kirchhoff conditions at the star graph vertex,

$$\psi_j(0) = \psi_k(0), \quad j,k = 1,\dots,N, \tag{2a}$$

$$\sum_{j=1}^{N} \psi_j'(0) = 0. \tag{2b}$$

Speaking of $C_0^\infty(\mathbb{R}_+)$, we suppose that the supports of the functions may contain zero, and $\psi_j(0)$ and $\psi_j'(0)$

are understood as right limits there. As such, the operator is densely defined and symmetric but not closed; it is straightforward to find its adjoint which acts as (1) again on the definition domain $D(H^*)$, consisting of all vector-valued functions $\psi \in \mathcal{H}$ such that $\psi_j \in H^2_{\mathrm{loc}}(\mathbb{R}_+)$ and $-\psi_j'' - x^4\psi_j$ understood in the sense of distributions belongs to $L^2(\mathbb{R}_+)$. The operator H is symmetric but not essentially self-adjoint because H^* is not symmetric; as is usual with Sturm-Liouville-type operators, this would require the boundary form

$$\mathcal{B}(\phi,\psi) := (H^*\phi,\psi) - (\phi,H^*\psi) \tag{3a}$$

to vanish for all $\phi,\psi \in D(H^*)$. This form can be expressed explicitly through integration by parts and decomposes naturally into the sum

$$\mathcal{B}(\phi,\psi) = \mathcal{B}_0(\phi,\psi) + \mathcal{B}_\infty(\phi,\psi), \tag{3b}$$

where

$$\mathcal{B}_0(\phi,\psi) := \sum_{j=1}^{N} \big(\bar\phi'\psi - \bar\phi\psi'\big)(0) \tag{3c}$$

and the other part related to the behaviour of functions from $D(H^*)$ at large values of the argument we shall specify later. The choice of the conditions (2) ensures that the operator is "locally self-adjoint", meaning that $\mathcal{B}_0(\phi,\psi) = 0$ holds, or in other words, that the probability current is conserved at the vertex. In view of the strong negative potential, however, it is not "globally" self-adjoint:

Proposition 2.1. *Operator* (1) *has deficiency indices* (N,N) *and is bounded neither from above nor from below. Any self-adjoint extension of it has a purely discrete spectrum of multiplicity not exceeding* N.

Proof. The "two-sided" unboundedness of H is easy to check. It is sufficient to choose a suitable family of functions of the domain, say, $\psi_\sigma = \big\{\delta_{j1}\sigma^{-\frac12} f\big(\frac{\cdot}{\sigma}\big)\big\}$ with $\sigma > 0$, where f is a non-vanishing function from $C_0^\infty(\mathbb{R}_+)$ with $\operatorname{supp} f \subset [1,2]$; then a straightforward computation yields the expression

$$(\psi_\sigma, H\psi_\sigma) = \sigma^{-2}\|f'\|^2 - \sigma^4\|x^2 f\|^2,$$

which tends to $\pm\infty$ as $\sigma \to 0+$ and $\sigma \to \infty$, respectively. Consider next the Dirichlet-decoupled counterpart to H, i.e. the direct sum $H^{\mathrm{D}} = \sum_j^{\oplus} H_j^{\mathrm{D}}$, where the operators H_j^{D} on $L^2(\mathbb{R}_+)$ act as (1) on functions from $C_0^\infty(\mathbb{R}_+)$ satisfying $\psi_j(0) = 0$. As H^{D} is a direct sum, its spectral properties are determined by those of its components. The latter have fixed boundary condition at zero and are limit circle at infinity as we shall see a little below, hence each of them has deficiency indices $(1,1)$, [7, Sec. XIII.6] or [5, App. to Sec. X.1], and consequently, the deficiency indices of H^{D} are (N,N).

