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Characterization of one-dimensional point interactions for the Schrödinger operator by means of boundary conditions

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Abstract

We find a new representation of all boundary conditions corresponding to the so-called point interactions. We show that there is one-to-one correspondence between one-dimensional point interactions and boundary conditions of the form

$$u'(0^+) + \mathrm{i}u(0^+) = \eta\alpha(u'(0^+) - \mathrm{i}u(0^+)) - \eta\bar{\beta}(u'(0^-) + \mathrm{i}u(0^-))$$
$$u'(0^-) - \mathrm{i}u(0^-) = \eta\beta(u'(0^+) - \mathrm{i}u(0^+)) + \eta\bar{\alpha}(u'(0^-) + \mathrm{i}u(0^-))$$

with $\alpha, \beta, \eta \in \mathbb{C}$ satisfying $|\eta| = |\alpha|^2 + |\beta|^2 = 1$.

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1. Introduction

The aim of this short paper is to find a representation of all point interactions for a one-dimensional Laplacian in terms of boundary conditions. It is well known that this is possible theoretically, see [17, theorem 4.7], yet the known representations lack a certain kind of concreteness.

We begin with the following example, see [4]. Consider a symmetric operator A defined on $\mathbb{H} := L^2(\mathbb{R}, \mathbb{C}^2)$ by

$$\mathcal{D}(A) = C_0^\infty(\mathbb{R} \setminus \{0\}, \mathbb{C}^2) \tag{1.1}$$

$$Af = \frac{1}{\mathrm{i}}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\frac{\mathrm{d}f}{\mathrm{d}x} \qquad f \in \mathcal{D}(A). \tag{1.2}$$

Note that $\mathcal{D}(A)$ is dense in $\mathbb{H}$. The proof of the following is standard.

Lemma 1.1. *$\mathcal{D}(A^*)$, the domain of the adjoint operator to A, consists of all elements u of $\mathbb{H}$ such that the restrictions of the weak derivative Du to the intervals $(0, \infty)$ and $(-\infty, 0)$ belong to the corresponding L^2 space. In other words, $u \in \mathcal{D}(A^*)$ iff $u \in \mathbb{H}$ and $u^- := 1_{(-\infty,0)}u$ and*

$u^+ := 1_{(0,\infty)}u$ *are absolutely continuous on* $(-\infty, 0)$ *and* $(0, \infty)$*, and their derivatives belong to the corresponding* L^2 *spaces.*

In particular, for each $u \in \mathcal{D}(A^*)$*, the following limits make sense:*

$$\lim_{s\nearrow 0} u(s) =: u(0^-) \in \mathbb{C}^2 \tag{1.3}$$

$$\lim_{s\searrow 0} u(s) =: u(0^+) \in \mathbb{C}^2. \tag{1.4}$$

By a standard integration by parts formula for absolutely continuous functions we derive from lemma 1.1 the following Green formula for the operator A.

Lemma 1.2. *If* $f, g \in \mathcal{D}(A^*)$ *then*

$$\langle A^* f, g\rangle - \langle f, A^* g\rangle = \frac{1}{\mathrm{i}}\left[\langle \delta_2 f, \delta_2 g\rangle - \langle \delta_1 f, \delta_1 g\rangle\right] \tag{1.5}$$

where $\delta_1, \delta_2 : \mathcal{D}(A^*) \to \mathbb{C}^2$ *are defined by (with* $f = (u, v)$*)*

$$\delta_1 f = \begin{pmatrix} u(0^+) \\ v(0^-) \end{pmatrix} \qquad \delta_2 f = \begin{pmatrix} u(0^-) \\ v(0^+) \end{pmatrix}. \tag{1.6}$$

The Green formula (1.5) can be used to characterize all possible self-adjoint extensions of the operator A. First of all one has:

Proposition 1.3. *If* $\Gamma : \mathbb{C}^2 \to \mathbb{C}^2$ *is linear and unitary, then the operator* $L = L_\Gamma$ *defined by*

$$\mathcal{D}(L) := \left\{ f \in \mathcal{D}(A^*) : \delta_2 f = \Gamma \delta_1 f \right\} \tag{1.7}$$

$$Lf := A^* f \qquad f \in \mathcal{D}(L) \tag{1.8}$$

is self-adjoint.

