ACADÉMIE
DES SCIENCES
INSTITUT DE FRANCE

Comptes Rendus

Mathématique

Mark M. Malamud and Vladimir V. Marchenko

On zero eigenvalue of invariant Schrödinger operators with point interactions at vertices of some regular polyhedra

Volume 363 (2025), p. 629-639

https://doi.org/10.5802/crmath.719

ACADÉMIE
DES SCIENCES
INSTITUT DE FRANCE

Comptes Rendus. Mathématique
2025, Vol. 363, p. 629-639
https://doi.org/10.5802/crmath.719

Research article / *Article de recherche*
Functional analysis / *Analyse fonctionnelle*

On zero eigenvalue of invariant Schrödinger operators with point interactions at vertices of some regular polyhedra

Sur la valeur propre nulle des opérateurs de Schrödinger invariants avec interactions ponctuelles aux sommets de certains polyèdres réguliers

Mark M. Malamud [a] and **Vladimir V. Marchenko** [b, c]

[a] Saint Petersburg State University, Saint Petersburg, Russia
[b] Bauman Moscow State Technical University, Moscow, Russia
[c] Institute of Applied Mathematics and Mechanics, Donetsk, Russia
E-mails: malamud3m@gmail.com, wmarchenko@rambler.ru

Abstract. Following Berezin and Faddeev, by a Schrödinger operator with point interactions:

$$-\Delta+\sum_{j=1}^{m}\alpha_j\delta(x-x_j),\quad X=\{x_j\}_1^m\subset\mathbb{R}^3,\quad \{\alpha_j\}_1^m\subset\mathbb{R},$$

one means any selfadjoint extension of the restriction Δ_X of the Laplace operator $-\Delta$ to the subset $\{f\in H^2(\mathbb{R}^3): f(x_j)=0,\ 1\le j\le m\}$ of the Sobolev space $H^2(\mathbb{R}^3)$.

In the present paper the above set of interactions X is assumed to be a vertex set of a certain regular polyhedron, and selfadjoint extensions (realizations) invariant under the symmetry group of $X=\{x_j\}_1^m$ are studied.

Such realizations $\mathbf{H}_B$ are parametrized by special matrices $B=B^*\in\mathbb{C}^{m\times m}$. We describe all such selfadjoint realizations with non-trivial kernels. By this we continue investigation by Grinevich–Novikov and ours relating to regular polygons. Besides, for arbitrary realizations the estimate $\dim(\ker\mathbf{H}_B)\le m-1$ is proved, and realizations with all feasible $\dim(\ker\mathbb{H}_B)$ are described.

Particular attention is paid to realizations with maximum value $\dim(\ker\mathbf{H}_B)=m-1$. One of them is the Krein realization, which is the minimal positive selfadjoint extension of the operator $\Delta_X\ge 0$.

Résumé. D'après Berezin et Faddeev, par un opérateur de Schrödinger avec des interactions ponctuelles:

$$-\Delta+\sum_{j=1}^{m}\alpha_j\delta(x-x_j),\quad X=\{x_j\}_1^m\subset\mathbb{R}^3,\quad \{\alpha_j\}_1^m\subset\mathbb{R},$$

on entend toute extension autoadjointe de la restriction Δ_X de l'opérateur de Laplace $-\Delta$ au sous-ensemble $\{f\in H^2(\mathbb{R}^3): f(x_j)=0,\ 1\le j\le m\}$ de l'espace de Sobolev $H^2(\mathbb{R}^3)$.

Dans le présent article, l'ensemble d'interactions X ci-dessus est supposé être un ensemble de sommets d'un certain polyèdre régulier, et des extensions (réalisations) autoadjointes invariantes sous le groupe de symétrie de $X=\{x_j\}_1^m$ sont étudiées.

De telles réalisations $\mathbf{H}_B$ sont paramétrées par des matrices spéciales $B=B^*\in\mathbb{C}^{m\times m}$. Nous décrivons toutes ces réalisations autoadjointes avec des noyaux non triviaux. Nous poursuivons ainsi l'investigation de Grinevich–Novikov et la nôtre concernant les polygones réguliers. De plus, pour des réalisations arbitraires,

ISSN (électronique) : 1778-3569

l'estimation $\dim(\ker \mathbf{H}_B) \le m-1$ est prouvée, et des réalisations avec tous les $\dim(\ker \mathbb{H}_B)$ réalisables sont décrites.

Une attention particulière est accordée aux réalisations avec la valeur maximale $\dim(\ker \mathbf{H}_B) = m-1$. L'une d'elles est la réalisation de Krein, qui est l'extension autoadjointe positive minimale de l'opérateur $\Delta_X \ge 0$.

Keywords. Schrödinger operators with point interactions, invariant operators, Krein realization, multiplicity of zero eigenvalue.

Mots-clés. Opérateurs de Schrödinger avec interactions ponctuelles, opérateurs invariants, réalisation de Krein, multiplicité de valeur propre nulle.

2020 Mathematics Subject Classification. 47A57.

Funding. The study of the first author in Sections 3–5 was carried out with the financial support of the Ministry of Science and Higher Education of the Russian Federation in the framework of a scientific project under agreement No. 075-15-2024-631. His research on Section 1, 2, and 6 was carried out by grant of the Russian Science Foundation No. 23-11-00153.

Manuscript received 12 November 2024, revised 8 January 2025, accepted 16 January 2025.

1. Introduction

It is well-known (see [9,13]) that positive spectrum of the Schrödinger operator $-\Delta + q$ in $L^2(\mathbb{R}^n)$, $n = 2,3$, with decaying potential $q(x) = O(1+|x|)^{-1-\varepsilon}$, $\varepsilon > 0$, is purely absolutely continuous. However, the operator $-\Delta + q$ may have the (embedded) zero eigenvalue. This effect for rational potentials $q(x_1, x_2)$ was discovered by Taimanov and Tsarev in [14,15] by means of the Moutard transformation.