Since the deficiency indices are finite and equal, every maximal symmetric extension of H^{D} is self-adjoint; the family of such extensions depends on N^2 real parameters. Let $\hat H^{\mathrm{D}}$ be a fixed self-adjoint extension. Its essential spectrum is empty: since for our edge potential $v(x) = -x^4$, both the functions $x \mapsto |v(x)|^{-\frac12} = x^{-2}$ and

$$x \mapsto \left(\left(\frac{v'}{|v|^{\frac32}}\right)' - \frac14\,\frac{(v')^2}{|v|^{\frac52}}\right)(x) = -16\,x^{-4}$$

belong to $L(1,\infty)$, we infer that $\sigma_{\mathrm{ess}}(H_j^{\mathrm{D}}) = \emptyset$ holds for $j = 1,\dots,N$, cf. [7, Sec. XIII.7.16], and the same is true for $\sigma_{\mathrm{ess}}(H^{\mathrm{D}})$, hence the spectrum of $\hat H^{\mathrm{D}}$ is purely discrete. We note that the adjoint of H^{D} is also a direct sum, $(H^{\mathrm{D}})^* = \sum_j^{\oplus}(H_j^{\mathrm{D}})^*$, and the family of self-adjoint extensions of H^{D} contains those which preserve the direct-sum form, obtained by imposing boundary condition at infinity componentwise. We pick one such extension with the property that the boundary condition at infinity is *the same* at each edge, denoting it as $\tilde H^{\mathrm{D}}$; as is usual with Sturm-Liouville problems, eigenvalues of its component operators are simple, and consequently, eigenvalues of $\tilde H^{\mathrm{D}}$, which is a direct sum of copies of the same operator, are of multiplicity N. We observe that $\hat H^{\mathrm{D}}$ and $\tilde H^{\mathrm{D}}$ are self-adjoint extensions of the same symmetric operator of the deficiency indices not exceeding N, namely H^{D}; in such a case, in each spectral gap of $\tilde H^{\mathrm{D}}$ there is at most N eigenvalues of $\hat H^{\mathrm{D}}$, counting multiplicity, cf. [8, Corr. 1 to Thm. 8.19], hence the multiplicity $\sigma_{\mathrm{disc}}(\hat H^{\mathrm{D}})$ cannot exceed that of $\sigma_{\mathrm{disc}}(\tilde H^{\mathrm{D}})$.

Next, we apply the analogous argument at the "other end" of the edges. We consider the self-adjoint extension $\hat H$ of the original operator H obtained by modifying $\hat H^{\mathrm{D}}$: we keep the requirements on the behavior of the functions at infinity that guarantee vanishing of the form $\mathcal{B}_\infty(\cdot,\cdot)$, but replace the Dirichlet condition at the vertex by (2). By Krein's formula [9] the resolvents of $\hat H$ and H^{D} differ by an operator of rank not exceeding N (in fact, equal to $N-1$), hence their essential spectra coincide and we get $\sigma_{\mathrm{ess}}(\hat H) = \emptyset$. Furthermore, both $\hat H$ and H^{D} are self-adjoint extensions of the same symmetric operator of the deficiency indices not exceeding N (the domain of which is obtained by imposing the conditions $\psi_j(0) = \psi_j'(0) = 0$ for $j = 1,\dots,N$), and since the eigenvalues come from zeros of (the determinant of) the denominator of the second term in Krein's formula which is an analytic matrix-valued function of the spectral parameter of the rank not exceeding N, the multiplicity $\sigma_{\mathrm{disc}}(\hat H)$ cannot exceed that of $\sigma_{\mathrm{disc}}(\hat H^{\mathrm{D}})$. ∎

After this preliminary, let us look how the self-adjoint extensions of H look like. Since every extension refers to a subspace of $D(H^*)$, we employ the standard decomposition of this set,

$$D(H^*) = D(\bar H) \oplus \mathcal{K}_+ \oplus \mathcal{K}_-, \tag{4}$$

where $\mathcal{K}_\pm = \mathrm{Ker}(H^* \mp i)$ are the deficiency spaces; we already know that in our case, their dimension is N. To construct the extensions, one can use different methods. The classical one, due to J. von Neumann, uses isometric maps from $\mathcal{K}_+$ to $\mathcal{K}_-$ [5, Sec. X.1]. If the operator in question is differential, it is usually simpler to employ appropriate boundary conditions; this approach finds its abstract form in the theory of boundary triples [10]. Here, we follow neither of the two paths, but our construction is closer to the latter since it expresses the second part of the form (3b) by means of generalised boundary values.