In fact the family L_Γ from proposition 1.3 constitutes the whole class of self-adjoint extensions of A. The following results are crucial steps in proving that fact.

Lemma 1.4. *The following maps:*

$$\hat{\delta}_1 := \delta_{1|\mathcal{D}(A^*)\cap\ker(\delta_2)} : \mathcal{D}(A^*) \cap \ker(\delta_2) \to \mathbb{C}^2 \tag{1.9}$$

$$\hat{\delta}_2 := \delta_{2|\mathcal{D}(A^*)\cap\ker(\delta_1)} : \mathcal{D}(A^*) \cap \ker(\delta_1) \to \mathbb{C}^2 \tag{1.10}$$

are onto.

Proof. The proof is obvious from (1.6). □

Lemma 1.5.

$$\mathcal{D}(A) \subset \ker \delta_1 \cap \ker \delta_2. \tag{1.11}$$

The following is a consequence of the previous lemma.

Lemma 1.6. *If* L *is any self-adjoint extension of* A*, then the maps* δ_i*,* $i = 1, 2$*, restricted to* $\mathcal{D}(L)$*, map the latter onto* $\mathbb{C}^2$*.*

We finish with:

Theorem 1.7. *If* L *is a self-adjoint extension of* A *then one can find a unitary operator* $\Gamma : \mathbb{C}^2 \to \mathbb{C}^2$ *such that* $L = L_\Gamma$*.*

There are many different ways to characterize all self-adjoint extensions of a symmetric operator (when such extensions exist). In von Neumann's approach [16, theorem X.2] (see also [1]), one indexes self-adjoint extensions by unitary maps from one deficiency subspace $\mathcal{K}_+ = \ker(\mathrm{i}I - A^*)$ onto the other $\mathcal{K}_- = \ker(\mathrm{i}I + A^*)$. For the operator above,

$$\mathcal{K}_+ = \operatorname{span}\left\{\begin{pmatrix}\sqrt{2}\mathrm{e}^{-x}1_{(0,\infty)}\\ 0\end{pmatrix}, \begin{pmatrix}0\\ \sqrt{2}\mathrm{e}^{x}1_{(-\infty,0)}\end{pmatrix}\right\} \tag{1.12}$$

$$\mathcal{K}_- = \operatorname{span}\left\{\begin{pmatrix}\sqrt{2}\mathrm{e}^{x}1_{(-\infty,0)}\\ 0\end{pmatrix}, \begin{pmatrix}0\\ \sqrt{2}\mathrm{e}^{-x}1_{(0,\infty)}\end{pmatrix}\right\}. \tag{1.13}$$

Let $\{u_+, v_+\}$ be the orthonormal basis (1.12) of $\mathcal{K}_+$ and $\{u_-, v_-\}$ the orthonormal basis (1.13) of $\mathcal{K}_-$. Then unitary maps $\Gamma : \mathbb{C}^2 \to \mathbb{C}^2$ correspond to unitary maps

$$c_1u_+ + c_2v_+ \longmapsto \left(\Gamma\begin{pmatrix}c_1\\ c_2\end{pmatrix}\right)_1 u_- + \left(\Gamma\begin{pmatrix}c_1\\ c_2\end{pmatrix}\right)_2 v_- \qquad c_1, c_2 \in \mathbb{C}$$

from the two-dimensional subspace $\mathcal{K}_+$ onto $\mathcal{K}_-$ and the self-adjoint extension A_Γ of A corresponding to Γ is given by

$$\mathcal{D}(A_\Gamma) = \left\{\phi + \phi_c + \psi_c : \phi \in \mathcal{D}(\overline{A}), c \in \mathbb{C}^2\right\}$$
$$\text{where}\quad \phi_c = c_1u_+ + c_2v_+ \qquad \text{and} \qquad \psi_c = (\Gamma c)_1\, u_- + (\Gamma c)_2\, v_-$$
$$A_\Gamma(\phi + \phi_c + \psi_c) = A^*\phi + \mathrm{i}\phi_c - \mathrm{i}\psi_c \qquad \text{for all}\quad \phi \in \mathcal{D}(\overline{A}) \quad c \in \mathbb{C}^2.$$