For the Schrödinger operator with point interactions in the set $X = \{x_j\}_1^m (\subset \mathbb{R}^3)$:

$$-\Delta + \sum_{j=1}^{m} \alpha_j \delta(x - x_j), \quad \{\alpha_j\}_1^m \subset \mathbb{R}, \tag{1}$$

this effect was discovered by Grinevich and Novikov in [7].

Recall that, following Berezin and Faddeev [2], by a Schrödinger operator with point interactions in $X = \{x_j\}_1^m (\subset \mathbb{R}^3)$ one means any realization (self-adjoint extension) $\mathbf{H}_B$ of the three-dimensional Laplace operator in $\mathfrak{H} = L^2(\mathbb{R}^3)$ restricted to the (dense in $\mathfrak{H}$) domain

$$\mathbf{H} = -\Delta \restriction \operatorname{dom}(\Delta_X), \quad \operatorname{dom}(\Delta_X) := \left\{ f \in W^{2,2}(\mathbb{R}^3) : f(x_j) = 0,\ j \in \{1, \dots, m\} \right\}. \tag{2}$$

The operator (2) is a closed nonnegative symmetric operator in $\mathfrak{H}$ with defect numbers $n_\pm(\mathbf{H}) = m$ with its adjoint $\mathbf{H}^*$ given by (6)–(7). A large number of papers are devoted to studying spectral properties of extensions of such operators (see, eg., [1,5,8,12], and references therein). It is well-known (see [1,5]) that positive spectrum of each realization is purely absolutely continuous, although negative spectrum is finite. In particular, it has no positive (embedded) eigenvalues. Assuming that $X = \{x_j\}_1^m (\subset \mathbb{R}^3)$ is a vertex set of a regular polygon or polyhedron, we described in [10] all realizations invariant under the symmetry group of X. Namely, we describe in [10] all "boundary" matrices $B = B^* \in \mathbb{C}^{m \times m}$ that parametrize all invariant realizations by formula $\mathbf{H}_B := \mathbf{H}^* \restriction \ker(\Gamma_1 - B\Gamma_0)$ (see (4)), where Γ_0 and Γ_1 are given by (8)–(9).

The paper [11] considers the case of a regular m-gon $X = \{x_j\}_1^m$ and describes all invariant realizations $\mathbf{H}_B$ satisfying $\ker \mathbf{H}_B \ne \{0\}$. In particular, [11] solves the problem, posed by Grinevich and Novikov in [7], on multiplicity of zero eigenvalue of $\mathbf{H}_B$.

In this note we continue the research initiated in [7,11] as well as describe all invariant realizations $\mathbf{H}_\mathbf{B}$ with non-trivial kernels, assuming that X is the vertex set of some regular polyhedra (tetrahedron, hexagedron, octahedron). As in [11] we study this problem in the framework of extension theory of the operator $\mathbf{H}$ by applying the boundary triples technique and the corresponding Weyl functions (see definitions in Section 2). We describe all invariant Schrödinger operators (extensions $\mathbf{H}_B$ of $\mathbf{H}$) with non-trivial kernels.

In particular, we complement the result of [7], where, in the case of a tetrahedron, invariant realizations $\mathbf{H_B}$ with non-trivial kernels and scalar matrices $B = \alpha I$, $\alpha \in \mathbb{R}$, are described.

Note that consideration of all "boundary" (not only scalar) matrices B leads to curious effects. Thus, it leads to a description of all invariant realizations $\mathbf{H_B}$ with maximal possible kernels: $\dim(\ker \mathbf{H}_B) = m-1$. Moreover, among them are contained non-negative realizations $\mathbf{H}_B \geq 0$, in particular, the Krein realization (the smallest one) $\widehat{\mathbf{H}}_K (\geq 0)$. Finally, we mention interesting features which essentially distinguish the considered case from the one of a regular m-gon:

(i) "boundary" matrices B are not necessarily Toeplitz;
(ii) C^*-algebras generated by "boundary" matrices contain more than one generator;
(iii) dimensions of $\ker \mathbf{H}_B$ have forbidden values missing some numbers from 1 to $m-2$ (see Section 8).

Besides, for $B \neq \alpha I$ there appear non-selfadjoint realizations $\mathbf{H}_B$ ($\Longleftrightarrow B \neq B^*$) with non-trivial kernels.

2. Boundary triples and Weyl functions

In this paragraph, following [3–6], we summarize the basic notions and facts of the boundary triples theory.

Let A be a symmetric operator in a separable Hilbert space $\mathfrak{H}$ with dense domain $\operatorname{dom}(A)$ and equal defect numbers $n_+(A) = n_-(A) \leq \infty$.

Definition 1. *The totality* $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$, *in which* $\mathcal{H}$ *is an auxiliary Hilbert space, and* $\Gamma_0, \Gamma_1 \colon \operatorname{dom}(A^*) \to \mathcal{H}$ *are linear mappings, is called a* boundary triple *of the operator* A^* *if:*

(i) *the following Green formula holds:*

$$(A^* f, g)_{\mathfrak{H}} - (f, A^* g)_{\mathfrak{H}} = (\Gamma_1 f, \Gamma_0 g)_{\mathcal{H}} - (\Gamma_0 f, \Gamma_1 g)_{\mathcal{H}}, \quad f, g \in \operatorname{dom}(A^*); \tag{3}$$

(ii) *the mapping* $\Gamma := (\Gamma_0, \Gamma_1)^\top \colon \operatorname{dom}(A^*) \to \mathcal{H} \oplus \mathcal{H}$ *is surjective.*

Definition 2. *An extension* $\widetilde{A} \supset A$ *is called* proper *if* $A \subset \widetilde{A} \subset A^*$.