To define them, we note that while we cannot solve the deficiency equations, $-\psi''(x) - (x^4 \pm i)\psi(x) = 0$, explicitly, the knowledge of the potential allows us to determine the asymptotic behaviour for large values of the argument, which is what would matter: components of any such solution are linear combinations of a pair of functions satisfying

$$\varphi_\pm(x) = \frac{\mathrm{e}^{\pm \frac{ix^3}{3}}}{x}\big(1 + \mathcal{O}(x^{-1})\big), \tag{5a}$$

$$\varphi'_\pm(x) = \pm ix\,\mathrm{e}^{\pm \frac{ix^3}{3}}\big(1 + \mathcal{O}(x^{-1})\big), \tag{5b}$$

cf. [11, Thm. 6.2.2]; since the solutions belong, in view of elliptic regularity, to $C^\infty(\mathbb{R}_+)$, both functions (5a) are obviously elements of $L^2(\mathbb{R}_+)$.

To use the asymptotics (5), one has to make sure that the sought boundary values will be determined by elements of the deficiency subspaces only.

Lemma 2.2. *The domain $D(\bar H)$ of the closure $\bar H$ consists of all the functions $\psi \in D(H^*)$ satisfying*

$$\lim_{x\to\infty} x\psi_j(x) = \lim_{x\to\infty} \frac{\psi'_j(x)}{x} = 0, \quad j = 1,\dots,N.$$

Proof. Recall that the decomposition (4) is orthogonal with respect to the scalar product $(\phi,\psi)_H := (\phi,\psi) + (H^*\phi, H^*\psi)$. In particular, any vectors $\psi \in D(\bar H)$ and $\phi \in \mathcal{K}_+$ are in this sense orthogonal, and since $H^*\phi = i\phi$, we have $(\psi,\phi) + i(H^*\psi,\phi) = 0$, or

$$\sum_{j=1}^N \big((\psi_j,\phi_j) + i(H^*\psi_j,\phi_j)\big) = 0 \tag{6}$$

(we use here the convention in which the scalar product is linear in the second argument). Next, we use the explicit expression of the second part on the left-hand side and move H^* to the other side of the scalar product using double integration by parts over the interval $[0,\tilde x)$, and since $H^*\phi_j = i\phi_j$ by assumption, we arrive at the relation

$$\lim_{\tilde x\to\infty} \sum_{j=1}^N \big[-\psi'_j(x)\overline{\phi_j(x)} + \psi_j(x)\overline{\phi'_j(x)}\,\big]_0^{\tilde x} = 0.$$

Furthermore, the contribution from the values at $x = 0$ vanishes in view of condition (2), and since there is no correlation between the values as $x \to \infty$, we get

$$\lim_{x\to\infty} \big[-\psi'_j(x)\overline{\phi_j(x)} + \psi_j(x)\overline{\phi'_j(x)}\,\big] = 0 \tag{7a}$$

for any $j = 1,\dots,N$. The vector $\psi \in D(\bar H)$ was supposed to be arbitrary, in particular, we can choose it real-valued; taking complex conjugate, we also get

$$\lim_{x\to\infty} \big[-\psi'_j(x)\phi_j(x) + \psi_j(x)\phi'_j(x)\,\big] = 0. \tag{7b}$$