If we denote by $\mathcal{D}(\overline{A})$ the domain of the *closure* $\overline{A}$ of A, then it is known from [17, theorem 3.8] that $\mathcal{D}(\overline{A})$ is the collection of all functions $f \in \mathcal{D}(A^*)$ with $f(0^+) = f(0^-) = 0$ and the operator $\overline{A}$ is the restriction of A^* to the linear subspace $\mathcal{D}(\overline{A})$ of $\mathcal{D}(A^*)$. A calculation shows that $A_\Gamma = L_\Gamma$.

A general approach to characterizing self-adjoint extensions in terms of boundary conditions is treated in [17, theorem 4.7]. If for each $u, v \in \mathcal{D}(A^*)$ we set

$$[u, v]_x = \mathrm{i}\,(u_0(x)\overline{v_0}(x) - u_1(x)\overline{v_1}(x))$$
$$= \mathrm{i}\left(\overline{v_0(x)}, -\overline{v_1(x)}\right)\begin{pmatrix}u_0(x)\\ u_1(x)\end{pmatrix}$$

for $x = 0^+$ or $x = 0^-$, then every self-adjoint extension of A is determined by vectors $\alpha_j = (\alpha_{j,0}, \alpha_{j,1})$ and $\beta_j = (\beta_{j,0}, \beta_{j,1})$ in $\mathbb{C}^2$ for $j = 1, 2$, such that the two vectors $(\alpha_{j,0}, \alpha_{j,1}, \beta_{j,0}, \beta_{j,1})$, $j = 1, 2$, in $\mathbb{C}^4$ are linearly independent and

$$[\alpha_j, \alpha_k] = [\beta_j, \beta_k] \tag{1.14}$$

for each $j, k = 1, 2$. Then the corresponding self-adjoint extension of A is given by the restriction of A^* to the linear subspace of all $f \in \mathcal{D}(A^*)$ such that

$$[f, \alpha_j]_{0^-} = [f, \beta_j]_{0^+} \qquad \text{for each} \quad j = 1, 2. \tag{1.15}$$

If we set

$$M = \begin{pmatrix}\alpha_{1,0} & \alpha_{2,0}\\ \beta_{1,1} & \beta_{2,1}\end{pmatrix} \text{ and } N = \begin{pmatrix}\beta_{1,0} & \beta_{2,0}\\ \alpha_{1,1} & \alpha_{2,1}\end{pmatrix}$$

then the compatibility condition (1.14) becomes $M^*M = N^*N$ and the boundary condition (1.15) reads as

$$M^*\begin{pmatrix}u(0^-)\\ v(0^+)\end{pmatrix} = N^*\begin{pmatrix}u(0^+)\\ v(0^-)\end{pmatrix} \qquad \text{for} \quad f = (u, v).$$

It turns out that M is invertible and $(M^*)^{-1}N^* = MN^{-1}$ is precisely the unitary matrix Γ given in equation (1.7).

Although we are led to the same self-adjoint extension by each method, the boundary condition (1.7) has a natural interpretation in terms of conservation of energy as travelling waves move across the origin, so that the evolution $t \mapsto e^{itL_\Gamma}$ forms a continuous unitary group of operators. A simpler example is discussed from this viewpoint in [16, pp 142–3].

2. The main result

Motivated by the previous example we will now formulate an abstract result which will then be used to study all point interactions of a one-dimensional Laplacian.

Theorem 2.1. *Suppose H is a complex Hilbert space and A is a densely defined symmetric operator in H. Suppose that G is another Hilbert space and $\gamma_i : \mathcal{D}(A^*) \to G$ for $i = 1, 2$, are two linear bounded operators satisfying the following conditions:*