Proposition 3 ([3]). *Let A be a symmetric operator in a Hilbert space $\mathfrak{H}$ with defect numbers $n_\pm(A) = m$, and let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triple of the operator A^*. Then the mapping*

$$B \longrightarrow A_B = A^* \upharpoonright \ker(\Gamma_1 - B\Gamma_0) \tag{4}$$

establishes a bijective correspondence between the set $\mathcal{C}(\mathcal{H})$ of closed linear operators B in $\mathcal{H}$ and the set of closed proper extensions A_B of the operator A which are disjoint with $A_0 := A^* \upharpoonright \ker(\Gamma_0)$, i. e., such that $\operatorname{dom} A_B \cap \operatorname{dom} A_0 = \operatorname{dom} A$.

Definition 4 ([3]). *Let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triple for A^*. The operator function $M(\cdot)$ defined by the equality*

$$M(z)\Gamma_0 f = \Gamma_1 f, \quad \text{where } f \in \mathfrak{N}_z = \ker(A^* - zI), \tag{5}$$

is called the Weyl function corresponding to the boundary triple Π.

3. Three-dimensional Schrödinger operators with point interactions

Proposition 5 ([5]). *Let* $\mathbf{H}$ *be the minimal Schrödinger operator* (2) *and let* $\xi_0 := \{\xi_{0j}\}_{j=1}^m$, $\xi_1 := \{\xi_{1j}\}_{j=1}^m \in \mathbb{C}^m$. *Then the following statements hold.*

(i) $\mathbf{H}$ *is a closed non-negative symmetric operator with deficiency indices* $n_\pm(\mathbf{H}) = m$.

(ii) *The adjoint operator* $\mathbf{H}^*$ *is given by the equalities*

$$\operatorname{dom}(\mathbf{H}^*) = \left\{ f = \sum_{j=1}^{m} \left(\xi_{0j} \frac{e^{-|x-x_j|}}{|x-x_j|} + \xi_{1j} e^{-|x-x_j|} \right) + f_H : \ \xi_0, \xi_1 \in \mathbb{C}^m, \ f_H \in \operatorname{dom}(\mathbf{H}) \right\}, \tag{6}$$

$$\mathbf{H}^* f = -\sum_{j=1}^{m} \left(\xi_{0j} \frac{e^{-|x-x_j|}}{|x-x_j|} + \xi_{1j} \left(e^{-|x-x_j|} - \frac{2e^{-|x-x_j|}}{|x-x_j|} \right) \right) - \Delta f_H. \tag{7}$$

(iii) *The totality* $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ *with*

$$\mathcal{H} = \mathbb{C}^m, \quad \Gamma_0 f := \{\Gamma_{0j} f\}_{j=1}^m = 4\pi \left\{ \lim_{x \to x_j} f(x)|x-x_j| \right\}_{j=1}^m = 4\pi \{\xi_{0j}\}_{j=1}^m, \tag{8}$$

$$\Gamma_1 f := \{\Gamma_{1j} f\}_{j=1}^m = \left\{ \lim_{x \to x_j} \left(f(x) - \tfrac{\xi_{0j}}{|x-x_j|} \right) \right\}_{j=1}^m, \tag{9}$$

forms a boundary triple for the operator $\mathbf{H}^*$.

(iv) *The corresponding Weyl function* $M(\cdot)$ *has the form*

$$M(z) = \left(\frac{i\sqrt{z}}{4\pi} \delta_{jk} + \widetilde{G}_{\sqrt{z}}(x_j - x_k) \right)_{j,k=1}^m, \quad z \in \mathbb{C}_+, \tag{10}$$

where

$$\widetilde{G}_{\sqrt{z}}(x) = \begin{cases} \frac{e^{i\sqrt{z}|x|}}{4\pi|x|}, & x \neq 0, \\ 0, & x = 0. \end{cases}$$

Here δ_{jk} *is the Kronecker symbol,* $\sqrt{\cdot}$ *is a branch of the root defined on* $\mathbb{C} \setminus \mathbb{R}_+$ *by the condition* $\sqrt{1} = 1$.

(v) *There exists the strong limit* $M(0) := \text{s-}\lim_{z \uparrow 0} M(z)$ *in* $\mathbb{C}^m$, *and* $M(0) = M(0)^*$.

(vi) $\mathbf{H}_0 := \mathbf{H}^* \upharpoonright \ker \Gamma_0 = \widehat{\mathbf{H}}_F = -\Delta$ *coincides with the Friedrichs (maximal positive) extension of the operator* $\mathbf{H}$. *Besides,* $\mathbf{H}_{M(0)} = \mathbf{H}^* \upharpoonright \ker\big(\Gamma_1 - M(0)\Gamma_0\big) = \widehat{\mathbf{H}}_K$ *is the Krein (minimal positive) extension of* $\mathbf{H}$.

Remark 6. The expression (1) is often identified with the realization $\mathbf{H}_B$ given in the boundary triple (8)–(9) by the equality (4) with the diagonal matrix $B = \operatorname{diag}(\alpha_1, \dots, \alpha_m)$.

4. Invariant Schrödinger operators

The concepts of this section are presented following [10].

For a set $X \subset \mathbb{R}^3$ by $\mathcal{S}_X$ we denote the symmetry group of X, i. e., the motions of the space $\mathbb{R}^3$ which preserve X.

A symmetry $u (\in \mathcal{S}_X)$ induces a unitary operator U in $L^2(\mathbb{R}^3)$ of the form

$$U f(x) = f\big(u(x)\big), \qquad U \colon L^2(\mathbb{R}^3) \longrightarrow L^2(\mathbb{R}^3). \tag{11}$$

Definition 7. *An operator* $A \colon L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ *is called invariant under a symmetry* u *if the equality* $AU = UA$ *holds on* $\operatorname{dom}(A)$. *If this equality holds for all symmetries* $u \in \mathcal{S}_X$, *then* A *is called invariant under the group* $\mathcal{S}_X$ *(or simply invariant).*

It is easily seen that the minimal operator $\mathbf{H}$ is invariant.