We denote the left-hand side of (7a) by $b(\psi_j,\phi_j)$ and choose for ϕ_j a vector with one of the asymptotics (5); then $b(\psi_j,\varphi_+) = \overline{b(\psi_j,\varphi_-)}$ equals

$$b(\psi_j,\varphi_+) = \lim_{x\to\infty}\Big[-\frac{\psi'_j(x)}{x} - ix\psi_j(x)\Big]\mathrm{e}^{-\frac{ix^3}{3}} = 0,$$

and similarly, from (7b) we get

$$b(\psi_j,\bar\varphi_-) = \lim_{x\to\infty}\Big[-\frac{\psi'_j(x)}{x} + ix\psi_j(x)\Big]\mathrm{e}^{-\frac{ix^3}{3}} = 0.$$

Thus the limits of the two square brackets have to be simultaneously zero, from which the claim follows. ∎

It follows from (5) and the above lemma that away from the vertex, the components of any vector $\psi \in D(H^*)$ can be expressed as

$$\psi_j(x) = A_j^{\mathrm{in}}(\psi)\,\frac{\mathrm{e}^{\frac{ix^3}{3}}}{x} + A_j^{\mathrm{out}}(\psi)\,\frac{\mathrm{e}^{-\frac{ix^3}{3}}}{x} + u_j(x) \tag{8}$$

with some $u = \{u_j\} \in D(\bar H)$ and the amplitudes

$$A_j^{\mathrm{in/out}}(\psi) := \frac{1}{2i}\lim_{x\to\infty}\Big(ix\psi_j(x) \pm \frac{\psi'_j(x)}{x}\Big)\mathrm{e}^{\mp\frac{ix^3}{3}}, \tag{9}$$

which are the sought generalised boundary values; by the lemma, $A_j^{\mathrm{in/out}}(\psi) = 0$ holds for any $\psi \in D(\bar H)$.

To find self-adjoint extension of H we have to evaluate the form $\mathcal{B}_\infty : D(H^*) \times D(H^*) \to \mathbb{C}$ given by

$$\mathcal{B}_\infty(\phi,\psi) := \lim_{x\to\infty}\sum_{j=1}^N \big(\bar\phi\psi' - \bar\phi'\psi\big)(x).$$

Substituting from (9) and using Lemma 2.2, we obtain by a straightforward computation

$$\mathcal{B}_\infty(\phi,\psi) = 2i\sum_{j=1}^N\Big(\overline{A_j^{\mathrm{in}}(\phi)}A_j^{\mathrm{in}}(\psi) - \overline{A_j^{\mathrm{out}}(\phi)}A_j^{\mathrm{out}}(\psi)\Big); \tag{10a}$$

introducing vector functions $A^{\mathrm{in/out}}(\cdot) = \{A_j^{\mathrm{in/out}}(\cdot)\}$ with values in $\mathbb{C}^N$, we can rewrite it concisely as

$$\mathcal{B}_\infty(\phi,\psi) = 2i\big((A^{\mathrm{in}}(\phi), A^{\mathrm{in}}(\psi)) - (A^{\mathrm{out}}(\phi), A^{\mathrm{out}}(\psi))\big). \tag{10b}$$

This has an easy consequence:

Theorem 2.3. *There is a bijective correspondence between self-adjoint extensions of operator H and 2×2 unitary matrices allowing us to use such matrices as the extension label. The domain of an extension H_U consist of those $\psi \in D(H^*)$, which satisfy*

$$A^{\mathrm{in}}(\psi) = UA^{\mathrm{out}}(\psi). \tag{11}$$

Remark 2.4. Mathematically speaking, it makes no difference if we put U or U^* on the right-hand side of (11). We made this choice to stress the heuristic "scattering-at-infinity" character of the condition (11), namely that the particle moving away from the vertex reaches infinity at a finite time and reenters the edges from their infinitely distant "endpoints".