(i) $\mathcal{D}(A) \subset \ker \gamma_1 \cap \ker \gamma_2$;
(ii) the restrictions of γ_1 and resp. γ_2 to $\mathcal{D}(A^*) \cap \ker \gamma_2$, resp. $\mathcal{D}(A^*) \cap \ker \gamma_1$, are onto,

and the following Green formula:

$$\langle A^* f, g\rangle - \langle f, A^* g\rangle = \mathrm{i}\left[\langle \gamma_2 f, \gamma_2 g\rangle - \langle \gamma_1 f, \gamma_1 g\rangle\right] \tag{2.1}$$

holds for all $f, g \in \mathcal{D}(A^*)$.
Then, for any unitary map $\Gamma : G \to G$, the operator $L = L_\Gamma$ defined by

$$\mathcal{D}(L_\Gamma) := \left\{f \in \mathcal{D}(A^*) : \gamma_2 f = \Gamma\gamma_1 f\right\} \tag{2.2}$$

$$L_\Gamma f := A^* f \qquad f \in \mathcal{D}(L_\Gamma) \tag{2.3}$$

is self-adjoint.

Moreover, if L is a self-adjoint extension of A then one can find a unitary operator $\Gamma : G \to G$ such that $L = L_\Gamma$.

The above stated result is a classical one and its origins can be traced to a seminal paper by Calkin [5], see also [9, theorem XII.4.31], Fulton [10], Crandall–Phillips [7] and Kochubei [14]. The point of this paper is to show that it pays to choose the Hilbert space G and maps $\gamma_j : \mathcal{D}(A^*) \to G$ appropriately.

Now let $H = L^2(a, b; \mathbb{C})$, where $-\infty < a < b < \infty$, and let A be a symmetric operator in H defined by

$$\mathcal{D}(A) = C_0^\infty((a, b), \mathbb{C}) \tag{2.4}$$

$$Af = -\frac{\mathrm{d}^2 f}{\mathrm{d}x^2} \qquad f \in \mathcal{D}(A). \tag{2.5}$$

The standard Green formula is of the following form:

$$\langle A^* f, g\rangle - \langle f, A^* g\rangle = u'(b)\bar{v}(b) - u(b)\bar{v}'(b) - \left[u'(a)\bar{v}(a) - u(a)\bar{v}'(a)\right] \tag{2.6}$$

for all $f, g \in \mathcal{D}(A^*)$. Let us recall at this point the well known fact that $\mathcal{D}(A^*)$ equals the Sobolev space $H^{2,2}(a, b; \mathbb{C})$ of all functions from $L^2(a, b; \mathbb{C})$ whose weak derivative up to order 2 belongs to $L^2(a, b; \mathbb{C})$ as well. Equivalently, $f \in \mathcal{D}(A^*)$ iff f is of C^1 class on the closed interval $[a, b]$ and its first derivative f' is absolutely continuous with f'' belonging to $L^2(a, b; \mathbb{C})$. Whatever the form, it follows that the maps δ_a, δ_b, δ'_a, δ'_b from $\mathcal{D}(A^*)$ into $\mathbb{C}$ defined by $f \mapsto f(a)$, $f(b)$, $f'(a)$ and $f'(b)$ are linear and bounded.

The problem with formula (2.6) is that it is not of the form (2.1). For example, it contains four terms instead of the two required. Fortunately the following two simple identities hold, again for all $u, v \in \mathcal{D}(A^*)$

$$\begin{aligned}\left(u'(b) + \mathrm{i}u(b)\right)\left(\bar{v}'(b) - \mathrm{i}\bar{v}(b)\right) - \left(u'(b) - \mathrm{i}u(b)\right)\left(\bar{v}'(b) + \mathrm{i}\bar{v}(b)\right)\\ = -2\mathrm{i}\left[u'(b)\bar{v}(b) - u(b)\bar{v}'(b)\right]\end{aligned} \tag{2.7}$$

and, analogously at a

$$\big(u'(a) + \mathrm{i}u(a)\big)\big(\bar{v}'(a) - \mathrm{i}\bar{v}(a)\big) - \big(u'(a) - \mathrm{i}u(a)\big)\big(\bar{v}'(a) + \mathrm{i}\bar{v}(a)\big)$$
$$= -2\mathrm{i}\left[u'(a)\bar{v}(a) - u(a)\bar{v}'(a)\right]. \tag{2.8}$$