5. Regular tetrahedron

Let X be a vertex set of a regular tetrahedron. According to Proposition 3, each realization $\mathbf{H}_B$ disjoint with the operator $\mathbf{H}_0 = -\Delta$ is the restriction of the operator $\mathbf{H}^*$ given by (6)–(7) to the domain $\operatorname{dom} \mathbf{H}_B = \ker(\Gamma_1 - B\Gamma_0)$, where Γ_0, Γ_1 are given by (8)–(9), and $B \in \mathbb{C}^{4\times 4}$.

Meanwhile, according to [10], the extension $\mathbf{H}_B$ is invariant (under the group $\mathscr{S}_X$) if and only if B is a special Toeplitz matrix of the following form:

$$B = \begin{pmatrix} a & b & b & b \\ b & a & b & b \\ b & b & a & b \\ b & b & b & a \end{pmatrix} \in \mathbb{C}^{4\times 4}. \tag{12}$$

According to [10], the Weyl function corresponding to the triple (8)–(9) in this case has the following form:

$$M(z) = \frac{1}{4\pi} \begin{pmatrix} i\sqrt{z} & \frac{e^{ir\sqrt{z}}}{r} & \frac{e^{ir\sqrt{z}}}{r} & \frac{e^{ir\sqrt{z}}}{r} \\ \frac{e^{ir\sqrt{z}}}{r} & i\sqrt{z} & \frac{e^{ir\sqrt{z}}}{r} & \frac{e^{ir\sqrt{z}}}{r} \\ \frac{e^{ir\sqrt{z}}}{r} & \frac{e^{ir\sqrt{z}}}{r} & i\sqrt{z} & \frac{e^{ir\sqrt{z}}}{r} \\ \frac{e^{ir\sqrt{z}}}{r} & \frac{e^{ir\sqrt{z}}}{r} & \frac{e^{ir\sqrt{z}}}{r} & i\sqrt{z} \end{pmatrix}, \quad r = |x_j - x_k|,\ j \neq k, \quad z \in \mathbb{C} \setminus \mathbb{R}_+. \tag{13}$$

Theorem 8. *An invariant realization* $\mathbf{H}_B$ *defined by a boundary matrix* B *of the form* (12) *has a non-trivial kernel if and only if*

$$a - b = -\frac{1}{4\pi r}. \tag{14}$$

Moreover, $\dim(\ker \mathbf{H}_B) = 3$, *and* $\ker \mathbf{H}_B$ *is spanned by the functions*

$$\begin{aligned} \psi_1(x) &= \tfrac{1}{4\pi}\left(\tfrac{1}{|x-x_1|} - \tfrac{1}{|x-x_2|}\right), \\ \psi_2(x) &= \tfrac{1}{4\pi}\left(\tfrac{1}{|x-x_1|} - \tfrac{1}{|x-x_3|}\right), \\ \psi_3(x) &= \tfrac{1}{4\pi}\left(\tfrac{1}{|x-x_1|} - \tfrac{1}{|x-x_4|}\right). \end{aligned} \tag{15}$$

Remark 9. In the case of a scalar matrix $B = aI \in \mathbb{R}^{4\times 4}$, i.e. when $b = 0$, this result in a different way was obtained by Grinevich and Novikov in [7, Example 1].

Theorem 10. *Let* $\mathbf{H}_B$ *be an invariant realization with a matrix* B *of the form* (12). *Let also* $E_4 (\in \mathbb{R}^{4\times 4})$ *be a matrix with all entries equal to* 1. *Then* $\ker \mathbf{H}_B \neq \{0\}$ *if and only if the matrix* B *is of the form*

$$B = B(a) := aE_4 + M(0), \qquad a \in \mathbb{C}.$$

Moreover, the following statements hold true:

(i) $\mathbf{H}_{B(a)} = \mathbf{H}^*_{B(a)}$ *precisely when* $a \in \mathbb{R}$;
(ii) $\mathbf{H}_{B(a)} \geq 0$ *precisely when* $a \geq 0$;
(iii) *in particular, for* $a = 0$ *the operator* $\mathbf{H}_{B(0)} = \mathbf{H}_{M(0)}$ *coincides with the Krein (smallest positive) realization* $\widehat{\mathbf{H}}_K$ *of the operator* $\mathbf{H}$.

Corollary 11. *In the case* $a < 0$ *the number of negative eigenvalues (counting multiplicity) of the operator* $\mathbf{H}_{B(a)}$ *equals*

$$\kappa_-(\mathbf{H}_{B(a)}) = \kappa_-\big(B(a) - M(0)\big) = \kappa_-(aE_4) = 1.$$

Now we specify the rate of decay at infinity of the eigenfunctions (15).

Proposition 12. *For the eigenfunctions* (15) *the following estimates hold:*

$$\psi_j(x) = O\left(\frac{1}{|x|^2}\right), \quad |x| \to +\infty, \quad j \in \{1,2,3\}. \tag{16}$$

6. Regular hexahedron (cube)

Let the set of interactions X be a vertex set of a cube.

According to Proposition 3, each realization $\mathbf{H}_B$ disjoint with the operator $\mathbf{H}_0 = -\Delta$ is the restriction of the operator $\mathbf{H}^*$ given by (6)–(7) to the domain $\operatorname{dom}\mathbf{H}_B = \ker(\Gamma_1 - B\Gamma_0)$, where Γ_0, Γ_1 are defined by the equalities (8)–(9), and $B \in \mathbb{C}^{8\times 8}$.