3. Properties of the extensions

Let us now look at properties of various self-adjoint extensions we have obtained. To begin with, it follows from (11) that for any H_U, we have

$$\sum_{j=1}^{N}\big(|A_j^{\mathrm{out}}(\psi)|^2-|A_j^{\mathrm{in}}(\psi)|^2\big)=0, \qquad (12)$$

which expresses the current conservation; recall that $J_j(\psi):=|A_j^{\mathrm{out}}(\psi)|^2-|A_j^{\mathrm{in}}(\psi)|^2$ is the *net outward probability current* on the j^{th} edge. In particular, the j^{th} current component vanishes if $A_j^{\mathrm{in}}(\psi)=\mathrm{e}^{i\theta_j}A_j^{\mathrm{in}}(\psi)$ for some $\theta_j\in\mathbb{R}$. The graph supports no current at all if and only if the matrix U is diagonal,

$$U=\mathrm{diag}\big(\mathrm{e}^{i\theta_1},\dots,\mathrm{e}^{i\theta_N}\big) \qquad (13)$$

for some $\theta_j\in(-\pi,\pi]$; in such a case, we speak of boundary conditions *fully separated at infinity*. The separation at infinity can be partial only; this happens if there is a nonempty $K\subset\{1,\dots,N\}$ with $\#K<N$ such that $A^{\mathrm{in}}(\psi)=\mathrm{e}^{i\theta_k}A^{\mathrm{out}}(\psi)$ for $k\in K$, i.e. when $U=D_M\oplus\tilde U$ where $\tilde U$ is an $(N-M)\times(N-M)$ non-diagonal unitary matrix and D_M is $M\times M$ of the type (13). One can label such a separation at infinity Dirichlet (Neumann, Robin), if $\theta_k=\pi$ ($\theta_k=0$ or $\theta_k\neq 0 \pmod{\pi}$), respectively. On any edge with separation at infinity, the probability current is naturally zero.

Another important class of the extension are those invariant with respect to the *time reversal*. In the absence of internal degrees of freedom, the swap of the time arrow orientation is described by the antilinear operator $\psi\mapsto\bar\psi$. The invariance thus means that $\bar U=U$, and since U is unitary, we see that H_U is time-reversal-invariant if and only if matrix U is *invariant with respect to the transposal*,

$$U=U^{\mathrm{T}}. \qquad (14)$$

Furthermore, it follows easily from (9) that

$$\overline{A_j^{\mathrm{in/out}}(\psi)}=A_j^{\mathrm{out/in}}(\bar\psi)\ \text{ for any }\ \psi\in D(H^*); \qquad (15)$$

thus indicating the dependence of the probability current on the chosen extension, we get

$$J_j(\psi;U^{\mathrm{T}})=-J_j(\psi;U),\quad j=1,\dots,N, \qquad (16)$$

as one should naturally expect.

Remark 3.1. The j^{th} component of the probability current vanishes for a given U if and only if $|A_j^{\mathrm{out}}(\psi)|=|A_j^{\mathrm{in}}(\psi)|$ holds for all $\psi\in D(H_U)$. The corresponding asymptotics of the j^{th} component of those functions, in particular, of any eigenvector of H_U, is then real-valued up to an overall phase factor, $\psi_j(x)=C_j\cos\big(\frac{x^3}{3}+\eta_j\big)\big(1+\mathcal{O}(x^{-1})\big)$ with some $\eta_j\in(-\pi,\pi]$ as $x\to\infty$.

Another subclass consists of the extension that are invariant *with respect to all permutations of the star edges*. Such a transformation leads to a simultaneous permutation of the rows and columns of the matrix U. Should this include all such permutations, it is easy to see that it singles out of the entire N^2-parameter family of the operators H_U a two-parameter subfamily, namely those with

$$U=\big(U_{ij}\big),\quad U_{ij}=b-a\delta_{ij}, \qquad (17a)$$

where the unitarity requires the numbers $a,b\in\mathbb{C}$ to obey

$$|a|=1 \quad\text{and}\quad |a+Nb|=1; \qquad (17b)$$

such a matrix is Hermitean having simple eigenvalue a and eigenvalue $a+Nb$ of multiplicity $N-1$, cf. [12]. A particular case with

$$a=-1,\quad b=\frac{2}{N}, \qquad (18)$$

is a natural counterpart of the condition (2) imposed at the vertex; we call it *Kirchhoff condition at infinity*.