Therefore, defining functions $\gamma_i : \mathcal{D}(A^*) \to \mathbb{C}^2$, for $i = 1, 2$, by

$$\gamma_1 u = \begin{pmatrix} u'(b) - \mathrm{i}u(b) \\ u'(a) + \mathrm{i}u(a) \end{pmatrix} \qquad \gamma_2 u = \begin{pmatrix} u'(b) + \mathrm{i}u(b) \\ u'(a) - \mathrm{i}u(a) \end{pmatrix} \tag{2.9}$$

for $u \in \mathcal{D}(A^*)$, we have

Lemma 2.2. *If $u, v \in \mathcal{D}(A^*)$ then*

$$\langle A^*u, v\rangle - \langle u, A^*v\rangle = \frac{\mathrm{i}}{2}\left[\langle\gamma_2 u, \gamma_2 v\rangle - \langle\gamma_1 u, \gamma_1 v\rangle\right]. \tag{2.10}$$

We are going to check the remaining two conditions of theorem 1.7. Obviously the first of them (i.e. (i)) holds true. We show the second. Using a partition of unity it is enough to show that for any $z \in \mathbb{C}$ there exists a $\mathcal{C}^2$ class function $u : [a, b] \to \mathbb{C}$ such that $u'(a) - \mathrm{i}u(a) = 0$ and $u'(a) + \mathrm{i}u(a) = z$. Certainly, there exists a function u of required regularity such that $u'(a) = \frac{z}{2}$ and $u(a) = -\frac{\mathrm{i}z}{2}$. Therefore, applying theorem 2.1 we obtain the following main result of our paper.

Theorem 2.3. *Each self-adjoint extension of the operator A is of the following form: for some unitary operator $\Gamma : \mathbb{C}^2 \to \mathbb{C}^2$,*

$$\mathcal{D}(L_\Gamma) := \left\{u \in H^{2,2}(a, b; \mathbb{C}) : \gamma_2 u = \Gamma\gamma_1 u\right\} \tag{2.11}$$

$$L_\Gamma f := -\frac{\mathrm{d}^2 f}{\mathrm{d}x^2} \qquad f \in \mathcal{D}(L_\Gamma). \tag{2.12}$$

Remark. If we take the orthonormal basis

$$\left(2^{\frac{1}{4}}\mathrm{e}^{\frac{1-\mathrm{i}}{\sqrt{2}}x}1_{(-\infty,0)}, 2^{\frac{1}{4}}\mathrm{e}^{-\frac{1-\mathrm{i}}{\sqrt{2}}x}1_{(0,\infty)}\right)$$

of the deficiency subspace $\ker(\mathrm{i}I - A^*)$ and the orthonormal basis

$$\left(2^{\frac{1}{4}}\mathrm{e}^{\frac{1+\mathrm{i}}{\sqrt{2}}x}1_{(-\infty,0)}, 2^{\frac{1}{4}}\mathrm{e}^{-\frac{1+\mathrm{i}}{\sqrt{2}}x}1_{(0,\infty)}\right)$$

of the other deficiency subspace $\ker(\mathrm{i}I + A^*)$, then on application of [9, theorem XII.4.31] the maps (2.9) are replaced by

$$\gamma_1' u = \begin{pmatrix} u'(b) + \mathrm{e}^{-\mathrm{i}\frac{\pi}{4}}u(b) \\ u'(a) - \mathrm{e}^{-\mathrm{i}\frac{\pi}{4}}u(a) \end{pmatrix} \qquad \gamma_2' u = \begin{pmatrix} u'(b) + \mathrm{e}^{\mathrm{i}\frac{\pi}{4}}u(b) \\ u'(a) - \mathrm{e}^{\mathrm{i}\frac{\pi}{4}}u(a) \end{pmatrix}. \tag{2.13}$$

The maps (2.9) are defined by a simpler formula than (2.13).

In fact, if we take any $z \in \mathbb{C}$ with non-zero imaginary part, and define the maps

$$\gamma_1(z)u = \begin{pmatrix} u'(b) + \bar{z}u(b) \\ u'(a) - \bar{z}u(a) \end{pmatrix}$$
$$\gamma_2(z)u = \begin{pmatrix} u'(b) + zu(b) \\ u'(a) - zu(a) \end{pmatrix}$$

then we obtain all self-adjoint extensions of A in the analogous manner. The maps (2.9) are obtained simply by taking $z = i$.