Meanwhile, according to [10], extension $\mathbf{H}_B$ is invariant (under the group $\mathscr{S}_X$) if and only if B is a special block Toeplitz matrix of the following form:

$$B = \left(\begin{array}{cccc|cccc} a & b & c & b & b & c & d & c \\ b & a & b & c & c & b & c & d \\ c & b & a & b & d & c & b & c \\ b & c & b & a & c & d & c & b \\ \hline b & c & d & c & a & b & c & b \\ c & b & c & d & b & a & b & c \\ d & c & b & c & c & b & a & b \\ c & d & c & b & b & c & b & a \end{array}\right) \in \mathbb{C}^{8\times 8}. \tag{17}$$

According to [10], the Weyl function corresponding to the triple (8)–(9) in this case has the following form:

$$M(z) = \frac{1}{4\pi}\left(\begin{array}{cccc|cccc}
i\sqrt{z} & \frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_2\sqrt{z}}}{r_2} & \frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_2\sqrt{z}}}{r_2} & \frac{e^{ir_3\sqrt{z}}}{r_3} & \frac{e^{ir_2\sqrt{z}}}{r_2} \\
\frac{e^{ir_1\sqrt{z}}}{r_1} & i\sqrt{z} & \frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_2\sqrt{z}}}{r_2} & \frac{e^{ir_2\sqrt{z}}}{r_2} & \frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_2\sqrt{z}}}{r_2} & \frac{e^{ir_3\sqrt{z}}}{r_3} \\
\frac{e^{ir_2\sqrt{z}}}{r_2} & \frac{e^{ir_1\sqrt{z}}}{r_1} & i\sqrt{z} & \frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_3\sqrt{z}}}{r_3} & \frac{e^{ir_2\sqrt{z}}}{r_2} & \frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_2\sqrt{z}}}{r_2} \\
\frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_2\sqrt{z}}}{r_2} & \frac{e^{ir_1\sqrt{z}}}{r_1} & i\sqrt{z} & \frac{e^{ir_2\sqrt{z}}}{r_2} & \frac{e^{ir_3\sqrt{z}}}{r_3} & \frac{e^{ir_2\sqrt{z}}}{r_2} & \frac{e^{ir_1\sqrt{z}}}{r_1} \\ \hline
\frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_2\sqrt{z}}}{r_2} & \frac{e^{ir_3\sqrt{z}}}{r_3} & \frac{e^{ir_2\sqrt{z}}}{r_2} & i\sqrt{z} & \frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_2\sqrt{z}}}{r_2} & \frac{e^{ir_1\sqrt{z}}}{r_1} \\
\frac{e^{ir_2\sqrt{z}}}{r_2} & \frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_2\sqrt{z}}}{r_2} & \frac{e^{ir_3\sqrt{z}}}{r_3} & \frac{e^{ir_1\sqrt{z}}}{r_1} & i\sqrt{z} & \frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_2\sqrt{z}}}{r_2} \\
\frac{e^{ir_3\sqrt{z}}}{r_3} & \frac{e^{ir_2\sqrt{z}}}{r_2} & \frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_2\sqrt{z}}}{r_2} & \frac{e^{ir_2\sqrt{z}}}{r_2} & \frac{e^{ir_1\sqrt{z}}}{r_1} & i\sqrt{z} & \frac{e^{ir_1\sqrt{z}}}{r_1} \\
\frac{e^{ir_2\sqrt{z}}}{r_2} & \frac{e^{ir_3\sqrt{z}}}{r_3} & \frac{e^{ir_2\sqrt{z}}}{r_2} & \frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_2\sqrt{z}}}{r_2} & \frac{e^{ir_1\sqrt{z}}}{r_1} & i\sqrt{z}
\end{array}\right), \tag{18}$$

where r_1, r_2, r_3 are three distinct distances between the cube vertices ($r_1 < r_2 < r_3$).

Theorem 13. *An invariant realization* $\mathbf{H}_B$ *defined by a boundary matrix* B *of the form* (17) *has a non-trivial kernel precisely when at least one of the following conditions holds:*

$$\begin{aligned} &\text{(i)} \quad a - b - c + d = \tfrac{1}{4\pi}\left(-\tfrac{1}{r_1} - \tfrac{1}{r_2} + \tfrac{1}{r_3}\right); \\ &\text{(ii)} \quad a + b - c - d = \tfrac{1}{4\pi}\left(\tfrac{1}{r_1} - \tfrac{1}{r_2} - \tfrac{1}{r_3}\right); \\ &\text{(iii)} \quad a - 3b + 3c - d = \tfrac{1}{4\pi}\left(-\tfrac{3}{r_1} + \tfrac{3}{r_2} - \tfrac{1}{r_3}\right). \end{aligned} \tag{19}$$

Moreover, in the first case, $\ker\mathbf{H}_B \supseteq \mathscr{H}_1^h$, *where* $\mathscr{H}_1^h$ *is the subspace spanned by the functions*

$$\begin{aligned} \psi_{1,1}(x) &= \tfrac{1}{4\pi}\left(\tfrac{1}{|x-x_3|} - \tfrac{1}{|x-x_4|} + \tfrac{1}{|x-x_5|} - \tfrac{1}{|x-x_6|}\right), \\ \psi_{2,1}(x) &= \tfrac{1}{4\pi}\left(\tfrac{1}{|x-x_1|} - \tfrac{1}{|x-x_3|} - \tfrac{1}{|x-x_5|} + \tfrac{1}{|x-x_7|}\right), \\ \psi_{3,1}(x) &= \tfrac{1}{4\pi}\left(\tfrac{1}{|x-x_2|} - \tfrac{1}{|x-x_3|} - \tfrac{1}{|x-x_5|} + \tfrac{1}{|x-x_8|}\right). \end{aligned} \tag{20}$$

In the second case, $\ker \mathbf{H}_B \supseteq \mathscr{H}_2^h$*, where* $\mathscr{H}_2^h$ *is the subspace spanned by the functions*

$$\begin{aligned}\psi_{1,2}(x) &= \frac{1}{4\pi}\left(\frac{1}{|x-x_3|} + \frac{1}{|x-x_4|} - \frac{1}{|x-x_5|} - \frac{1}{|x-x_6|}\right),\\ \psi_{2,2}(x) &= \frac{1}{4\pi}\left(\frac{1}{|x-x_1|} - \frac{1}{|x-x_3|} + \frac{1}{|x-x_5|} - \frac{1}{|x-x_7|}\right),\\ \psi_{3,2}(x) &= \frac{1}{4\pi}\left(\frac{1}{|x-x_2|} + \frac{1}{|x-x_3|} - \frac{1}{|x-x_5|} - \frac{1}{|x-x_8|}\right).\end{aligned} \tag{21}$$