A wider, N-parameter family of extensions corresponds to the situations when the matrix is *circulant* [13]. Recall that in general, such matrices are of the form

$$\begin{pmatrix} c_0 & c_1 & \cdots & c_{n-2} & c_{n-1}\\ c_{n-1} & c_0 & c_1 & & c_{n-2}\\ \vdots & c_{n-1} & c_0 & \ddots & \vdots\\ c_2 & & \ddots & \ddots & c_1\\ c_1 & c_2 & \cdots & c_{n-1} & c_0 \end{pmatrix} \qquad (19)$$

and that they belong to the class of Toeplitz matrices in which they are distinguished by the "two-sided cyclicity" in the antidiagonal direction; matrices (17) represent a particular case with $c_0=b-a$ and $c_k=b$ for $k=1,\dots,N-1$. Not every such matrix is unitary, of course; to find the condition which ensures unitarity, generalising (17b), we recall that all circulant matrices of the same dimension have a common orthonormal basis of eigenvectors, namely

$$v_k=\frac{1}{\sqrt{N}}\Big(1,\omega^k,\omega^{2k},\dots,\omega^{(N-1)k}\Big)^{\mathrm{T}} \qquad (20)$$

with $k=0,1,\dots,N-1$, where $\omega:=\mathrm{e}^{\frac{2\pi i}{N}}$ are complex roots of unity, and the k^{th} eigenvalue is

$$\lambda_k=c_0+c_1\omega^k+c_2\omega^{2k}+\dots+c_{N-1}\omega^{(N-1)k}; \qquad (21)$$

therefore, to get a unitary circulant matrix, the generating sequence $(c_0,\dots,c_{N-1})$ must satisfy $|\lambda_k|=1$ for $k=0,\dots,N-1$. Let us also recall that every circulant matrix is diagonalised by the discrete Fourier transform represented by the matrix

$$F=\begin{pmatrix} 1 & 1 & 1 & 1 & \dots & 1\\ 1 & \omega & \omega^2 & \omega^3 & \dots & \omega^{(N-1)}\\ 1 & \omega^2 & \omega^4 & \omega^6 & \dots & \omega^{2(N-1)}\\ \vdots & \vdots & \vdots & \vdots & & \vdots\\ 1 & \omega^{N-1} & \omega^{2(N-1)} & \omega^{3(N-1)} & \dots & \omega^{(N-1)^2} \end{pmatrix},$$

so that

$$D = \frac{1}{N} F^* C F = \operatorname{diag}\big(\lambda_0, \lambda_1, \dots, \lambda_{N-1}\big). \tag{22}$$

Since F is unitary, we have $C = \frac{1}{N} F D F^*$, which yields

$$c_k = \frac{1}{N}\Big(\lambda_0 + \lambda_1 \omega^{-k} + \dots + \lambda_{N-1}\omega^{-(N-1)k}\Big); \tag{23}$$

hence $N \times N$ unitary circulant matrices can be indeed characterised by N real parameters.

The symmetries considered up to now did not require to consider the star graph as embedded in a Euclidean space; if this is the case, other possibilities open. For simplicity, let us restrict to the situation where the star is *planar*, that is, embedded in $\mathbb{R}^2$. The edges numbering then defines the order in which they appear if we go around the vertex. Observing such a graph in a mirror, the order is reversed, which means that we can associate the *parity* transformation of a planar star graph with the passage from H_U to $H_{U^{\mathrm{T}}}$. A comparison with (15) then shows that star graphs with a circulant coupling are $\mathcal{PT}$*-symmetric*, i.e. invariant with respect to the combination of the parity and time reversal transformations.