Examples

In the following the unitary maps $\Gamma : \mathbb{C}^2 \to \mathbb{C}^2$ are expressed by matrices in the canonical basis of $\mathbb{C}^2$.

We begin with $\Gamma = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$. Easy calculations show that in this case the boundary conditions (2.11) take the form

$$u(a) = u(b) = 0$$

i.e. of Dirichlet.

If $\Gamma = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, the boundary conditions in (2.11) take the form

$$u'(a) = u(b) = 0.$$

The matrix $\Gamma = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$ corresponds to the Neumann boundary conditions

$$u'(a) = u'(b) = 0.$$

3. Comments

The so-called point interactions are the self-adjoint extensions of the following modification of the operator A from the last section. Now let $H = L^2(\mathbb{R}; \mathbb{C})$ and A be a symmetric operator in H defined by

$$\mathcal{D}(A) = C_0^\infty(\mathbb{R} \setminus \{0\}, \mathbb{C}) \tag{3.1}$$

$$Af = -\frac{d^2 f}{dx^2} \qquad f \in \mathcal{D}(A). \tag{3.2}$$

It is indeed well known that A is a densely defined symmetric operator in H and that its deficiency index is (2, 2). Chernoff and Hughes [6], see also [2, 3, 8, 12, 13, 15], describe all self-adjoint extensions of the operator A by means of the following boundary conditions

$$\begin{aligned} u(0^+) &= \omega a u(0^-) + \omega b u'(0^-) \\ u'(0^+) &= \omega c u(0^-) + \omega d u'(0^-) \end{aligned} \tag{3.3}$$

where $\omega \in \mathbb{C}$; $a, b, c, d \in \mathbb{R} \cup \{\infty\}$, satisfy $|\omega| = 1$ and $ad - bc = 1$. Three cases are classical. $b = c = 0$ corresponds to the Friedrichs extension of A, $b = \infty$, $c = 0$ corresponds to the Neumann boundary conditions and $c = \infty$, $b = 0$ corresponds to the Dirichlet boundary conditions. In this case our boundary conditions read

$$\begin{pmatrix} u'(0^+) + iu(0^+) \\ u'(0^-) - iu(0^-) \end{pmatrix} = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \begin{pmatrix} u'(0^+) - iu(0^+) \\ u'(0^-) + iu(0^-) \end{pmatrix} \tag{3.4}$$

where $\Gamma = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}$ is a 2×2 unitary matrix.

Since any unitary matrix is of the form $\eta \begin{pmatrix} \alpha & -\bar{\beta} \\ \beta & \bar{\alpha} \end{pmatrix}$, $\alpha, \beta, \eta \in \mathbb{C}$, $|\eta| = |\alpha|^2 + |\beta|^2 = 1$, the latter take the form

$$\begin{aligned} u'(0^+) + iu(0^+) &= \eta\alpha(u'(0^+) - iu(0^+)) - \eta\bar{\beta}(u'(0^-) + iu(0^-)) \\ u'(0^-) - iu(0^-) &= \eta\beta(u'(0^+) - iu(0^+)) + \eta\bar{\alpha}(u'(0^-) + iu(0^-)). \end{aligned} \tag{3.5}$$

Comparing our boundary conditions with (3.3) we see that ours are somehow more natural. In particular, we do not require any of the coefficients to be equal to ∞. These different characterizations can be explained in different parameterizations of the unitary group $U(2)$. From the point of view of quantum mechanics, we have represented the probability flux across zero of a state ψ in the domain of a possible Hamiltonian operator as a constant times $|\gamma_2\psi|^2 - |\gamma_1\psi|^2$. As noted earlier, there are many possible ways to achieve this representation. Hence, Hamiltonian operators H_Γ are in one-to-one correspondence with unitary maps $\Gamma : \mathbb{C}^2 \to \mathbb{C}^2$ such that $\gamma_2\psi = \Gamma\gamma_1\psi$, so that total probability is conserved, i.e. e^{-itH_Γ} is a unitary operator for all times $t \in \mathbb{R}$.

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