In the third case, $\ker \mathbf{H}_B \supseteq \mathscr{H}_3^h$*, where* $\mathscr{H}_3^h$ *is the subspace spanned by the function*

$$\psi_{1,3}(x) = \frac{1}{4\pi}\left(\frac{1}{|x-x_1|} - \frac{1}{|x-x_2|} + \frac{1}{|x-x_3|} - \frac{1}{|x-x_4|} - \frac{1}{|x-x_5|} + \frac{1}{|x-x_6|} - \frac{1}{|x-x_7|} + \frac{1}{|x-x_8|}\right). \tag{22}$$

Besides, $\ker \mathbf{H}_B = \mathscr{H}_k^h$ *if and only if the* k*th condition in* (19) *holds, and the other two fail. In this case,* $\dim(\ker \mathbf{H}_B) = 3$ *for* $k = 1$*,* $k = 2$*, and* $\dim(\ker \mathbf{H}_B) = 1$ *for* $k = 3$*.*

Remark 14. The conditions (i), (ii), (iii) can hold either in pairs (in any combinations) or all three at once. However, in the case of a scalar matrix $B = aI$ only one of the above conditions is feasible.

The full list of all possible dimensions of $\ker \mathbf{H}_B$ is derived from Theorem 13.

Corollary 15. *Under the conditions of Theorem 13 the following description of* $\dim(\ker \mathbf{H}_B)$ *holds:*

$$\dim(\ker \mathbf{H}_B) = \begin{cases} 1 & \textit{if } \text{(iii)} \textit{ holds, but both } \text{(i)} \textit{ and } \text{(ii)} \textit{ fail;}\\ 3 & \textit{if precisely one of } \text{(i)} \textit{ and } \text{(ii)} \textit{ holds, but } \text{(iii)} \textit{ fails;}\\ 4 & \textit{if } \text{(iii)} \textit{ and precisely one of } \text{(i)} \textit{ and } \text{(ii)} \textit{ hold;}\\ 6 & \textit{if both } \text{(i)} \textit{ and } \text{(ii)} \textit{ hold, but } \text{(iii)} \textit{ fails;}\\ 7 & \textit{if all three conditions } \text{(i), (ii)} \textit{ and } \text{(iii)} \textit{ hold.}\end{cases}$$

Meanwhile, in the case of a scalar matrix $B = aI$ *(*$b = c = d = 0$*) the dimension of* $\ker \mathbf{H}_B$ *takes only two values:*

$$\dim(\ker \mathbf{H}_B) = \begin{cases} 1 & \textit{if } \text{(iii)} \textit{ holds;}\\ 3 & \textit{if } \text{(i)} \textit{ or } \text{(ii)} \textit{ holds.}\end{cases}$$

The following theorem explicitly describes all realizations $\mathbf{H}_B$ with maximum value of $\dim(\ker \mathbf{H}_B)$.

Theorem 16. *Let* $\mathbf{H}_B$ *be an invariant realization with a matrix* B *of the form* (17)*. Let also* $E_8 (\in \mathbb{R}^{8\times 8})$ *be a matrix with all entries equal to* 1*. Then the zero eigenvalue of the operator* $\mathbf{H}_B$ *is of maximal multiplicity*

$$\dim(\ker \mathbf{H}_B) = 7 \tag{23}$$

precisely when any of the following equivalent conditions holds:

- $b = a + \frac{1}{4\pi r_1}$, $c = a + \frac{1}{4\pi r_2}$, $d = a + \frac{1}{4\pi r_3}$;
- $B = B(a) := aE_m + M(0)$, $a \in \mathbb{C}$.

Moreover, the following statements hold true:

(i) $\mathbf{H}_{B(a)} = \mathbf{H}^*_{B(a)}$ *precisely when* $a \in \mathbb{R}$*;*
(ii) $\mathbf{H}_{B(a)} \geq 0$ *precisely when* $a \geq 0$*;*
(iii) *in particular, for* $a = 0$ *the operator* $\mathbf{H}_{B(0)} = \mathbf{H}_{M(0)}$ *coincides with the Krein (smallest positive) realization* $\widehat{\mathbf{H}}_K$ *of the operator* $\mathbf{H}$*.*

Corollary 17. *In the case* $a < 0$ *the number of negative eigenvalues (counting multiplicity) of the operator* $\mathbf{H}_{B(a)}$ *equals*

$$\kappa_-(\mathbf{H}_{B(a)}) = \kappa_-\big(B(a) - M(0)\big) = \kappa_-(aE_8) = 1.$$

Now we specify the rate of decay at infinity of the eigenfunctions (20)–(22).

Proposition 18. *For the eigenfunctions* (20)–(22) *the following (distinct) estimates hold:*

$$\psi_{j,k}(x) = O\left(\frac{1}{|x|^3}\right),\ j \in \{1,2,3\},\ k \in \{1,2\}, \qquad \psi_{1,3}(x) = O\left(\frac{1}{|x|^4}\right), \qquad |x| \to +\infty. \tag{24}$$

7. Regular octahedron

Let X be a vertex set of a regular octahedron. According to Proposition 3, each realization $\mathbf{H}_B$ disjoint with the operator $\mathbf{H}_0 = -\Delta$ is the restriction of the operator $\mathbf{H}^*$ given by (6)–(7) to the domain $\operatorname{dom}\mathbf{H}_B = \ker(\Gamma_1 - B\Gamma_0)$, where Γ_0, Γ_1 are given by the equalities (8)–(9), and $B \in \mathbb{C}^{6\times 6}$.