In more detail, an $\big(\lfloor \frac{N}{2} \rfloor + 1\big)$-parameter part of this family exhibits these symmetries separately, while its $\big(\lfloor \frac{N-1}{2} \rfloor\big)$-parameter counterpart for which $U \neq U^{\mathrm{T}}$ shows a "genuine" $\mathcal{PT}$-symmetry. To put this observation in context, let us add that circulant matrices in relation to quantum graphs were first considered by Astudillo et al. [14], but those authors looked, in the spirit of [15], for graphs with non-selfadjoint dynamics having a real spectrum. A nontrivial $\mathcal{PT}$-symmetry of self-adjoint quantum graph Hamiltonians was noted in [16] for graphs with the "usual" vertices; the present discussion shows that the observation also extends to situations with a "coupling at infinity".

4. Spectrum of H_U

Let us turn to spectral properties of the obtained self-adjoint extensions. We know from Proposition 2.1 that the spectrum of any operator H_U is purely discrete and its multiplicity does not exceed N; now we can say more. As a preliminary, let us fix a family of parameters characterising $N \times N$ unitary matrices, as a subset of $\mathbb{R}^{N^2}$. We use the relation $U = \frac{\coth A + i}{\coth A - i}$, which defines a bijection between our unitary matrices and Hermitean matrices A with $\|A\| \leq 1$, and use the elements of the unit ball in $\mathbb{R}^{N^2}$ with the coordinates being N real numbers for the diagonal elements of A together with $\frac{1}{2}N(N-1)$ pairs of real numbers characterising the complex above-diagonal elements.

Theorem 4.1. *(i) The spectrum is not simple if the H_U is time-reversal invariant and there are an index j and a function $\psi \in D(H_U)$ such that $J_j(\psi) \neq 0$.*

(ii) As a function of U, the spectrum of H_U is generically simple, that is, the subset of the parameter space for which this is not true has Lebesgue measure zero.

(iii) There are matrices U such that every eigenvalue of H_U is either simple or it has multiplicity $N-1$.

Proof. (i) If ψ is an eigenfunction of a time-reversal invariant operator H_U, the same is true for its complex conjugate function $\bar{\psi}$. Since $|A_j^{\mathrm{out}}(\psi)| \neq |A_j^{\mathrm{in}}(\psi)|$ by assumption, the asymptotics of ψ cannot be represented by a real function, cf. Remark 3.1, which means that ψ and $\bar{\psi}$ must be linearly independent.

(ii) We employ the above described parametrisation. By negation of the previous claim, if the spectrum is simple, then $U \neq U^{\mathrm{T}}$ or $J_j(\psi) = 0$ for all j and $\psi \in D(H_U)$. The first condition excludes only transposal-invariant matrices U to which transposal invariant Hermitean matrices A correspond, i.e. those with real off-diagonal elements. They refer to vectors in the intersection of the ball with the hyperplane at which $\frac{1}{2}N(N-1)$ out of the N^2 coordinates of the parameter vector are zero, certainly a zero measure set. The second condition excludes only separated boundary conditions with U given by (13) to which a diagonal A corresponds, i.e. the parameters belonging to the intersection of the ball with the hyperplane of vectors with even $N(N-1)$ components vanishing, no doubt a zero measure set again.

(iii) Each matrix U can be, of course, diagonalised: there is a unitary V such that

$$V U V^* = \operatorname{diag}\big(\mathrm{e}^{i\theta_1}, \dots, \mathrm{e}^{i\theta_N}\big), \tag{24}$$

and since $V A^{\mathrm{in/out}}(\psi) = A^{\mathrm{in/out}}(V\psi)$ obviously holds, relation (11) defining the self-adjoint extension gives

$$A_j^{\mathrm{in}}(V\psi) = \mathrm{e}^{i\theta_j} A_j^{\mathrm{out}}(V\psi), \quad j = 1, \dots, N. \tag{25}$$