Similarly to the cases of a tetrahedron and cube, which were considered in [10], we show that in the case of an octahedron the extension $\mathbf{H}_B$ is invariant (under the group $\mathscr{S}_X$) if and only if B is of the following form

$$B = \begin{pmatrix} a & b & c & b & b & b \\ b & a & b & c & b & b \\ c & b & a & b & b & b \\ b & c & b & a & b & b \\ b & b & b & b & a & c \\ b & b & b & b & c & a \end{pmatrix} \in \mathbb{C}^{6\times 6}. \tag{25}$$

Moreover, it is also shown that the Weyl function corresponding to the triple (8)–(9) in this case has the following form:

$$M(z) = \frac{1}{4\pi}\begin{pmatrix} i\sqrt{z} & \frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_2\sqrt{z}}}{r_2} & \frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_1\sqrt{z}}}{r_1} \\ \frac{e^{ir_1\sqrt{z}}}{r_1} & i\sqrt{z} & \frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_2\sqrt{z}}}{r_2} & \frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_1\sqrt{z}}}{r_1} \\ \frac{e^{ir_2\sqrt{z}}}{r_2} & \frac{e^{ir_1\sqrt{z}}}{r_1} & i\sqrt{z} & \frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_1\sqrt{z}}}{r_1} \\ \frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_2\sqrt{z}}}{r_2} & \frac{e^{ir_1\sqrt{z}}}{r_1} & i\sqrt{z} & \frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_1\sqrt{z}}}{r_1} \\ \frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_1\sqrt{z}}}{r_1} & i\sqrt{z} & \frac{e^{ir_2\sqrt{z}}}{r_2} \\ \frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_1\sqrt{z}}}{r_1} & \frac{e^{ir_2\sqrt{z}}}{r_2} & i\sqrt{z} \end{pmatrix}. \tag{26}$$

Here r_1 and r_2 are distinct distances between the octahedron vertices ($r_1 < r_2$). Hence, for each $z \in \mathbb{C}_\pm$ the matrix $M(z)$ is of the form (25) with certain a, b, c.

Theorem 19. *An invariant realization* $\mathbf{H}_B$ *with a boundary matrix* B *of the form* (25) *has a nontrivial kernel precisely when at least one of the following conditions holds:*

$$\begin{aligned} &\text{(i)}\ \ a - c = -\tfrac{1}{4\pi r_2}; \\ &\text{(ii)}\ \ a - 2b + c = \tfrac{1}{4\pi}\left(-\tfrac{2}{r_1} + \tfrac{1}{r_2}\right). \end{aligned} \tag{27}$$

Moreover, in the first case, $\ker\mathbf{H}_B \supseteq \mathscr{H}_1^o$, *where* $\mathscr{H}_1^o$ *is the subspace spanned by the functions*

$$\begin{aligned} \psi_{1,1}(x) &= \tfrac{1}{4\pi}\left(\tfrac{1}{|x-x_1|} - \tfrac{1}{|x-x_3|}\right), \\ \psi_{2,1}(x) &= \tfrac{1}{4\pi}\left(\tfrac{1}{|x-x_2|} - \tfrac{1}{|x-x_4|}\right), \\ \psi_{3,1}(x) &= \tfrac{1}{4\pi}\left(\tfrac{1}{|x-x_5|} - \tfrac{1}{|x-x_6|}\right). \end{aligned} \tag{28}$$

In the second case, $\ker\mathbf{H}_B \supseteq \mathscr{H}_2^o$, *where* $\mathscr{H}_2^o$ *is the subspace spanned by the functions*

$$\begin{aligned} \psi_{1,2}(x) &= \tfrac{1}{4\pi}\left(\tfrac{1}{|x-x_1|} - \tfrac{1}{|x-x_2|} + \tfrac{1}{|x-x_3|} - \tfrac{1}{|x-x_4|}\right), \\ \psi_{2,2}(x) &= \tfrac{1}{4\pi}\left(\tfrac{1}{|x-x_1|} + \tfrac{1}{|x-x_3|} - \tfrac{1}{|x-x_5|} - \tfrac{1}{|x-x_6|}\right). \end{aligned} \tag{29}$$

Besides, $\ker\mathbf{H}_B = \mathscr{H}_k^o$ *if and only if the* k*th condition in* (27) *holds, and the other fails. In this case,* $\dim(\ker\mathbf{H}_B) = 3$ *for* $k = 1$, *and* $\dim(\ker\mathbf{H}_B) = 2$ *for* $k = 2$.

Remark 20. The conditions (i) and (ii) can hold simultaneously. However, in the case of a scalar matrix $B = aI$ only one of the above conditions is feasible.

The following description of all possible dimensions of $\ker \mathbf{H}_B$ is easily derived from Theorem 19.

Corollary 21. *Under the conditions of Theorem 19 the dimension of* $\ker \mathbf{H}_B$ *takes the following values:*

$$\dim(\ker \mathbf{H}_B) = \begin{cases} 2 & \text{if (ii) holds, but (i) fails,} \\ 3 & \text{if (i) holds, but (ii) fails,} \\ 5 & \text{if both (i) and (ii) hold.} \end{cases}$$

Meanwhile, in the case of a scalar matrix $B = aI$ ($b = c = 0$) the dimension $\ker \mathbf{H}_B$ *takes only two values:*

$$\dim(\ker \mathbf{H}_B) = \begin{cases} 2 & \text{if (ii) holds;} \\ 3 & \text{if (i) holds.} \end{cases}$$

The following theorem explicitly describes all realizations $\mathbf{H}_B$ with maximum value of $\dim(\ker \mathbf{H}_B)$.

Theorem 22. *Let $\mathbf{H}_B$ be an invariant realization with a matrix B of the form* (25)*. Let also $E_6 (\in \mathbb{R}^{6\times 6})$ be a matrix with all entries equal to* 1*. Then the zero eigenvalue of the operator $\mathbf{H}_B$ is of maximum multiplicity*

$$\dim(\ker \mathbf{H}_B) = 5 \tag{30}$$

if and only if any of the following equivalent conditions hold:

- $b = a + \frac{1}{4\pi r_1}$, $c = a + \frac{1}{4\pi r_2}$;
- $B = B(a) := aE_6 + M(0)$, $a \in \mathbb{C}$.

Moreover, the following statements hold true:

(i) $\mathbf{H}_{B(a)} = \mathbf{H}^*_{B(a)}$ *precisely when* $a \in \mathbb{R}$;
(ii) $\mathbf{H}_{B(a)} \geq 0$ *precisely when* $a \geq 0$;
(iii) *in particular, for $a = 0$ the operator $\mathbf{H}_{B(0)} = \mathbf{H}_{M(0)}$ coincides with the Krein (smallest positive) realization $\widehat{\mathbf{H}}_K$ of the operator* $\mathbf{H}$.

Corollary 23. *In the case $a < 0$ the number of negative eigenvalues (counting multiplicity) of the operator $\mathbf{H}_{B(a)}$ is given by*

$$\kappa_-(\mathbf{H}_{B(a)}) = \kappa_-\big(B(a) - M(0)\big) = \kappa_-(aE_6) = 1.$$

Now we specify the rate of decay at infinity of the eigenfunctions (28), (29).

Proposition 24. *For the eigenfunctions* (28), (29) *the following (distinct) estimates hold:*

$$\psi_{j,1}(x) = O\left(\frac{1}{|x|^2}\right),\ j \in \{1,2,3\}, \qquad \psi_{k,2}(x) = O\left(\frac{1}{|x|^3}\right),\ k \in \{1,2\}, \qquad |x| \to +\infty. \tag{31}$$

8. Concluding remarks

We emphasize that the entries of the matrices B in Theorems 8, 13, and 19 might take complex values. Therefore, the matrices B and, thus, the realizations induced by them for all three considered cases with the property $\ker \mathbf{H}_B \neq \{0\}$ are not necessarily selfadjoint. But for scalar matrices $B = \alpha I$ the condition $\alpha \in \mathbb{R}$, i.e. $B = B^*$, follows from the property $\ker \mathbf{H}_B \neq \{0\}$.

It is interesting to note that for regular polyhedra, in contrast to the case of a regular $2l$-gon, $\dim(\ker \mathbf{H}_B)$ miss some values from 1 to $m-2$. Thus, it does not take the values 1 and 2 in the case of a tetrahedron, 2 and 5 in the case of a cube, and 1 and 4 in the case of an octahedron.

We also emphasize that the maximal multiplicity of zero eigenvalue of local interactions parameterized by scalar matrices B does not exceed 3, while the multiplicity 3 is attained for every polyhedron. This follows from Theorem 8, Corollary 15, and Corollary 21.

In this paper we have considered three of the five regular polyhedra in $\mathbb{R}^3$. The remaining two (icosahedron and dodecahedron) seem to be more complicated due to certain computational difficulties. Nevertheless, we hope to consider them in one of the upcoming publications.

Declaration of interests

The authors do not work for, advise, own shares in, or receive funds from any organization that could benefit from this article, and have declared no affiliations other than their research organizations.

References

[1] S. Albeverio, F. Gesztesy, R. Høegh-Krohn and H. Holden, *Solvable models in quantum mechanics*, Texts and Monographs in Physics, Springer, 1988, pp. xiv+452.

[2] F. A. Berezin and L. D. Faddeev, “A remark on Schrödinger’s equation with a singular potential”, *Sov. Math., Dokl.* **2** (1961), pp. 372–375.

[3] V. O. Derkach and M. M. Malamud, “Generalized resolvents and the boundary value problems for Hermitian operators with gaps”, *J. Funct. Anal.* **95** (1991), no. 1, pp. 1–95.

[4] V. O. Derkach and M. M. Malamud, *Extension theory of symmetric operators and boundary value problems*, Institute of Mathematics, NAS of Ukraine, 2017, p. 573.

[5] N. I. Goloshchapova, M. M. Malamud and V. P. Zastavnyi, “Radial positive definite functions and spectral theory of the Schrödinger operators with point interactions”, *Math. Nachr.* **285** (2012), no. 14-15, pp. 1839–1859.

[6] V. I. Gorbachuk and M. L. Gorbachuk, *Boundary value problems for operator differential equations*, Mathematics and its Applications (Soviet Series), Kluwer Academic Publishers, 1991, pp. xii+347. Translated and revised from the 1984 Russian original.

[7] P. G. Grinevich and R. G. Novikov, “Multipoint scatterers with bound states at zero energy”, *Theor. Math. Phys.* **193** (2017), no. 2, pp. 309–314.

[8] P. G. Grinevich and R. G. Novikov, “Spectral inequality for Schrödinger’s equation with multipoint potential”, *Russ. Math. Surv.* **77** (2022), no. 6, pp. 69–76.

[9] T. Kato, *Perturbation theory for linear operators*, Grundlehren der Mathematischen Wissenschaften, Springer, 1966, pp. xix+592.

[10] M. M. Malamud and V. V. Marchenko, “Invariant Schrödinger operators with point interactions at the vertices of a regular polyhedron”, *Math. Notes* **110** (2021), no. 3-4, pp. 463–469.

[11] M. M. Malamud and V. V. Marchenko, “On kernels of invariant Schrödinger operators with point interactions. Grinevich-Novikov conjecture”, *Dokl. Math.* **109** (2024), no. 2, pp. 125–129.

[12] M. M. Malamud and K. Schmüdgen, “Spectral theory of Schrödinger operators with infinitely many point interactions and radial positive definite functions”, *J. Funct. Anal.* **263** (2012), no. 10, pp. 3144–3194.

[13] M. Reed and B. Simon, *Methods of modern mathematical physics. I. Functional analysis*, Academic Press Inc., 1972, pp. xvii+325.

[14] I. A. Taĭmanov and S. P. Tsarëv, "Two-dimensional Schrödinger operators with rapidly decaying rational potential and multidimensional L_2-kernel", *Russ. Math. Surv.* **62** (2007), no. 3, pp. 631–633.

[15] I. A. Taĭmanov and S. P. Tsarëv, "Two-dimensional rational solitons and their blowup via the Moutard transformation", *Theor. Math. Phys.* **157** (2008), no. 2, pp. 1525–1541.