In particular, if all the θ_j are the same, i.e. $U = \mathrm{e}^{i\theta} I$ for some $\theta \in (-\pi, \pi]$, any unitary matrix V does the job. We can then choose V which diagonalizes similarly the coupling (2) at the star vertex. It is well known that this leads to the simple Neumann condition and the Dirichlet one of multiplicity $N-1$. In this way, the problem is unitarily equivalent to the analysis of a direct sum of N halfline operators. All of them satisfy the condition $A_j^{\mathrm{in}}(V\psi) = \mathrm{e}^{i\theta} A_j^{\mathrm{out}}(V\psi)$ at infinity; one is Neumann at the origin and $N-1$ satisfy Dirichlet condition there. Consequently, the spectrum of the operators H_U with $U = \mathrm{e}^{i\theta} I$ consists of two interlaced series of eigenvalues: the elements of one of them have all multiplicity $N-1$ while the elements of the other referring to the Neumann condition at the origin are simple. ∎

Remarks 4.2. (a) We proved claim (ii) for a particular parametrisation of the family of matrices U but its validity extends to other parametrisations as long as the corresponding parameter space is related to the indicated one by a bijective and bicontinous mapping preserving zero Lebesgue measure sets, in particular, to various commonly used parametrisations.

(b) A natural counterpart to (2) is the Kirchhoff condition at infinity (18). In this case, there is a matrix V, which diagonalises the problem at zero and infinity simultaneously, and the problem splits into a family of halfline ones, a single with Neumann condition at zero and infinity, $(A^{\mathrm{in}}(V\psi))_1 = (A^{\mathrm{out}}(V\psi))_1$, and $N-1$ copies of the one with Dirichlet at zero and infinity, $(A^{\mathrm{in}}(V\psi))_j = -(A^{\mathrm{out}}(V\psi))_j$ for $j = 2, \dots, N-1$. The latter give rise to eigenvalues of multiplicity $N-1$, but we do not know whether those coincide with the eigenvalues of the Neumann part of the problem or not.

(c) If we replace the initial operator H satisfying condition (2) by H^{D} from the proof of Proposition 2.1, Dirichlet decoupled at the vertex, and choose $U = \mathrm{e}^{i\theta} I$, we get an operator each eigenvalue of which has multiplicity N. If U is non-diagonal, we get a graph the edges of which are decoupled at the vertex, but some or all of them are coupled at infinity.

(d) The case $N = 2$ considered in [6], i.e. Schrödinger operator on line with the potential $-x^4$, fits the scheme. The matrix U has now a conventional parametrization

$$U = \mathrm{e}^{i\eta} \begin{pmatrix} r\,\mathrm{e}^{i\theta} & -\sqrt{1-r^2}\,\mathrm{e}^{-i\phi} \\ \sqrt{1-r^2}\,\mathrm{e}^{i\phi} & r\,\mathrm{e}^{-i\theta} \end{pmatrix},$$

and the spectrum of H_U is simple unless $r \in [0,1)$ and $\phi = \pm\frac{\pi}{2}$; otherwise, it has multiplicity two. In contrast, for $N > 2$ the eigenvalue multiplicities may be different as the claim (iii) of Theorem 4.1 shows and we cannot even guarantee that all non-simple eigenvalues have the same multiplicity.

5. Concluding remarks

The present example underlines one more time the importance of self-adjointness in quantum mechanics: a formally "Hermitean" operator can have a nontrivial family of self-adjoint realisations, each of which describes a different physics. In some situations, this fact is obvious; even a hard-core physicist would not object against the necessity to impose condition matching wave functions at the graph vertices. What we tried to illustrate here was that the necessity to check the self-adjointness may come from less conspicuous places.

The situation we discussed in this short paper is rather particular and the conclusions allow for various generalisations. For instance, the graph topology can be more complicated; the same reasoning would clearly work as long as the graph has a compact core to which a finite number of edges is attached. Likewise, the attractive potential on the leads, which is the reason behind the quantum-mechanical incompleteness, can be modified; staying in the class of powerlike ones only, $-x^p$ with any $p > 2$ will do.

This does not say that the analysis of our example is complete. One can ask, for example, about the asymptotic distribution of the eigenvalues of both directions, or for the allowed values of multiplicities in the situations where the spectrum is not simple. Another question concerns the existence of effects analogous to those discussed in [16] in cases when the matrix U is circulant and the time-reversal invariance is violated. We leave these problems to a future publication.

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